



# TMS2013

**142<sup>nd</sup> Annual Meeting & Exhibition**

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**March 3-7, 2013 • Henry B. Gonzalez Convention Center  
San Antonio, Texas, USA**

## ***Technical Program***

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## 2013 Aluminum Keynote: Impurities in the Aluminum Supply Chain: 2013 Aluminum Keynote Session

*Sponsored by:* TMS Light Metals Division

*Program Organizers:* Les Edwards, Rain CII Carbon; Barry Sadler, Net Carbon Consulting Pty Ltd

Monday AM  
March 4, 2013

Room: Lila Cockrell Theatre  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* Les Edwards, Rain CII Carbon

### 8:30 AM Introductory Comments

8:35 AM

**Raw Material Impurities and the Challenge Ahead:** *Stephen Lindsay*<sup>1</sup>; <sup>1</sup>Alcoa, Inc.

9:00 AM

**Impacts of Impurities Introduced into the Aluminium Reduction Cell:** *James Metson*<sup>1</sup>; David Wong<sup>1</sup>; Jenny Hung<sup>1</sup>; Mark Taylor<sup>1</sup>; <sup>1</sup>University of Auckland

9:25 AM

**Changes in Global Refining and Its Impact on Anode Quality Petroleum Coke:** *Karl Bartholomew*; ICIS Consulting

9:50 AM

**Impact of Higher Vanadium Levels on Smelter Operations:** Chuck Coney<sup>1</sup>; Lew Crabtree<sup>1</sup>; John Gavin<sup>1</sup>; Wes Marcum<sup>1</sup>; *Andrea Weber*<sup>1</sup>; Les Edwards<sup>2</sup>; <sup>1</sup>RTA Seabree; <sup>2</sup>Rain CII Carbon

10:15 AM Break

10:35 AM

**Impact on Smelter Operations of Operating High Purity Reduction Cells:** *Stewart Hamilton*<sup>1</sup>; <sup>1</sup>New Zealand Aluminium Smelters Ltd

11:00 AM

**Management of Impurities in Cast House with Particular Reference to Ni and V:** *Muhammad Rhamdhani*<sup>1</sup>; John Grandfield<sup>2</sup>; Abdul Khaliq<sup>1</sup>; Geoffrey Brooks<sup>1</sup>; <sup>1</sup>Swinburne University of Technology; <sup>2</sup>Grandfield Technology Pty Ltd

11:25 AM

**An Initial Assessment of the Effects of Increased Ni and V Content in AA6063 and A356 Alloys:** Lisa Sweet<sup>1</sup>; *John Grandfield*<sup>2</sup>; Cameron Davidson<sup>3</sup>; Jason Mitchell<sup>3</sup>; Aiden Beer<sup>3</sup>; Suming Zhu<sup>3</sup>; Xiaobo Chen<sup>3</sup>; Mark Easton<sup>3</sup>; <sup>1</sup>CAST; <sup>2</sup>Grandfield Technology Pty Ltd; <sup>3</sup>CAST

11:50 AM Panel Discussion

This will be a question-and-answer style panel discussion with the keynote speakers.

## 2013 and Beyond: Flexible Electronics: Flexible Bioelectronics in the Central and Peripheral Nervous Systems

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Biomaterials Committee, TMS: Nanomaterials Committee

*Program Organizer:* Walter Voit, UT Dallas

Monday AM  
March 4, 2013

Room: 204A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* To Be Announced

### 8:30 AM Introductory Comments by Walter Voit, UT Dallas

8:35 AM Invited

**Low-Temperature Materials for a Neuromorphic Architecture:** *Eric Vogel*<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

9:05 AM Question and Answer Period

9:15 AM

**Shape Memory Polymer Substrates for Softening, 3D Neural Interfaces:** *Taylor Ware*<sup>1</sup>; Dustin Simon<sup>1</sup>; Walter Voit<sup>1</sup>; <sup>1</sup>The University of Texas at Dallas

9:45 AM Question and Answer Period

9:55 AM Break

**10:15 AM Use of Compliant Materials in the Fabrication of a Flexible Utah Neural Interface Electrode Array:** *Brian Baker*<sup>1</sup>; Rohit Sharma<sup>2</sup>; Prashant Tathireddy<sup>2</sup>; Loren Rieth<sup>2</sup>; Florian Solzbacher<sup>2</sup>; <sup>1</sup>Utah Nanofab; <sup>2</sup>University of Utah

10:45 AM Question and Answer Period

10:55 AM

**Graphene Coated with Titanium Nitride as Electrode Materials for Neural Interfaces:** *David Arreaga-Salas*<sup>1</sup>; Walter Voit<sup>1</sup>; <sup>1</sup>UT Dallas

11:15 AM Question and Answer Period

11:25 AM

**Brain Matched Magnetic Susceptibility in Metallic Alloys for Use during MR Imaging:** *Charles Fisher*<sup>1</sup>; Garrett Astary<sup>1</sup>; Rachel Stewart<sup>1</sup>; Marcus Peprah<sup>1</sup>; Tom Mareci<sup>1</sup>; Mark Meisel<sup>1</sup>; Paul Carney<sup>1</sup>; Malisa Sarntinoranont<sup>1</sup>; Michele Manuel<sup>1</sup>; <sup>1</sup>University of Florida

11:45 AM Question and Answer Period

11:55 AM

**Electrochemical Properties of Neural Interfaces on Smart, Softening Substrates:** *Ryan Marcotte*<sup>1</sup>; Dustin Simon<sup>1</sup>; Taylor Ware<sup>1</sup>; David Arreaga-Salas<sup>1</sup>; Walter Voit<sup>1</sup>; <sup>1</sup>University of Texas at Dallas

12:15 PM Question and Answer Period

12:25 PM Concluding Comments

## 2013 Functional Nanomaterials: Synthesis, Properties and Applications: Nanomaterials for Energy Technologies

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Nanomaterials Committee

*Program Organizers:* Seong Jin Koh, University of Texas at Arlington; Nitin Chopra, University of Alabama; Jiyoung Kim, University of Texas at Dallas; Yuanbing Mao, University of Texas-Pan American; Ashwin Ramasubramaniam, University of Massachusetts; Gregory Thompson, University of Alabama

Monday AM  
March 4, 2013

Room: 201  
Location: Henry B. Gonzalez  
Convention Center

*Funding support provided by:* Qualcomm, Inc.

*Session Chairs:* Seong Jin Koh, University of Texas at Arlington; Seung Kang, Qualcomm, Inc

### 8:30 AM Introductory Comments

#### 8:40 AM Invited

**Nanostructured Energy Materials for Advanced Technical Applications:** *Sungho Jin*<sup>1</sup>; <sup>1</sup>UC San Diego

#### 9:15 AM Invited

**Molecularly-Sculpted Nanomaterials and Interfaces for Energy and Electronics:** *Ganpati Ramanath*<sup>1</sup>; <sup>1</sup>Rensselaer Polytechnic Institute

#### 9:50 AM

**Improved Performance of Bulk-Heterojunction Organic Solar Cells with the Use of Antireflective Zinc Oxide Nanorod Arrays on Seedless Substrates:** *Hyung Woo Choi*<sup>1</sup>; Kyu-Sung Lee<sup>2</sup>; T. Alford<sup>1</sup>; <sup>1</sup>Arizona State University; <sup>2</sup>Electronics and Telecommunications Research Institute (ETRI)

#### 10:10 AM Break

#### 10:25 AM Invited

**Energy Harvesting and Cooling with Flexible and Light-Weight Organic Nanocomposites:** *Choongho Yu*<sup>1</sup>; <sup>1</sup>Texas A&M University

#### 11:00 AM Invited

**Next Generation Polymer Nanocomposite Electrolytes for Lithium Ion Batteries:** *Haleh Ardebili*<sup>1</sup>; <sup>1</sup>University of Houston

#### 11:35 AM

**In-Situ Stress Study of Vanadium Oxide Thin Films as Li-Ion Storage Electrodes:** *Dawei Liu*<sup>1</sup>; Aaron Kessman<sup>2</sup>; Jay Sheth<sup>3</sup>; Brian Sheldon<sup>3</sup>; <sup>1</sup>Alfred University; <sup>2</sup>Brown University; <sup>3</sup>Brown University

#### 11:55 AM

**Atomic-Scale Characterization of Nb-Doped SrTiO<sub>3</sub> Nanostructures for Energy Harvesting and Applications:** *Riad Alzghier*<sup>1</sup>; Jeremiah Abiad<sup>1</sup>; <sup>1</sup>Department of Mechanical & Industrial Engineering, University of Illinois at Chicago

#### 12:15 PM

**Metal Oxide Nanofibers Produced by a ForceSpinning Method for Battery Electrodes:** *Edna Garcia*<sup>1</sup>; Yuanbing Mao<sup>1</sup>; <sup>1</sup>University of Texas-Pan American

## 4th International Symposium on High-Temperature Metallurgical Processing: High Efficiency New Metallurgical Technology

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

*Program Organizers:* Tao Jiang, Central South University; Jiann-Yang Hwang, Michigan Technological University; Phillip Mackey, Consultant; Onuralp Yücel, ITU; Guifeng Zhou, Wuhan Iron and Steel

Monday AM  
March 4, 2013

Room: 008B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Tao Jiang, Central South University; Lawrence F. McHugh, Orchard Material Technology

### 8:30 AM Introductory Comments

#### 8:35 AM

**A New Copper Smelting Technology – Bottom Blown Oxygen Furnace Developed at Dongying Fangyuan Nonferrous Metals:** *Baojun Zhao*<sup>1</sup>; Zhixiang Cui<sup>2</sup>; Zhi Wang<sup>2</sup>; <sup>1</sup>The University of Queensland; <sup>2</sup>Dongying Fangyuan Nonferrous Metals Co., Ltd

#### 8:55 AM

**A Novel Vacuum Aluminothermic Reduction Lithium Process:** *Di Yuezhang*<sup>1</sup>; Wang Zhihui<sup>1</sup>; Tao Shaohu<sup>1</sup>; Feng Naixiang<sup>1</sup>; <sup>1</sup>Northeastern University

#### 9:15 AM

**Study on Double-Layered Pellet Roasting of Sulfur & Arsenic-Bearing Gold Concentrate:** Jiang Tao<sup>1</sup>; Li Xi-Shan<sup>1</sup>; Ge Jie<sup>1</sup>; Cui Li-na<sup>1</sup>; Li Qian<sup>1</sup>; *Yang Yong-bin*<sup>1</sup>; <sup>1</sup>Central South University

#### 9:35 AM

**Electrochemical Preparation of Tungsten. Tungsten Carbide and Cemented Carbide:** Diem-Hang Tran-Nguyen<sup>1</sup>; Daniel Jewell<sup>1</sup>; *Derek Fray*<sup>1</sup>; <sup>1</sup>University of Cambridge

#### 9:50 AM

**Preparation of MoO<sub>3</sub> from Ammonium Tetramolybdate in Microwave Fields:** *Li Jian*<sup>1</sup>; <sup>1</sup>Kun Ming University of Science and Technology

#### 10:10 AM Break

#### 10:20 AM

**Looping Sulfide Oxidation Process for Anode Copper Production:** Leonid Shekhter<sup>1</sup>; Corby Anderson<sup>2</sup>; *Daniel Gribbin*<sup>1</sup>; Esra Cankaya-Yalcin<sup>1</sup>; Joseph Lessard<sup>1</sup>; Lawrence McHugh<sup>1</sup>; <sup>1</sup>Orchard Material Technology; <sup>2</sup>Kroll Institute for Extractive Metallurgy

#### 10:40 AM

**Direct Reduction of Ti-V Magnetite Via ITmk3 Technology:** *Nikolay Panishev*<sup>1</sup>; Boris Dubrovsky<sup>1</sup>; Anatoly Starikov<sup>1</sup>; Eugene Redin<sup>1</sup>; Edward Knyazev<sup>1</sup>; <sup>1</sup>Magnitogorsk Iron & Steel Works

#### 11:00 AM

**Research and Industrial Applications of Oxygen-rich Side-blow Bath Smelting Technology:** *Lin Chen*<sup>1</sup>; Wanda Bin<sup>1</sup>; Tianzu Yang<sup>1</sup>; Weifeng Liu<sup>1</sup>; Shu Bin<sup>1</sup>; <sup>1</sup>Central South University

#### 11:20 AM

**New Innovative Gas Purging System for Stationary and Tilting Copper Anode Furnaces:** *Klaus Gamweger*<sup>1</sup>; <sup>1</sup>RHI AG



11:35 AM

**Thermal Plasma Torches for Metallurgical Applications:** Lakshminarayana Rao<sup>1</sup>; Pierre Carabin<sup>1</sup>; *Gillian Holcroft*<sup>2</sup>; <sup>1</sup>PyroGenesis Canada Inc.; <sup>2</sup>PyroGenesis Canada Inc.

11:50 AM

**Research on Removal of Potassium and Sodium by Pre-reduction Sintering:** *Li Qian*<sup>1</sup>; Jing Zhao<sup>1</sup>; Jiang Tao<sup>1</sup>; Yang Yong-bin<sup>1</sup>; Li Guang-hui<sup>1</sup>; Chen Xu-ling<sup>1</sup>; <sup>1</sup>Central South University

12:05 PM

**Reactive Foils Using Ni/Al Multilayers with Sputtering Followed by Pressurizing:** *SeoungWoo Kuk*<sup>1</sup>; Jin Yu<sup>1</sup>; <sup>1</sup>KAIST

12:20 PM

**NOx Reduction by Sintering Flue Gas Circulation for Iron Ores:** *Guanghui Li*<sup>1</sup>; Chen Liu<sup>1</sup>; Tao Jiang<sup>1</sup>; Yuanbo Zhang<sup>1</sup>; Zhengwei Yu<sup>1</sup>; Chongzhong Ouyang<sup>1</sup>; <sup>1</sup>Central South University

## Advanced Materials and Reservoir Engineering for Extreme Oil & Gas Environments: Nanocrystalline Metals I

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Nanomaterials Committee

*Program Organizers:* Indranil Roy, Schlumberger; Brajendra Mishra, Colorado School of Mines; Manuel Marya, Schlumberger Technology Corporation; Kuo-Chiang Chen, Schlumberger; Partha Ganguly, Schlumberger; Richard Lewis, Schlumberger; Suveen Mathaudhu, U.S. Army Research Office; Nitin Chopra, The University of Alabama; Xinghang Zhang, Texas A&M University; Greg Kusinski, Chevron; John Meng, BP America Inc.; Jefferson Rodrigues, Petrobras; Justin Cheney, Scoperta

Monday AM

March 4, 2013

Room: Lone Star Salon A

Location: Grand Hyatt

*Session Chairs:* Partha Ganguly, Schlumberger; Kuo-Chiang Chen, Schlumberger

8:30 AM AMREE Oil and Gas I - Introductory Comments and talk by Greg Kusinski, Director Deepstar, Chevron

8:55 AM Keynote

**Advanced Materials and Processes for Extreme Environments:** *Enrique Lavernia*<sup>1</sup>; <sup>1</sup>University of California, Davis

9:25 AM Invited

**Achieving Ultra-High Strength and High Ductility in Cu-Cr-Zr Alloy by Combination of Ultrafine-Grain Formation and Static/Dynamic Precipitation:** *Gencaga Purcek*<sup>1</sup>; Onur Saray<sup>1</sup>; Harun Yanar<sup>1</sup>; Ibrahim Karaman; Hans Maier<sup>2</sup>; <sup>1</sup>Karadeniz Technical University; <sup>2</sup>University of Paderborn

9:45 AM Invited

**Grain Size Effect on Densities of Dislocations with Edge Components in Nanocrystalline Body-Centered Cubic Mo:** *Yuntian Zhu*<sup>1</sup>; Guangming Cheng<sup>1</sup>; Paul Millet<sup>2</sup>; <sup>1</sup>North Carolina State University; <sup>2</sup>Idaho National Lab

10:05 AM Break

10:20 AM

**Nanocrystalline and Nanotwinned Metals under Extreme Environment:** *Xinghang Zhang*<sup>1</sup>; Y. Chen<sup>1</sup>; D. Bufford<sup>1</sup>; C. Sun<sup>1</sup>; Y. Liu<sup>1</sup>; K.Y. Yu<sup>1</sup>; H. Wang<sup>1</sup>; <sup>1</sup>Texas A&M University

10:40 AM Keynote

**Nanoengineered Surfaces & Coatings for Efficiency Enhancements in Oil & Gas Industry:** *Kripa Varanasi*<sup>1</sup>; <sup>1</sup>MIT

11:10 AM Invited

**Plastic Deformation of Metal Surfaces:** *Niels Hansen*<sup>1</sup>; Xiaodan Zhang<sup>1</sup>; Xiaoxu Huang<sup>1</sup>; <sup>1</sup>Technical University of Denmark

11:30 AM Invited

**SPD-Processed Bulk Nanostructured Materials for Extreme Environments:** *Ruslan Valiev*<sup>1</sup>; Maxim Murashkin<sup>1</sup>; Nariman Enikeev<sup>1</sup>; Julia Ivanisenko<sup>2</sup>; Horst Hahn<sup>2</sup>; <sup>1</sup>Ufa State Aviation Technical University; <sup>2</sup>KIT Institute of Nanotechnology

11:50 AM

**Corrosion of Bulk Nanocrystalline Materials in Hostile Environments:** *Indranil Roy*<sup>1</sup>; Manuel Marya<sup>1</sup>; Troy Topping<sup>2</sup>; Rashmi Bhavsar<sup>1</sup>; Kuo-Chiang Chen<sup>1</sup>; Enrique Lavernia<sup>2</sup>; <sup>1</sup>Schlumberger; <sup>2</sup>University of California, Davis

12:10 PM

**Thermally Stabilized Ultrahigh-Strength Nanocrystalline Alloys for Extreme Environments:** *Kristopher Darling*<sup>1</sup>; Heidi Maupin<sup>1</sup>; Laszlo Kecskes<sup>1</sup>; Suveen Mathaudhu<sup>2</sup>; <sup>1</sup>U.S. Army Research Laboratory; <sup>2</sup>U.S. Army Research Office

12:30 PM

**Study of Deformation Mechanism of Nanocrystalline 304L Stainless Steel:** *C. Sun*<sup>1</sup>; D. C. Foley<sup>1</sup>; K. Hartwig<sup>1</sup>; S. A. Maloy<sup>2</sup>; H. Wang<sup>1</sup>; X. Zhang<sup>1</sup>; <sup>1</sup>Texas A&M University; <sup>2</sup>Los Alamos National Laboratory

## Advances in Surface Engineering: Alloyed and Composite Coatings II: Functional Coatings I

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

*Program Organizers:* Srinivasa Bakshi, Indian Institute of Technology Madras; Graham McCartney, University of Nottingham; Arvind Agarwal, Florida International University; Sandip Harimkar, Oklahoma State University

Monday AM

March 4, 2013

Room: Bowie B

Location: Grand Hyatt

*Funding support provided by:* Bulk Nanostructured Materials Programs, Office of Naval Research

*Session Chair:* To Be Announced

8:30 AM Introductory Comments

8:35 AM Invited

**Multifunctional Nanocomposite Thin Films:** *Efstathios Meletis*<sup>1</sup>; <sup>1</sup>University of Texas at Arlington

8:55 AM Invited

**Nanocomposite Coatings to Eliminate Bridging Oxidation on Boiling Water Reactor Safety Relief Valves:** *Kent Coulter*<sup>1</sup>; Craig Engel<sup>1</sup>; Ronghua Wei<sup>1</sup>; <sup>1</sup>Southwest Research Institute

9:15 AM Invited

**Role of CeO<sub>2</sub> Addition on Catalytic Conversion of Plasma Sprayed Al<sub>2</sub>O<sub>3</sub> Coatings:** Neelima Mahato<sup>1</sup>; S Ariharan<sup>1</sup>; *Kantesh Balani*<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Kanpur

9:35 AM

**The Role of Cu-Sn Coating on the Adhesion between Steel and SBR Based Rubber:** Atanu Banerjee<sup>1</sup>; Monojit Dutta<sup>1</sup>; Anil Bhowmick<sup>2</sup>; *Tapas Laha*<sup>3</sup>; <sup>1</sup>Tata Steel; <sup>2</sup>Indian Institute of Technology Patna; <sup>3</sup>Indian Institute of Technology Kharagpur

**9:50 AM Break**

**10:05 AM**

**Oxidation-Resistant Cu-Cr Coatings for High-Temperature Applications:** *Kuang-Tsan Chiang*<sup>1</sup>; <sup>1</sup>Southwest Research Institute

**10:20 AM**

**Microstructural Effects on Work Function of OsRu Coatings Used for Dispenser Cathodes:** *Phillip Swartzentruber*<sup>1</sup>; Michael Effgen<sup>2</sup>; Scott Roberts<sup>2</sup>; John Balk<sup>1</sup>; <sup>1</sup>University of Kentucky; <sup>2</sup>Semicon Associates

**10:35 AM**

**Effect of Ag Thickness on Electrical and Optical Properties of TiO<sub>2</sub>/Ag/TiO<sub>2</sub> Multilayers as Transparent Composite Electrodes (TCEs) on Flexible Substrates:** *Aritra Dhar*<sup>1</sup>; *Terry Alford*<sup>1</sup>; <sup>1</sup>Arizona State University

**10:50 AM**

**Through-the-thickness Measurement of Residual Stress in Functionally Graded WC-Co:** *Leila Tahvilian*<sup>1</sup>; *Z. Zak Fang*<sup>1</sup>; <sup>1</sup>University of Utah

**11:05 AM**

**Effect of Thermal Cycling and Sliding on the Structure of Cu-Nb Nanolaminates:** *David Economy*<sup>1</sup>; Emilio Jimenez<sup>2</sup>; Bobak Ranjbaran<sup>3</sup>; Bradley Schultz<sup>1</sup>; Marian Kennedy<sup>1</sup>; <sup>1</sup>Clemson University; <sup>2</sup>James Madison University; <sup>3</sup>Washington State University

**11:20 AM**

**Virtually Arc Free High Power Pulsed Magnetron Sputtering Based on Oscillatory Voltage Wave Forms for Insulating Film Depositions:** *Jianliang Lin*<sup>1</sup>; William Sproul<sup>1</sup>; Bo Wang<sup>1</sup>; Isaac Dahan<sup>2</sup>; <sup>1</sup>Colorado School of Mines; <sup>2</sup>Nuclear Research Center-NEGEV

**Alloys and Compounds for Thermoelectric and Solar Cell Applications: Thermoelectric I**

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Alloy Phases Committee, TMS: Energy Conversion and Storage Committee

*Program Organizers:* Sinn-wen Chen, National Tsing Hua University; Yoshisato Kimura, Tokyo Institute of Technology; Chih-Huang Lai, National Tsing-Hua University; CW Nan, Tsinghua University; G. Jeffrey Snyder, California Institute of Technology; Hubert Scherrer, Ecole des Mines

Monday AM  
March 4, 2013

Room: 007C  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Sinn-wen Chen, National Tsing Hua University; G. Snyder, California Institute of Technology

**8:30 AM Introductory Comments**

**8:35 AM Invited**

**Atomic Scale Investigations of Interfaces in Telluride-Based Thermoelectric Materials:** *Douglas Medlin*<sup>1</sup>; <sup>1</sup>Sandia National Laboratories

**9:00 AM Invited**

**Carrier Pocket Engineering to Improve Thermoelectric Transport:** *G. Jeffrey Snyder*<sup>1</sup>; <sup>1</sup>California Institute of Technology

**9:25 AM**

**Size Control and Alignment of the Microstructure in the Bi<sub>2</sub>Te<sub>3</sub>-In<sub>2</sub>Te<sub>3</sub> System:** *Nicholas Heinz*<sup>1</sup>; Teruyuki Ikeda<sup>1</sup>; G. Jeffrey Snyder<sup>1</sup>; <sup>1</sup>California Institute of Technology

**9:45 AM**

**Synthesis and Stability of Nanocrystalline Tellurides:** *Samuel Humphry-Baker*<sup>1</sup>; Christopher Schuh<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology

**10:05 AM Break**

**10:20 AM Invited**

**Bond Networks, Conduction Channels, and More: Diamond-like Compounds as a Novel Thermoelectric Materials:** *Wenqing Zhang*<sup>1</sup>; <sup>1</sup>Shanghai Institute of Ceramics

**10:45 AM**

**Interdiffusion Experiments in the Thermoelectric Mg<sub>2</sub>Si/Mg<sub>2</sub>Sn Ternary System:** *Stephane Gorsse*<sup>1</sup>; Solange Vives<sup>1</sup>; Philippe Bellanger<sup>1</sup>; <sup>1</sup>ICMCB-CNRS

**11:05 AM**

**Ternary Eutectic Growth of Nanostructured Thermoelectric Ag-Pb-Te Materials:** *Hsin-Jay Wu*<sup>1</sup>; Wei-jian Foo<sup>2</sup>; Sinn-wen Chen<sup>1</sup>; G Snyder<sup>3</sup>; <sup>1</sup>National Tsing Hua University; <sup>2</sup>Engineering Science Programme, National University of Singapore; <sup>3</sup>Materials Science, California Institute of Technology

**11:25 AM**

**The Properties of High Performance p-Type GeTe Based Materials for Thermoelectric Generators:** *ChiaChan Hsu*<sup>1</sup>; Hsiu-Ying Chung<sup>2</sup>; Jenn-Dong Hwang<sup>3</sup>; Tsai-Kun Huang<sup>4</sup>; Jing-Yi Huang<sup>4</sup>; Huey-Lin Hsieh<sup>4</sup>; <sup>1</sup>Industrial Technology Research Institute; <sup>2</sup>Feng Chia University; <sup>3</sup>Industrial Technology Research Institute; <sup>4</sup>China Steel Corporation

**11:45 AM**

**Thermoelectric Properties of Pb<sub>1+x</sub>Te Prepared by High Pressure Method:** *Taichao Su*<sup>1</sup>; <sup>1</sup>Institute of Materials Science and Engineering, Henan Polytechnic University

**Biological Materials Science Symposium: Mechanical Behavior of Biological Materials I: Bone and Teeth**

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS Structural Materials Division, TMS: Biomaterials Committee

*Program Organizers:* Candan Tamerler, University of Washington; Molly Gentleman, Texas A & M University; Po-Yu Chen, National Tsing Hua University; Kajal Mallick, University of Warwick; Rajendra Kumar Kasinath, University of Montana; Paul G. Allison, US Army Corp of Engineers

Monday AM  
March 4, 2013

Room: 214C  
Location: Henry B. Gonzalez  
Convention Center

*Funding support provided by:* Biomaterials Program, National Science Foundation

*Session Chairs:* Candan Tamerler, University of Washington; Molly Gentleman, Stony Brook

**8:30 AM Introductory Comments**

**8:35 AM Keynote**

**Multi-scale Study of Deformation and Fracture in Bone at Physiological Strain Rates:** *Elizabeth Zimmermann*<sup>1</sup>; Bernd Gludovatz<sup>2</sup>; Eric Schaible<sup>2</sup>; Hrishikesh Bale<sup>1</sup>; *Robert Ritchie*<sup>1</sup>; <sup>1</sup>University of California Berkeley; <sup>2</sup>Lawrence Berkeley National Laboratory

9:15 AM

**Osteocytes and Cementocytes: Their Role in Structure and Mechanical Properties of Bone and Teeth:** *Hanson Fong*<sup>1</sup>; Yunfeng (Bruce) Li<sup>1</sup>; Hai Zhang<sup>1</sup>; <sup>1</sup>University of Washington

9:35 AM

**Micromechanical Fatigue Testing of Bovine Cortical Bone:** *Kelly Kranjc*<sup>1</sup>; Katharine Flores<sup>2</sup>; <sup>1</sup>Ohio State University; <sup>2</sup>Washington University

9:50 AM

**Initial Anisotropy in Demineralized Bovine Cortical Bone in Compressive Cyclic Loading-unloading:** *Ekaterina Novitskaya*<sup>1</sup>; Steve Lee<sup>1</sup>; Vlado Lubarda<sup>1</sup>; Joanna McKittrick<sup>1</sup>; <sup>1</sup>UC San Diego

10:05 AM Break

10:25 AM Invited

**In Situ Behavior of Mineral vs. Bulk Properties of Bone:** *Xiaodu Wang*<sup>1</sup>; <sup>1</sup>The University of Texas at San Antonio

10:55 AM

**Surface Energy and Bone Growth:** *Molly Gentleman*<sup>1</sup>; Eileen Gentleman<sup>2</sup>; <sup>1</sup>Stony Brook University; <sup>2</sup>King's College London

11:15 AM

**Evaluating the Durability of Adhesive Bonds to Dentin and Enamel: A Mechanistic Approach:** *Mustafa Mutluay*<sup>1</sup>; Mobin Yahyazadehfar<sup>2</sup>; Heonjune Ryou<sup>2</sup>; Hessam Majd<sup>2</sup>; Dominic Do<sup>2</sup>; *Dwayne Arola*<sup>2</sup>; <sup>1</sup>University of Turku; <sup>2</sup>University of Maryland Baltimore County

11:35 AM

**Importance of Microstructure on the Crack Growth Resistance of Dentin:** *Juliana Ivancik*<sup>1</sup>; Dwayne Arola<sup>1</sup>; <sup>1</sup>University of Maryland Baltimore County

11:55 AM Invited

**Microengineering Biopolymer Scaffolds: Tools to Enhance Tissue Regeneration:** *George Pins*<sup>1</sup>; <sup>1</sup>Worcester Polytechnic Institute

12:15 PM

**Why Human Dentin Behaves Like a Rubber:** *Peter Panfilov*<sup>1</sup>; Dmitry Zaytsev<sup>1</sup>; Olga Antonova<sup>2</sup>; Victoria Alpatova<sup>3</sup>; Larissa Kiselnikova<sup>3</sup>; <sup>1</sup>Ural Federal University; <sup>2</sup>Institute of Metalphysics; <sup>3</sup>Moscow State Medical Stomatologic University

## Bulk Metallic Glasses X: Alloy Development and Application I

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

*Program Organizers:* Peter Liaw, The University of Tennessee; Hahn Choo, The University of Tennessee; Yanfei Gao, The University of Tennessee; Gongyao Wang, University of Tennessee

Monday AM

Room: Lone Star Salon D

March 4, 2013

Location: Grand Hyatt

*Funding support provided by:* Materials Processing and Manufacturing Division, National Science Foundation

*Session Chairs:* William Johnson, California Institute of Technology; Peter Liaw, The University of Tennessee

8:30 AM Keynote

**Development and Processing of Multicomponent Bulk Metallic Glasses:** *William Johnson*<sup>1</sup>; Marios Demetriou<sup>1</sup>; <sup>1</sup>California Institute of Technology

9:00 AM

**Fabrication Of Bulk Metallic Glass Composites With High Magnesium Content:** *Olga Biletska*<sup>1</sup>; Kevin Laws<sup>1</sup>; Mark Gibson<sup>2</sup>; Michael Ferry<sup>1</sup>; <sup>1</sup>University of NSW; <sup>2</sup>CSIRO Process Science and Engineering

9:15 AM Invited

**Micro Factory Concept for Metallic Glasses:** *Y. Yokoyama*<sup>1</sup>; <sup>1</sup>Institute for Materials Research

9:35 AM

**Al-Based Metallic Glass Incorporated Novel Ag Electrode for Si Solar Cell:** *Jin Man Park*<sup>1</sup>; Suk Jun Kim<sup>1</sup>; Sang Soo Jee<sup>1</sup>; Se Yun Kim<sup>1</sup>; Keum Hwan Park<sup>1</sup>; Won Tae Kim<sup>2</sup>; Do Hyang Kim<sup>3</sup>; Jurgen Eckert<sup>4</sup>; Eun-Sung Lee<sup>1</sup>; <sup>1</sup>Electronic Materials Lab, Samsung Advanced Institute of Technology (SAIT); <sup>2</sup>IT Division, Cheongju University; <sup>3</sup>Center for Noncrystalline Materials, Department of Materials Science and Engineering, Yonsei University; <sup>4</sup>Institute for Complex Materials, IFW Dresden

9:50 AM Invited

**Design and Development of Bulk Metallic Glasses for Enabling Applications:** *Atakan Peker*<sup>1</sup>; <sup>1</sup>Washington State University

10:10 AM Break

10:25 AM Invited

**Development of Bio-Inspired Magnetoelastic Sentinels Based on Amorphous Metallic Glasses:** *Suiqiong Li*<sup>1</sup>; Shin Horikawa<sup>1</sup>; Yating Chai<sup>1</sup>; Mi-kyung Park<sup>1</sup>; Kanchana Weerakoon<sup>1</sup>; *Bryan Chin*<sup>1</sup>; <sup>1</sup>Auburn University

10:45 AM

**A Laser-Assisted Combinatorial Approach for Designing Metallic Glass Alloys:** *Peter Tsai*<sup>1</sup>; Katharine Flores<sup>1</sup>; <sup>1</sup>Washington University in St. Louis

11:00 AM Invited

**Aerospace and Spacecraft Applications for Bulk Metallic Glasses and Matrix Composites:** *Douglas Hofmann*<sup>1</sup>; <sup>1</sup>NASA JPL/Caltech

11:20 AM

**Fabrication, Mechanical Properties and Corrosion Behavior of Ti<sub>75</sub>Zr<sub>10</sub>Si<sub>15</sub>-Based Alloys for Implant Applications:** *Somayeh Abdi*<sup>1</sup>; Steffen Oswald<sup>1</sup>; Anna Hynowska<sup>2</sup>; Mariana Calin<sup>1</sup>; Ludwig Schultz<sup>1</sup>; Jürgen Eckert<sup>1</sup>; Maria Dolors Baró<sup>2</sup>; Jordi Sort<sup>2</sup>; Annett Gebert<sup>1</sup>; <sup>1</sup>IFW institute; <sup>2</sup>Universitat Autònoma de Barcelona

11:35 AM Invited

**Phase Selection in Systems Driven Far from Equilibrium:** *Matthew Kramer*<sup>1</sup>; R. Ott<sup>1</sup>; E. Park<sup>1</sup>; F. Zhang<sup>1</sup>; C. Wang<sup>1</sup>; K. Ho<sup>1</sup>; <sup>1</sup>Iowa State University

11:55 AM

**Metallic Glass Based NanoScale Composites: New Approach for Developing Usable Ductility:** *Alla Sergueeva*<sup>1</sup>; Brian Meacham<sup>1</sup>; Sheng Cheng<sup>1</sup>; Daniel Branagan<sup>1</sup>; <sup>1</sup>The NanoSteel Company

12:10 PM

**Design and Formation Mechanism of Crystalline/Amorphous Composite Powder in Liquid Immiscible Alloy Systems:** *Yan Yu*<sup>1</sup>; Rongpei Shi<sup>1</sup>; Cuiping Wang<sup>1</sup>; *Xingjun Liu*<sup>1</sup>; Ryosuke Kainuma<sup>2</sup>; Kiyohito Ishida<sup>2</sup>; <sup>1</sup>Xiamen University; <sup>2</sup>Tohoku University

12:25 PM

**Fabrication of Mg-Cu-Zn-Y-Zr Amorphous Matrix Composites:** *You Junhua*<sup>1</sup>; *Wang Houchun*<sup>1</sup>; <sup>1</sup>Shenyang University of Technology

## Characterization of Materials through High Resolution Coherent Imaging: X-ray Based Techniques I

*Sponsored by:* TMS Structural Materials Division, TMS: Advanced Characterization, Testing, and Simulation Committee  
*Program Organizers:* John Carpenter, Los Alamos National Laboratory; Ross Harder, Argonne National Laboratory; Richard Sandberg, Los Alamos National Laboratory

Monday AM  
March 4, 2013

Room: 206B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Richard Sandberg, Los Alamos National Laboratory;  
Ross Harder, Argonne National Laboratory

### 8:30 AM Keynote

**Coherent Diffraction Imaging of Materials by Using an X-ray Free Electron Laser:** *Jianwei (John) Miao*<sup>1</sup>; <sup>1</sup>University of California, Los Angeles

### 9:00 AM Invited

**Coherent Diffraction Imaging of Strain on the Nanoscale:** *Ross Harder*<sup>1</sup>; <sup>1</sup>Argonne National Laboratory

### 9:20 AM

**Study of Charge-Ordering in Manganites via Serial Femtosecond Crystallography:** *Kenneth Beyerlein*<sup>1</sup>; <sup>1</sup>DESY

### 9:40 AM Invited

**Advanced Reconstruction Algorithms for Ptychography:** *Pierre Thibault*<sup>1</sup>; <sup>1</sup>Technical University of Munich

### 10:00 AM Break

### 10:20 AM Keynote

**XFEL Materials Imaging at the LCLS CXI Endstation:** *Garth Williams*<sup>1</sup>; <sup>1</sup>SLAC National Accelerator Lab

### 10:50 AM Invited

**Nanoscale X-Ray Imaging:** *Oleg Shpyrko*<sup>1</sup>; <sup>1</sup>University of California, San Diego

### 11:10 AM

**Ptychographic Tomography: A Quantitative Tool for Nanoscale 3D Microscopy:** *Ana Diaz*<sup>1</sup>; Pavel Trtik<sup>2</sup>; Manuel Guizar-Sicairos<sup>1</sup>; Andreas Menzel<sup>1</sup>; Oliver Bunk<sup>1</sup>; <sup>1</sup>Paul Scherrer Institute; <sup>2</sup>EMPA

### 11:30 AM

**Diffraction Imaging at Large Fresnel Number and the Challenge of Dynamic Mesoscale Imaging of Materials:** *Cris Barnes*<sup>1</sup>; John Barber<sup>1</sup>; Richard Sandberg<sup>1</sup>; Richard Sheffield<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

## Characterization of Minerals, Metals and Materials 2013: Characterization of Ferrous Metals I

*Sponsored by:* TMS Extraction and Processing Division, TMS: Materials Characterization Committee  
*Program Organizers:* Jiann-Yang Hwang, Michigan Technological University; Chen-Guang Bai, Chongqing University; John Carpenter, DOE LANL; Shadia Ikhamyies, Al Isra University; Bowen Li, Michigan Technological University; Mingming Zhang, ArcelorMittal Global R&D; Sergio Monteiro, State University of North Rio de Janeiro; Zhiwei Peng, Michigan Technological University

Monday AM  
March 4, 2013

Room: 206A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Jiann Yang Hwang, Michigan Technological University;  
Jian Li, CANMET

### 9:00 AM Joint Lecture

Attendees are encouraged to attend the Extraction and Processing Division Distinguished Lecturer Presentation in Room 006D at 9:00 AM.

**Towards Sustainable Metal Production by Molten Oxide Electrolysis:** Antoine Allanore<sup>1</sup> on behalf of Donald Sadoway<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology

### 9:30 AM

**Application of Thermoelectric Power Technique to Study the Static Strain Ageing of Heavily Cold Drawn Steel:** *Aude Lamontagne*<sup>1</sup>; Xavier Kleber<sup>1</sup>; Véronique Massardier<sup>1</sup>; Daniele Mari<sup>2</sup>; <sup>1</sup>INSA de Lyon, MATEIS - UMR CNRS 5510; <sup>2</sup>Ecole Polytechnique Fédérale de Lausanne, Institute of Condensed Matter Physics

### 9:50 AM

**Analysis of the Welded 100-Meter Heavy Rails for Passenger Dedicated Lines Being Broken during the Straightening Process:** *Ren Chao*<sup>1</sup>; <sup>1</sup>Wuhan University of Science and Technology

### 10:10 AM

**Effect of Continuous Cooling Rate on Microstructural Transformation of 60Si<sub>2</sub>CrVAT Spring Steel:** *Biao Zhou*<sup>1</sup>; Yi-Long Liang<sup>2</sup>; Qun Luo<sup>1</sup>; Jie-Yu Zhang<sup>1</sup>; Qian Li<sup>1</sup>; Kuo-Chih Chou<sup>1</sup>; <sup>1</sup>Shanghai University; <sup>2</sup>Guizhou University

### 10:30 AM

**An Investigation on Texture-Property Correlation in CRNO Steels:** *Santosh Sahoo*<sup>1</sup>; Dibyanjan Prusty<sup>1</sup>; Hitendra Pradhan<sup>1</sup>; Vijay Hiwarkar<sup>2</sup>; <sup>1</sup>National Institute of Technology Rourkela; <sup>2</sup>Crompton Greaves Limited

### 10:50 AM

**Effect of Centrifugal And Gravity Casting Technique over Metallographic and Mechanical Properties of Spheroidal Graphite Iron:** *Desai Gowda H S*<sup>1</sup>; Mukunda Pudukottah<sup>1</sup>; Mervin Herbert<sup>2</sup>; <sup>1</sup>Nitte Meenakshi Institute of Technology; <sup>2</sup>National Institute of Technology Karnataka

### 11:10 AM

**Crystallographic Research on the Morphology of AlN and MnS Complex Precipitation in Steel:** *Feifei Sun*<sup>1</sup>; <sup>1</sup>Shanghai University



## Computational Discovery of Novel Materials: Novel Methods for Materials Discovery

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Integrated Computational Materials Engineering Committee  
*Program Organizers:* Richard Hennig, Cornell University; Dallas Trinkle, University of Illinois at Urbana-Champaign

Monday AM  
March 4, 2013

Room: 207B  
Location: Henry B. Gonzalez  
Convention Center

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

### 8:30 AM Invited

**High-Throughput Diffusion Modeling for Materials Data and Discovery:** *Dane Morgan*<sup>1</sup>; Tam Mayeshiba<sup>1</sup>; Tom Angsten<sup>1</sup>; <sup>1</sup>University of Wisconsin - Madison

### 9:05 AM

**Combination of Computational Thermodynamics, Gaussian Processes and Genetic Algorithms for Superalloy Design:** *Franck Tancrét*<sup>1</sup>; <sup>1</sup>Université de Nantes

### 9:25 AM Invited

**Sparse Bayesian Cluster Expansions:** *Jesper Kristensen*<sup>1</sup>; Meenakshi Sundaram<sup>1</sup>; Ilias Bilonis<sup>1</sup>; Nicholas Zabaras<sup>1</sup>; <sup>1</sup>Materials Process Design and Control Laboratory

### 10:00 AM Break

### 10:15 AM

**Design of Multifunctional Material Architectures Using Topology Optimization:** *James Guest*<sup>1</sup>; Seunghyun Ha<sup>1</sup>; Reza Lotfi<sup>1</sup>; <sup>1</sup>Johns Hopkins University

### 10:35 AM Invited

**First-Principles Guided Nano-to-Microscale Design of Material Interfaces:** *Santanu Chaudhuri*<sup>1</sup>; Jie Xiao<sup>1</sup>; Shahryar Fotovati<sup>1</sup>; Hyunwook Kwak<sup>1</sup>; <sup>1</sup>Washington State University

### 11:10 AM

**Hybrid Genetic Algorithm and Mesh Adaptive Direct Search Algorithm Approach for the Thermodynamic Assessment of Multi-component Alloys:** *Sean Gibbons*<sup>1</sup>; Raymundo Arroyave<sup>1</sup>; ShengYen Li<sup>1</sup>; <sup>1</sup>Texas A&M University

### 11:30 AM

**Symmetry in Material Property Relationships: A Tool for the Discovery of New Alloys:** *Isaac Toda-Caraballo*<sup>1</sup>; Enrique Galindo-Nava<sup>1</sup>; Pedro Rivera-Díaz-del-Castillo<sup>1</sup>; <sup>1</sup>University of Cambridge

### 11:50 AM

**Strength/Elongation Optimisation in Materials: A Case for Accelerated Metallurgy Research:** *Isaac Toda-Caraballo*<sup>1</sup>; Enrique Galindo-Nava<sup>1</sup>; Pedro Rivera-Díaz-del-Castillo<sup>1</sup>; <sup>1</sup>University of Cambridge

## Computational Thermodynamics and Kinetics: First-principles Thermodynamics

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Alloy Phases Committee, TMS: Chemistry and Physics of Materials Committee, TMS/ASM: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS/ASM: Phase Transformations Committee, TMS: Process Technology and Modeling Committee

*Program Organizers:* Jörg Neugebauer, Max-Planck-Institut für Eisenforschung GmbH; Carelyn Campbell, NIST; Dongwon Shin, Oakridge National Lab; Zi Kui Liu, Penn State; Michael Demkowicz, Massachusetts Institute of Technology; Raymundo Arroyave, Texas A & M University; Shenyang Hu, Pacific Northwest National Laboratory

Monday AM  
March 4, 2013

Room: 207A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Dongwon Shin, Oak Ridge National Laboratory; Tetsuo Mohri, Hokkaido University

### 8:30 AM Invited

**First-Principles Calculation of Spinodal Ordering for Fe-Based Alloys:** *Tetsuo Mohri*<sup>1</sup>; <sup>1</sup>Hokkaido University

### 8:55 AM Invited

**First-Principles Thermodynamics of Paramagnetic Gamma Iron:** *Fritz Körmann*<sup>1</sup>; Blazej Grabowski<sup>1</sup>; Tilmann Hickel<sup>1</sup>; Jörg Neugebauer<sup>1</sup>; <sup>1</sup>Max-Planck-Institut für Eisenforschung

### 9:20 AM

**Phonon Stiffening Due to Hybridization of Electronic States in Au-Fe Alloys:** *Jorge Munoz*<sup>1</sup>; Matthew Lucas<sup>2</sup>; Brent Fultz<sup>1</sup>; <sup>1</sup>California Institute of Technology; <sup>2</sup>Air Force Research Laboratory

### 9:35 AM

**Atomic Configurations of PbTiO<sub>3</sub> Investigated by Ab-Initio Molecular Dynamic Simulations:** *Huazhi Fang*<sup>1</sup>; Yi Wang<sup>1</sup>; Shun Li Shang<sup>1</sup>; Zi-Kui Liu<sup>1</sup>; <sup>1</sup>The Pennsylvania State University

### 9:50 AM Break

### 10:10 AM Invited

**Topologically Close-Packed Phases in Transition-Metal Alloys - Assessing an Empirical Structure Map with High-throughput Ab-Initio Calculations:** *Thomas Hammerschmidt*<sup>1</sup>; Bernhard Seiser<sup>2</sup>; Arthur Bialon<sup>1</sup>; David Pettifor<sup>2</sup>; Ralf Drautz<sup>1</sup>; <sup>1</sup>ICAMS, Ruhr-University Bochum; <sup>2</sup>MML, University of Oxford

### 10:35 AM

**Ab Initio Calculations of the U-Zr System:** *Wei Xie*<sup>1</sup>; Wei Xiong<sup>1</sup>; Chao Shen<sup>1</sup>; Chris Marianetti<sup>2</sup>; Austin Chang<sup>1</sup>; Dane Morgan<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison; <sup>2</sup>Columbia University

### 10:50 AM

**Interface Structure and Segregation for MoSi<sub>2</sub>-NbSi<sub>3</sub> Alloys: A First Principles Study:** *Koretaka Yuge*<sup>1</sup>; Yuichiro Koizumi<sup>2</sup>; Koji Hagihara<sup>3</sup>; Takayoshi Nakano<sup>4</sup>; Kyosuke Kishida<sup>1</sup>; Haruyuki Inui<sup>1</sup>; <sup>1</sup>Department of Materials Science and Engineering, Kyoto University; <sup>2</sup>Institute for Materials Research, Tohoku University; <sup>3</sup>Department of Adaptive Machine Systems, Graduate School of Engineering, Osaka University; <sup>4</sup>Division of Materials & Manufacturing Science, Graduate School of Engineering, Osaka University



11:05 AM

**Thermodynamics of Precipitate Nanolayers in Th-Doped and Ce-Doped Ir:** *James Morris*<sup>1</sup>; Frank Averill<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

11:20 AM

**Ab Initio Molecular Dynamics Simulation Study on the Carbothermal Reduction of Alumina under Vacuum:** *Xiumin Chen*<sup>1</sup>; Bin Yang<sup>1</sup>; Heng Xiong<sup>1</sup>; Ping Long<sup>1</sup>; Baoqiang Xu<sup>1</sup>; Dachun Liu<sup>1</sup>; <sup>1</sup>Kunming University of Science and Technology

11:35 AM

**Effects of Phonon Kinematics and Phonon Anharmonicity on the Thermodynamics of Rutile TiO<sub>2</sub> and SnO<sub>2</sub>:** *Tian Lan*<sup>1</sup>; Chen Li<sup>1</sup>; Brent Fultz<sup>1</sup>; <sup>1</sup>California Institute of Tech

## Cost Affordable Titanium IV: Overview and Low Cost Processing

*Sponsored by:* TMS Structural Materials Division, TMS: Titanium Committee

*Program Organizers:* M. Ashraf Imam, Naval Research Lab; Sam Froes, University of Idaho (Retired); Ramana Reddy, The University of Alabama

Monday AM  
March 4, 2013

Room: 217C  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* M. Ashraf Imam, Naval Research Laboratory; Ramana Reddy, The University of Alabama

8:30 AM Keynote

**Cost Effective Developments for Fabrication of Titanium Components:** *F. H. (Sam) Froes*<sup>1</sup>; M. Ashraf Imam<sup>2</sup>; Ramana Reddy<sup>3</sup>; <sup>1</sup>University of Idaho; <sup>2</sup>Naval Research Lab; <sup>3</sup>The University of Alabama

9:10 AM Invited

**There is Low Cost Titanium Componentry Today:** *James Withers*<sup>1</sup>; V. Shapovalov<sup>1</sup>; R. Storm<sup>1</sup>; R. O. Loutfy<sup>1</sup>; <sup>1</sup>MER Corporation

9:30 AM Invited

**The Impact of Porosity on the Microstructural Kinetics of the Electro-Deoxidation of Titanium Dioxide in Molten Calcium Chloride:** Duncan Alexander<sup>1</sup>; *Carsten Schwandt*<sup>2</sup>; Derek Fray<sup>2</sup>; <sup>1</sup>Interdisciplinary Centre for Electron Microscopy, École Polytechnique Fédérale de Lausanne; <sup>2</sup>Department of Materials Science and Metallurgy, University of Cambridge

9:50 AM Break

10:10 AM Invited

**Application of the FFC Cambridge Process for the Production of Titanium Alloys:** *Rohit Bhagat*<sup>1</sup>; Kartik Rao<sup>2</sup>; David Dye<sup>3</sup>; Gregory Gibbons<sup>1</sup>; Richard Dashwood<sup>1</sup>; <sup>1</sup>Warwick University; <sup>2</sup>Metalysis Ltd; <sup>3</sup>Imperial College London

10:30 AM Invited

**Development of a Continuous Process to Produce Ti via Metallothermic Reduction of TiCl<sub>4</sub> in Molten Salt:** *David van Vuuren*<sup>1</sup>; Salomon Oosthuizen<sup>1</sup>; Jaco Swanepoel<sup>1</sup>; <sup>1</sup>CSIR

10:50 AM Invited

**The Metalysis Process: From Patents to Production:** *Kartik Rao*<sup>1</sup>; Steve Holloway<sup>1</sup>; Ian Mellor<sup>1</sup>; James Deane<sup>1</sup>; Lucy Grainger<sup>1</sup>; Guppy Dhariwal<sup>1</sup>; <sup>1</sup>Metalysis

11:10 AM

**Behavior of Intermediate CaTiO<sub>3</sub> in Reduction Process of TiO<sub>2</sub> by Calcium Vapor:** Jingang Jia<sup>1</sup>; *Baoqiang Xu*<sup>1</sup>; Bin Yang<sup>1</sup>; Heng Xiong<sup>1</sup>; Dachun Liu<sup>1</sup>; Dongsheng Wang<sup>1</sup>; <sup>1</sup>Kunming University of Science and Technology

11:30 AM

**The TiRO™ Process for the Continuous Direct Production of Titanium Powder:** *Christian Doblin*<sup>1</sup>; <sup>1</sup>CSIRO

11:50 AM

**Factors Affecting The Yield of Ti-Al Alloy in the TiPro Process:** *Kenneth Sichone*<sup>1</sup>; Deliang Zhang<sup>1</sup>; Stella Raynova<sup>1</sup>; <sup>1</sup>The University of Waikato

## Fatigue and Fracture of Thin Films and Nanomaterials: Fatigue of Thin Films and Nanomaterials

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS/ASM: Mechanical Behavior of Materials Committee, TMS: Nanomechanical Materials Behavior Committee

*Program Organizers:* Megan Cordill, Erich Schmid Institute of Materials Science; Daniel Kiener, Montanuniversitaet Leoben; Xinghang Zhang, Texas A & M University; Daniel Gianola, University of Pennsylvania; Corinne Packard, Colorado School of Mines

Monday AM  
March 4, 2013

Room: Bowie C  
Location: Grand Hyatt

*Funding support provided by:* Hysitron, Inc. and Nanomechanics, Inc.

*Session Chairs:* Daniel Gianola, University of Pennsylvania; Benoit Merle, University Erlangen-Nürnberg

8:30 AM Invited

**Deformation in Several Nanotwinned Metals:** Tim Furnish<sup>1</sup>; Leonardo Velasco<sup>1</sup>; Carla Shute<sup>2</sup>; Yifeng Liao<sup>2</sup>; Andrea Hodge<sup>1</sup>; *Julia Weertman*<sup>2</sup>; <sup>1</sup>USC; <sup>2</sup>Northwestern University

9:00 AM

**The Evolution of Nanocrystalline Grain Boundary Networks under Thermomechanical Cycling:** David Bober<sup>1</sup>; *Timothy Rupert*<sup>1</sup>; <sup>1</sup>University of California, Irvine

9:20 AM

**Fatigue Testing of Gold Thin Films with the Bulge Test:** *Benoit Merle*<sup>1</sup>; Mathias Goken<sup>1</sup>; <sup>1</sup>University Erlangen-Nürnberg, Department of Materials Science and Engineering, Institute I

9:40 AM

**Fatigue Behavior of a Nanocrystalline Austenitic Steel:** *Oliver Renk*<sup>1</sup>; Reinhard Pippan<sup>1</sup>; Erich Schmid Institute of Materials Science

10:00 AM Break

10:20 AM Invited

**Plasticity, Fracture and Fatigue of Ultra Thin Metallic Films on Polyimide Substrates:** *Patric Gruber*<sup>1</sup>; <sup>1</sup>KIT Institute for Applied Materials

10:50 AM

**Fatigue Behavior of Nanoscale Au Films on a Flexible Substrate:** *Guang-Ping Zhang*<sup>1</sup>; *Xiao-Fei Zhu*<sup>2</sup>; *Xue-Mei Luo*<sup>2</sup>; *Bin Zhang*<sup>3</sup>; <sup>1</sup>Institute of Metal Research, Chinese Academy of Sciences, China; <sup>2</sup>Institute of Metal Research, Chinese Academy of Sciences; <sup>3</sup>Key Laboratory for Anisotropy and Texture of Materials of Ministry of Education, Northeastern University, China

11:10 AM

**Design and Fabrication of Fatigue Damage Free Metal Electrode with 2D Nanohole Arrays:** *Byoung-Joon Kim*<sup>1</sup>; *Young-Chang Joo*<sup>1</sup>; *In-suk Choi*<sup>2</sup>; <sup>1</sup>Seoul National University; <sup>2</sup>Korea Institute of Science and Technology

11:30 AM

**Influence of Nanoscale Atomic-Layered-Deposited Coatings on the Fatigue Properties of Si and Ni Films:** *Eva Baumert*<sup>1</sup>; *Thomas Straub*<sup>2</sup>; *Chris Eberl*<sup>2</sup>; *Olivier Pierron*<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology; <sup>2</sup>Karlsruhe Institute of Technology

## High Temperature Electrochemistry: High Temperature Electrochemistry Plenary Session

*Sponsored by:* TMS Extraction and Processing Division, TMS; Pyrometallurgy Committee

*Program Organizers:* Prabhat Tripathy, Idaho National Laboratory; Guy Fredrickson, Idaho National Lab

Monday AM  
March 4, 2013

Room: 006D  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Jerome Downey, Montana Tech of The University of Montana; Boyd Davis, Kingston Process Metallurgy

8:30 AM

**Electrochemical Applications of Molten Salts:** *Derek Fray*<sup>1</sup>; <sup>1</sup>University of Cambridge

9:00 AM

**Towards Sustainable Metal Production by Molten Oxide Electrolysis:** *Antoine Allanore*<sup>1</sup>; *Donald Sadoway*<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology

9:30 AM Break

9:50 AM

**Electrolytic Production of Metals from Oxides Dissolved in Molten Salts:** *Uday Pal*<sup>1</sup>; <sup>1</sup>Boston University

10:20 AM

**Sensor Technology for Real Time Monitoring of Molten Salt Electrolytes During Nuclear Fuel Electrowinning:** *Michael Simpson*<sup>1</sup>; *Guy Fredrickson*<sup>1</sup>; *Brenda Serrano-Rodriguez*<sup>1</sup>; *Natalie Gese*<sup>1</sup>; *Marat Khafizov*<sup>1</sup>; *Supathorn Phongikaroon*<sup>2</sup>; *Kerry Allahar*<sup>3</sup>; <sup>1</sup>Idaho National Laboratory; <sup>2</sup>University of Idaho; <sup>3</sup>Boise State University

10:50 AM

**Thermochemical Consideration of Pyrochemical Treatment of Spent Nitride Fuels:** *Hirokazu Hayashi*<sup>1</sup>; *Takumi Satoh*<sup>1</sup>; *Hiroki Shibata*<sup>1</sup>; *Masaki Kurata*<sup>1</sup>; *Takashi Iwai*<sup>1</sup>; *Yasuo Arai*<sup>1</sup>; <sup>1</sup>Japan Atomic Energy Agency

11:20 AM

**Various Cathodic Processes during Electro-Reduction of Solid Oxides in High Temperature Molten Salt:** *Dihua Wang*<sup>1</sup>; *Wei Xiao*<sup>1</sup>; <sup>1</sup>Wuhan University

11:50 AM

**How High Temperature Electrochemical Cell Experiments Led to Industrial Trials for Using Waste ZnO for Desulfurising Hot Metal:** *Ramachandran Kumar*<sup>1</sup>; <sup>1</sup>University of Cambridge

12:20 PM

**The Molten Salt Electrolytic Winning of Oxygen and Metal from Lunar Regolith:** *Carsten Schwandt*<sup>1</sup>; *James Hamilton*<sup>2</sup>; *Derek Fray*<sup>1</sup>; *Ian Crawford*<sup>3</sup>; <sup>1</sup>Department of Materials Science and Metallurgy, University of Cambridge; <sup>2</sup>Green Metals Ltd; <sup>3</sup>Department of Earth and Planetary Sciences, Birkbeck College, University of London

## Hume-Rothery Award Symposium: Electronic Structure Theory of Stability and Bonding in Alloys: Electronic Structure

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Alloy Phases Committee

*Program Organizer:* Chris Wolverton, Northwestern University

Monday AM  
March 4, 2013

Room: 205  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Chris Wolverton, Northwestern University; Mark Asta, University California Berkeley

8:30 AM Introductory Comments

8:40 AM Keynote

**2013 William Hume-Rothery Award Winner: First Principles Alloy Theory - A Retrospective:** *Alex Zunger*<sup>1</sup>; <sup>1</sup>University of Colorado

9:25 AM Invited

**A Family of Nonempirical Density Functionals for the Exchange-Correlation Energy:** *John Perdew*<sup>1</sup>; <sup>1</sup>Tulane University

9:55 AM Break

10:15 AM Invited

**Computational Nano-Materials Design for Spinodal Nanotechnology as a New Class of Bottom-up Nanotechnology: Design vs. Experimental Realization:** *Hiroshi Katayama-Yoshida*<sup>1</sup>; <sup>1</sup>Osaka University

10:45 AM Invited

**Development of Reduced Tight-Binding and Bond-Order Potential Models for Si-N Nanocomposite Coatings:** *David Pettifor*<sup>1</sup>; *Jan Gehrman*<sup>1</sup>; *Martin Reese*<sup>2</sup>; *Matous Mrovec*<sup>2</sup>; *Christian Elsaesser*<sup>2</sup>; *Bernd Meyer*<sup>3</sup>; *Aleksey Kolmogorov*<sup>1</sup>; *Ralf Drautz*<sup>1</sup>; <sup>1</sup>University of Oxford; <sup>2</sup>Fraunhofer-Institut; <sup>3</sup>Friedrich-Alexander University of Erlangen-Nurnberg

11:15 AM Invited

**Perspectives on Phonons and Electron-Phonon Scattering in High-Temperature Superconductors:** *Barry Klein*<sup>1</sup>; <sup>1</sup>UC Davis

## Hybrid and Hierarchical Composite Materials: Processing

*Sponsored by:* TMS Structural Materials Division, TMS/ASM: Composite Materials Committee

*Program Organizers:* Tomoko Sano, US Army Research Laboratory; Charles Randow, US Army Research Laboratory; Chang Soo Kim, University of Wisconsin - Milwaukee

Monday AM  
March 4, 2013

Room: 215  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* Chang Soo Kim, University of Wisconsin - Milwaukee

8:30 AM

**Hierarchical Composites from Simple Building Blocks: Computation, Theory and Experiment:** *Markus Buehler*<sup>1</sup>; Leon Dimas<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology

9:00 AM

**Effects of Processing Conditions During Freeze Casting of Alumina Composites:** *Octavio Cervantes*<sup>1</sup>; Hilary Bowen<sup>2</sup>; Alexander Gash<sup>1</sup>; John Molitoris<sup>1</sup>; Luke Brewer<sup>3</sup>; Joseph Hooper<sup>3</sup>; <sup>1</sup>LLNL; <sup>2</sup>United States Air Force Academy; <sup>3</sup>Naval Postgraduate School / Center for Materials Research

9:20 AM

**Enabling Nanoparticle Networking in Semi-Crystalline Polymer Matrices:** *Meisha Shofner*<sup>1</sup>; Jasmeet Kaur<sup>1</sup>; Ji Hoon Lee<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

9:40 AM

**Bonding and Mechanical Testing of 3D Woven Lattice Material:** *Yong Zhang*<sup>1</sup>; Seunghyun Ha<sup>1</sup>; Jamie Guest<sup>1</sup>; Keith Sharp<sup>2</sup>; Richard Fonda<sup>3</sup>; Andy Geltmacher<sup>3</sup>; Timothy Weihs<sup>1</sup>; Kevin Hemker<sup>1</sup>; <sup>1</sup>Johns Hopkins University; <sup>2</sup>3TEX, Inc; <sup>3</sup>Naval Research Laboratory

10:00 AM Break

10:15 AM

**Effect of Graphene NanoPlatelets on Consolidation and Mechanical Properties of Spark Plasma Sintered Tantalum Carbide:** *Andy Nieto*<sup>1</sup>; Debrupa Lahiri<sup>1</sup>; Arvind Agarwal<sup>1</sup>; <sup>1</sup>Florida International University

10:35 AM

**Fiber Reinforced Chemical Bonded Phosphate Ceramics Matrix Composites:** *Henry A. Colorado*<sup>1</sup>; Clem Hiel<sup>2</sup>; Jenn-Ming Yang<sup>1</sup>; <sup>1</sup>University of California, Los Angeles; <sup>2</sup>Composite Support and Solutions Inc

10:55 AM

**High Performance Multi-Walled Carbon Nanotubes Reinforced Epoxy Nanocomposites:** *Hongbo Gu*<sup>1</sup>; Yudong Huang<sup>2</sup>; Suying Wei<sup>1</sup>; Zhanhu Guo<sup>1</sup>; <sup>1</sup>Lamar University; <sup>2</sup>Harbin Institute of Technology

11:15 AM

**Mechanical Properties and Dispersion Characteristics of Aluminum Composites Reinforced with Carbon Nanotubes of Different Diameters:** Prathap Chandran<sup>1</sup>; Shyam Kumar<sup>1</sup>; Niraj Chawake<sup>1</sup>; Karthiselva N<sup>1</sup>; Niraj Nayan<sup>2</sup>; SVS Narayana Murty<sup>2</sup>; *Srinivasa Bakshi*<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Madras; <sup>2</sup>Vikram Sarabhai Space Center

## Integrated Computational Modeling of Materials for Nuclear Energy: Fuel Modeling I: Lower Scale Modeling

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS/ASM: Computational Materials Science and Engineering Committee, TMS/ASM: Nuclear Materials Committee

*Program Organizers:* Remi Dingreville, Sandia National Laboratories; Koenraad Janssens, Paul Scherrer Institute; Timothy Bartel, Sandia National Laboratories

Monday AM  
March 4, 2013

Room: 202B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* To Be Announced

8:30 AM Invited

**Latest Improvements for the Treatment of Strong Correlations and Dispersive Bonds in First-Principles Studies of Actinide-Based Nuclear Materials:** Emerson Vathonne<sup>1</sup>; *Michel Freyss*<sup>1</sup>; Marjorie Bertolus<sup>1</sup>; Bernard Amadon<sup>2</sup>; <sup>1</sup>CEA, DEN; <sup>2</sup>CEA, DAM

9:00 AM

**Computational Study of Energetics and Defect-Ordering Tendencies for Y and La in UO<sub>2</sub>:** *Jonathan Solomon*<sup>1</sup>; Vitaly Alexandrov<sup>2</sup>; Tatiana Shvareva<sup>2</sup>; Babak Sadigh<sup>3</sup>; Alexandra Navrotsky<sup>2</sup>; Mark Asta<sup>1</sup>; <sup>1</sup>University of California, Berkeley; <sup>2</sup>University of California, Davis; <sup>3</sup>Lawrence Livermore National Laboratory

9:20 AM

**Fission Gas Bubble Nucleation in Bulk and at Grain-Boundaries of UO<sub>2</sub>:** *Xiang-Yang Liu*<sup>1</sup>; David Andersson<sup>1</sup>; Blas Uberuaga<sup>1</sup>; <sup>1</sup>Los Alamos National Lab

9:40 AM Invited

**Mechanism of Irradiation-Induced Point-Defect Cluster Formation in Metal Oxides by Molecular Dynamics Simulation:** *Dieter Wolf*<sup>1</sup>; Dilpuneet Aidhy<sup>2</sup>; Simon Phillpot<sup>3</sup>; <sup>1</sup>Argonne National Laboratory; <sup>2</sup>IBM India Research Laboratory; <sup>3</sup>University of Florida

10:10 AM Break

10:30 AM

**Atomistic Studies of Defect Cluster Migration Mechanisms in UO<sub>2</sub>:** *Xian-Ming Bai*<sup>1</sup>; Jianguo Yu<sup>1</sup>; Anter El-Azab<sup>2</sup>; Todd Allen<sup>3</sup>; <sup>1</sup>Idaho National Laboratory; <sup>2</sup>Purdue University; <sup>3</sup>University of Wisconsin - Madison

10:50 AM

**Atomic Level Investigation of Defect Evolution in Irradiated Thoria (ThO<sub>2</sub>):** *Rakesh Behera*<sup>1</sup>; Dilpuneet Aidhy<sup>2</sup>; Chaitanya Deo<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology; <sup>2</sup>IBM

11:10 AM

**Molecular Dynamics Study of Voids and Bubbles in BCC Uranium:** *Benjamin Beeler*<sup>1</sup>; Chaitanya Deo<sup>1</sup>; Michael Baskes<sup>2</sup>; Maria Okuniewski<sup>3</sup>; <sup>1</sup>Georgia Institute of Technology; <sup>2</sup>University of California, San Diego; <sup>3</sup>Idaho National Laboratory



## Magnesium Technology 2013: Plenary

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

*Program Organizers:* Norbert Hort, Helmholtz-Zentrum Geesthacht; Suveen Mathaudu, US Army Research Office; Neale Neelameggham, IND LLC; Martyn Alderman, Magnesium Elektron

Monday AM  
March 4, 2013

Room: 214A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Norbert Hort, Helmholtz-Zentrum Geesthacht; Martyn Alderman, Magnesium Elektron North America; Suveen Mathaudu, U.S. Army Research Office; Neale Neelameggham, IND LLC

### 8:30 AM Introductory Comments

8:40 AM

**From Elektron to Bio Implants – Magnesium Alloys in the 21st Century:** *Karl Kainer*<sup>1</sup>; <sup>1</sup>Helmholtz-Zentrum Geesthacht

9:10 AM Invited

**A Brief History of the Development of Grain Refinement Technology for Cast Magnesium Alloys:** *David StJohn*<sup>1</sup>; Peng Cao<sup>2</sup>; Ma Qian<sup>1</sup>; Mark Easton<sup>3</sup>; <sup>1</sup>The University of Queensland; <sup>2</sup>University of Auckland; <sup>3</sup>CAST CRC, Monash University

9:40 AM

**The USAMP Magnesium Front End Research and Development Project – Results of the Magnesium “Demonstration” Structure:** Alan Luo; J. Quinn; Ravi Verma; Yar-Ming Wang; David Wagner; *Joy Forsmark*<sup>1</sup>; X. Su; J. Zindel; Mei Li; S. Logan; S. Bilkhur; Robert C. McCune; <sup>1</sup>Ford Motor Company

10:10 AM Break

10:30 AM

**The Use of AC-DC-AC Methods in Assessing Corrosion Resistance Performance of Coating Systems for Magnesium Alloys:** *Robert C. McCune*<sup>1</sup>; Vinod Upadhyay<sup>2</sup>; Yar-Ming Wang<sup>3</sup>; Dante Battocchi<sup>2</sup>; <sup>1</sup>Robert C McCune & Associates LLC; <sup>2</sup>NDSU Center for Surface Protection; <sup>3</sup>General Motors Research Laboratory (retired)

11:00 AM

**Thermodynamics of Phase Formation in Mg-La-Ce-Nd Alloys:** *Rainer Schmid-Fetzer*<sup>1</sup>; Joachim Groebner<sup>1</sup>; Artem Kozlov<sup>1</sup>; Milan Hamp<sup>1</sup>; Mark Easton<sup>2</sup>; Suming Zhu<sup>2</sup>; Mark Gibson<sup>3</sup>; Jian-Feng Nie<sup>2</sup>; <sup>1</sup>Clausthal University of Technology; <sup>2</sup>Monash University; <sup>3</sup>CSIRO Process Science & Engineering

11:30 AM

**Non-Flammable Magnesium Alloys with High Strength:** *Yoshihito Kawamura*<sup>1</sup>; Tsuyoshi Ito<sup>1</sup>; <sup>1</sup>Kumamoto University

## Magnetic Materials for Energy Applications -III: Status and Challenges

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Energy Committee, TMS: Energy Conversion and Storage Committee, TMS: Magnetic Materials Committee

*Program Organizers:* Sivaraman Guruswamy, University of Utah; Thomas Woodcock, IFW Dresden; Yongmei Jin, Michigan Technological University; Raju Ramanujan, Nanyang Technological University; Frank Johnson, GE Global Research; Oliver Gutfleisch, Technische Universität Darmstadt

Monday AM  
March 4, 2013

Room: 217D  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Robert Shull, National Institute of Standards and Technology; Victorino Franco, Universidad de Sevilla; Sivaraman Guruswamy, University of Utah

### 8:30 AM Introductory Comments

8:35 AM Keynote

**Current Status and Future Prospects of Magnetocaloric Materials:** *Karl Gschneidner*<sup>1</sup>; Yaroslav Mudryk<sup>2</sup>; Vitalij Pecharsky<sup>1</sup>; <sup>1</sup>Iowa State University; <sup>2</sup>Ames Laboratory (USDOE)

9:15 AM Invited

**The Search for Enhanced Magnetic Materials:** Steve Constantinides<sup>1</sup>; <sup>1</sup>Arnold Magnetic Technologies

9:50 AM Break

10:10 AM Invited

**Bonded Permanent Magnets – An Overview:** *Viswanathan Panchanathan*<sup>1</sup>; Mitchell Spencer<sup>1</sup>; <sup>1</sup>Polaris Rare Earth Materials LLC

10:45 AM Invited

**Challenges of Magnetic Material Development for Vehicle Electrification:** *Matthew Willard*<sup>1</sup>; <sup>1</sup>U.S. Naval Research Laboratory

11:20 AM Invited

**Anisotropic Curie Temperature Materials:** *Harsh Chopra*<sup>1</sup>; Jason Armstrong<sup>2</sup>; Susan Hua<sup>2</sup>; <sup>1</sup>State University of New York at Buffalo; <sup>2</sup>University at Buffalo, The State University of New York

## Materials and Fuels for the Current and Advanced Nuclear Reactors II: Modeling

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

*Program Organizers:* Ramprashad Prabhakaran, Idaho National Laboratory; Dennis Keiser, Idaho National Laboratory; Raul Rebak, GE Global Research

Monday AM  
March 4, 2013

Room: 202A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Brian Wirth, University of Tennessee; Ramprashad Prabhakaran, Idaho National Laboratory

8:30 AM

**A Rate-Theory Approach to Irradiation Damage Modeling with Random Cascades in Space and Time:** *Jesse Carter*<sup>1</sup>; Richard Smith<sup>1</sup>; William Howland<sup>1</sup>; <sup>1</sup>Bettis Atomic Power Laboratory

8:50 AM

**Computational Studies of Oxygen Transport along Grain Boundaries during Zirconium Corrosion:** *Xian-Ming Bai*<sup>1</sup>; <sup>1</sup>Idaho National Laboratory

9:10 AM

**Computational Modeling of Metallic Nuclear Fuel Casting Processes – A Separate Effects Study:** *Justin Crapps*<sup>1</sup>; Jack Galloway<sup>1</sup>; Dave Decroix<sup>1</sup>; David Korzekwa<sup>1</sup>; Rob Aikin<sup>1</sup>; Cetin Unal<sup>1</sup>; Randall Fielding<sup>2</sup>; Rory Kennedy<sup>2</sup>; <sup>1</sup>Los Alamos National Laboratory; <sup>2</sup>Idaho National Laboratory

9:30 AM

**Structure and Properties of the Y<sub>2</sub>O<sub>3</sub>/Fe Interface from First Principles Calculations:** *Samrat Choudhury*<sup>1</sup>; Christopher Stanek<sup>1</sup>; Blas Uberuaga<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

9:50 AM Break

10:10 AM

**Defect and Diffusion in UO<sub>2-x</sub> by Quantum Mechanics and Statistical Thermodynamic Approaches:** *Zhi-Gang Mei*<sup>1</sup>; Marius Stan<sup>1</sup>; Petrica Cristea<sup>2</sup>; David Andersson<sup>3</sup>; <sup>1</sup>Argonne National Laboratory; <sup>2</sup>University of Bucharest; <sup>3</sup>Los Alamos National Laboratory

10:30 AM

**Interface Affected Cascading In Nuclear Materials and Role of Fractal Dimensions:** You sung Han<sup>1</sup>; *Vikas Tomar*<sup>1</sup>; <sup>1</sup>Purdue University

10:50 AM

**Effects of Surface Strain on Oxygen Adsorption on Zr (0001) Surface:** *Xing Wang*<sup>1</sup>; Izabela Szlufarska<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison

11:10 AM

**Modelling of Dynamic Recrystallization Process Considering Orientation Effects in 316LN Stainless Steel:** *Xie Ganlin*<sup>1</sup>; Wang Xitao<sup>1</sup>; Wang Genqi<sup>2</sup>; <sup>1</sup>University of Science and Technology Beijing; <sup>2</sup>Yantai Taihai Manoir Nuclear Equipment Co. Ltd

## Materials in Clean Power Systems VIII: Durability of Materials : Materials for Fuel Cells and CSP Applications

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

*Program Organizers:* Sebastien Dryepont, ORNL; Kinga Unocic, ORNL; Jeffrey Fergus, Auburn University; Xingbo Liu, West Virginia University

Monday AM  
March 4, 2013

Room: 007A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Sebastien Dryepont, Oak Ridge National Laboratory; Jeffrey Fergus, Auburn University

8:30 AM Invited

**An Overview of the Mechanical Behavior of Solid Oxide Fuel Cell Substrates:** *Amit Shyam*<sup>1</sup>; Dana McClurg<sup>2</sup>; Amit Pandey<sup>2</sup>; Rosa Trejo<sup>2</sup>; Rick Lowden<sup>2</sup>; Andres Marquez<sup>2</sup>; Edgar Lara-Curzio<sup>2</sup>; Richard Goettler<sup>3</sup>; <sup>1</sup>ORNL; <sup>2</sup>Oak Ridge National Laboratory; <sup>3</sup>LG Fuel Cells

9:00 AM Invited

**Advanced Conductive Coating Performance under Long-term SOFC Operating Conditions:** *Jung Pyung Choi*<sup>1</sup>; Jeffry Stevenson<sup>1</sup>; Ryan Scott<sup>1</sup>; Matt Chou<sup>1</sup>; Gordon Xia<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory

9:30 AM

**ALCHEMI Studies of Cation Site Occupancies in Doped Manganese Cobaltite Spinels:** *Louis Gambino*<sup>1</sup>; Neal Magdefrau<sup>2</sup>; Yingjia Liu<sup>3</sup>; Jeffrey Fergus<sup>3</sup>; Ellen Sun<sup>2</sup>; Mark Aindow<sup>1</sup>; <sup>1</sup>University of Connecticut; <sup>2</sup>United Technologies Research Center; <sup>3</sup>Auburn University

9:50 AM

**The Effect of Constituent, Interfacial Properties and Morphology on the Dielectric Response of MIEC Membranes:** *Kyle Brinkman*<sup>1</sup>; Kenneth Reifsnider<sup>2</sup>; Fazle Rabbi<sup>2</sup>; <sup>1</sup>Savannah River National Laboratory (SRNL); <sup>2</sup>University of South Carolina

10:10 AM Break

10:20 AM Invited

**Comparison of Binary and Calcium Nitrate Ternary Systems for Solar Power Concentration: Saltt Stability and Materials Performance:** *Francisco Pérez Trujillo*<sup>1</sup>; Angel Fernandez Diaz-Carralero<sup>1</sup>; Isabel Lasanta<sup>1</sup>; <sup>1</sup>Universidad Complutense de Madrid

10:50 AM Invited

**Impact of Heat Transfer Media on Materials for Concentrated Solar Power:** *Dane Wilson*<sup>1</sup>; <sup>1</sup>ORNL

11:20 AM

**Corrosion Fatigue Studies of High Nickel Tubular Samples Containing Molten Salt:** *James Keiser*<sup>1</sup>; Sebastien Dryepont<sup>2</sup>; Donald Erdman<sup>2</sup>; Charles Hawkins<sup>2</sup>; <sup>1</sup>Oak Ridge National Laboratory; <sup>2</sup>ORNL

## Materials Research Applied to National Needs (MARANN) in Honor of Professor Morris E. Fine: Materials Research Applied to National Needs (MARANN) I

*Sponsored by:* TMS Structural Materials Division, TMS: Chemistry and Physics of Materials Committee

*Program Organizers:* Peter Liaw, Univ of Tennessee; Gongyao Wang, University of Tennessee; Semyon Vaynman, Northwestern University; Yip Wah Chung, Northwestern University

Monday AM  
March 4, 2013

Room: 006A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Yip-Wah Chung, Northwestern University; Peter Liaw, The University of Tennessee

8:30 AM Introductory Comments

8:35 AM Invited

**Lightweight Materials for the Automotive Industry - Materials Research Applied to National Energy Agenda:** *Alan Taub*<sup>1</sup>; <sup>1</sup>University of Michigan

9:15 AM Invited

**Development of a New Bridge Steel: From Atoms to Implementation:** *Julia Weertman*<sup>1</sup>; <sup>1</sup>Northwestern University

9:55 AM Break

10:15 AM Invited

**Computational Materials Design: From Genome to Flight:** *Greg Olson*<sup>1</sup>; <sup>1</sup>Northwestern University

10:55 AM Invited

**Fracture of Crystalline Silicon Nanopillars during Electrochemical Lithium Insertion:** *William Nix*<sup>1</sup>; Soek Woo Lee<sup>1</sup>; Matt McDowell<sup>1</sup>; Lucas Berla<sup>1</sup>; Ill Ryu<sup>1</sup>; Yi Cui<sup>1</sup>; <sup>1</sup>Stanford University

11:35 AM Invited

**Modeling and Simulation as a Tool to Advance Discovery in Materials Science:** Clark Cooper<sup>1</sup>; <sup>1</sup>National Science Foundation

## Materials Science in Reduced Gravity: Structure and Kinetics

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

*Program Organizers:* Douglas Matson, Tufts University; Robert Hyers, University of Massachusetts Amherst; Hani Henein, University of Alberta

Monday AM  
March 4, 2013

Room: Lone Star Salon E  
Location: Grand Hyatt

*Session Chair:* Douglas Matson, Tufts University

8:30 AM Introductory Comments

8:40 AM Invited

**Bias Fields: The Cause of Dendritic Branching:** Martin Glicksman<sup>1</sup>; <sup>1</sup>Florida Institute of Technology

9:10 AM Invited

**Integrated Shrinkage and Shape Distortion Analysis of Liquid-Phase Sintering Affected by Gravity:** Eugene Olevsky<sup>1</sup>; José Alvarado-Contreras<sup>1</sup>; Randall German<sup>1</sup>; <sup>1</sup>San Diego State University

9:40 AM

**Non-Equilibrium Solidification, Modeling for Microstructure Engineering of Industrial Alloys (NEQUISOL):** Dieter Herlach<sup>1</sup>; Jan Gegner<sup>1</sup>; Charles-André Gandin<sup>2</sup>; Damien Tournet<sup>2</sup>; Hani Henein<sup>3</sup>; Asuncion Garcia-Escorial<sup>4</sup>; Gerd-Ulrich Grün<sup>5</sup>; Marc Schneider<sup>6</sup>; <sup>1</sup>Deutsches Zentrum für Luft- und Raumfahrt; <sup>2</sup>ARMINES-CEMEF; <sup>3</sup>University of Alberta; <sup>4</sup>CENIM-CSIC; <sup>5</sup>HYDRO Aluminium Rolled Products GmbH; <sup>6</sup>MAGMA Gießereitechnologie

10:00 AM

**Phase Selection in Undercooled FeCo Alloys:** Douglas Matson<sup>1</sup>; <sup>1</sup>Tufts University

10:20 AM Break

10:40 AM Invited

**Effect of Microgravity on Solidification Processes in Fe-Based Undercooled Melts:** Wolfgang Loser<sup>1</sup>; Thomas Volkmann<sup>2</sup>; ; Douglas Matson<sup>3</sup>; <sup>1</sup>IFW Dresden; <sup>2</sup>DLR Cologne; <sup>3</sup>Tufts University

11:10 AM Invited

**Phase Selection in Undercooled Nd-Fe-B Alloy Melts:** Thomas Volkmann<sup>1</sup>; Wolfgang Loser<sup>2</sup>; Jianrong Gao<sup>3</sup>; Jorn Strohmer<sup>1</sup>; Sven Reutzel<sup>1</sup>; <sup>1</sup>German Aerospace Center DLR; <sup>2</sup>IFW Dresden; <sup>3</sup>Northeastern University

11:40 AM

**Measurement of Dendrite Growth Velocity as a Function of Undercooling on Al<sub>68.5</sub>Ni<sub>31.5</sub> Alloy in Reduced Gravity:** Stefan Klein<sup>1</sup>; Dieter Herlach<sup>1</sup>; Matthias Kolbe<sup>1</sup>; <sup>1</sup>German Aerospace Center (DLR)

12:00 PM

**Effects of Static Magnetic Fields on Dendritic Growth Kinetics in Undercooled Metallic Melts:** Jianrong Gao<sup>1</sup>; Yingjie Zhang<sup>1</sup>; Chao Yang<sup>1</sup>; <sup>1</sup>Northeastern University

12:20 PM Concluding Comments

## Mesoscale Computational Materials Science of Energy Materials: Battery Materials and Electrochemical Processes I

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

*Program Organizers:* Pascal Bellon, University of Illinois; Alfredo Caro, LANL; Long Qing Chen, Penn State University; Anter El-Azab, Florida State University; Ming Tang, Lawrence Livermore National Laboratory

Monday AM  
March 4, 2013

Room: 218  
Location: Henry B. Gonzalez Convention Center

*Session Chairs:* Yue Qi, General Motors R&D Center; Ming Tang, Lawrence Livermore National Laboratory

8:30 AM Invited

**Electrochemical and Mechanical Reliability of Three Dimensionally Reconstructed Electrode Microstructures:** R. Edwin Garcia<sup>1</sup>; <sup>1</sup>Purdue University

9:00 AM Invited

**Electrochemical Shock of Lithium Battery Materials:** William Woodford<sup>1</sup>; Yet-Ming Chiang<sup>1</sup>; W. Craig Carter<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology

9:30 AM

**Nonlinear Phase-Field Model of Interface Evolution Resulted from Electrode Reactions:** Linyun Liang<sup>1</sup>; Long Qing Chen<sup>1</sup>; Yue Qi<sup>2</sup>; Stephen Harris<sup>2</sup>; <sup>1</sup>Penn State University; <sup>2</sup>General Motors Corporation

9:50 AM Break

10:10 AM

**Mesoscale Modeling of Electrochemical Crystal Growth and the Interfacial Double Layer:** Michael Welland<sup>1</sup>; John Guyer<sup>2</sup>; Dieter Wolf<sup>1</sup>; <sup>1</sup>Argonne National Laboratory; <sup>2</sup>National Institute of Standards and Technology

10:30 AM Invited

**Morphological Evolution of Lithium Iron Phosphate Cathodes:** Bernardo Orvananos<sup>1</sup>; Hui-Chia Yu<sup>1</sup>; Katsuyo Thornton<sup>2</sup>; <sup>1</sup>Department of Materials Science & Engineering, University of Michigan; <sup>2</sup>Department of Materials Science & Engineering, University of Michigan

11:00 AM Invited

**Mesoscale Modeling of the Morphology and the Mechanical Properties of Proton Exchange Membranes:** Yue Qi<sup>1</sup>; Yeh-Hung Lai<sup>1</sup>; <sup>1</sup>General Motors R&D

11:30 AM

**Phase Field Simulation on the Concurrent Plastic Deformation, Phase Transformation, and Mass Diffusion in Silicon Anode for Lithium Ion Batteries:** Yonghao An<sup>1</sup>; Hanqing Jiang<sup>2</sup>; Ming Tang<sup>3</sup>; <sup>1</sup>Arizona State University, Lawrence Livermore National Laboratory; <sup>2</sup>Arizona State University; <sup>3</sup>Lawrence Livermore National Laboratory

11:50 AM

**Effect of Anisotropic Charge Transport, Elasticity and Particle Geometry on the Phase Transformation Morphology and Kinetics in Olivine Cathode Particles:** Ming Tang<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Laboratory



## Microstructural Processes in Irradiated Materials: Ferritic/Martensitic Steels I

*Sponsored by:* TMS Structural Materials Division, TMS/ASM: Nuclear Materials Committee

*Program Organizers:* Thak Sang Byun, Oak Ridge National Laboratory; Dane Morgan, University of Wisconsin-Madison; Yasuyoshi Nagai, Tohoku University; Zhijie Jiao, University of Michigan-Ann Arbor; Christine Guéneau, CEA-Saclay

Monday AM  
March 4, 2013

Room: 203A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Masatake Yamaguchi, Japan Atomic Energy Agency; Gary Was, University of Michigan

### 8:30 AM Introductory Comments

#### 8:40 AM Invited

**Microstructures of F-M Alloys at Very High Doses:** Gary Was<sup>1</sup>; Zhijie Jiao<sup>1</sup>; Elizabeth Beckett<sup>1</sup>; Kai Sun<sup>1</sup>; Janelle Wharry<sup>1</sup>; <sup>1</sup>University of Michigan

#### 9:10 AM

**The Mechanism of Radiation-Induced Segregation in Ferritic-Martensitic Alloys:** Janelle Wharry<sup>1</sup>; Gary Was<sup>1</sup>; <sup>1</sup>University of Michigan

#### 9:30 AM

**Intra- and Inter-Granular Cr and Impurities Behaviour on the Nanostructural Evolution of Fe-Cr Model Alloys under Neutron Irradiation: Comparison with Ion Irradiation:** Philippe Pareige<sup>1</sup>; Cristelle PAREIGE<sup>1</sup>; Viatcheslav Kuksenko<sup>1</sup>; <sup>1</sup>Rouen University

#### 9:50 AM

**Miscibility Gap and Short-Range Ordering in Non-Irradiated and He-Ion Irradiated Fe-Cr15 Alloy:** Stanislaw Dubiel<sup>1</sup>; Jan Zukrowski<sup>1</sup>; <sup>1</sup>AGH University

#### 10:10 AM Break

#### 10:30 AM

**In-Situ Observation of Dislocation Loop Formation and Growth in Electron-Irradiated Pure Iron and Fe-8Cr Alloys:** Naoyuki Hashimoto<sup>1</sup>; Bumsu Park<sup>1</sup>; Seiji Sakuraya<sup>1</sup>; Somei Ohnuki<sup>1</sup>; <sup>1</sup>Hokkaido University

#### 10:40 AM Invited

**First-Principles Study on the Intergranular Decohesion in Iron by Solute Segregation: Temper and Hydrogen-Induced Embrittlement:** Masatake Yamaguchi<sup>1</sup>; Jun Kameda<sup>2</sup>; <sup>1</sup>Japan Atomic Energy Agency; <sup>2</sup>Tohoku University

#### 11:10 AM

**Point Defect Cluster Interactions with Grain Boundaries in Nanocrystalline Fe and Fe-Cr:** Greg Vetterick<sup>1</sup>; Chris Barr<sup>1</sup>; John Baldwin<sup>2</sup>; Pete Baldo<sup>3</sup>; Mark Kirk<sup>3</sup>; Amit Misra<sup>2</sup>; Mitra Taheri<sup>1</sup>; <sup>1</sup>Drexel University; <sup>2</sup>Los Alamos National Laboratory; <sup>3</sup>Argonne National Laboratory

#### 11:30 AM

**Irradiated Microstructure of 9 and 12 Cr Model Alloys:** Yuedong Wu<sup>1</sup>; Zhijie Jiao<sup>2</sup>; Yong Yang<sup>1</sup>; <sup>1</sup>University of Florida; <sup>2</sup>University of Michigan

#### 11:50 AM

**Microstructural Evolution and Fracture Toughness Recovery by Thermal Annealing in HT9 Steel Irradiated to High Doses:** Osman Anderoglu<sup>1</sup>; Stuart Maloy<sup>2</sup>; Thak Sang Byun<sup>3</sup>; Bulent Sencer<sup>4</sup>; <sup>1</sup>Los Alamos National Laboratory; <sup>2</sup>LANL; <sup>3</sup>Oak Ridge National Laboratory; <sup>4</sup>Idaho National Laboratory

#### 12:10 PM

**Irradiation-Induced Formation of Clusters with C15 Laves Phase Structure in Bcc Iron:** Mihai-Cosmin Marinica<sup>1</sup>; Francois Willaume<sup>1</sup>; Jean-Paul Crocombette<sup>1</sup>; <sup>1</sup>CEA, Service de Recherches de Metallurgie Physique

## Modeling and Experimental Validation of Multiscale Mechanical Behavior from Atomic Scale to Macro Scale: Failure and Fracture

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Integrated Computational Materials Engineering Committee, TMS/ASM: Mechanical Behavior of Materials Committee, TMS: Nanomechanical Materials Behavior Committee, TMS: Process Technology and Modeling Committee, TMS: Shaping and Forming Committee

*Program Organizers:* Nathan Mara, Los Alamos National Laboratory; Jian Wang, Los Alamos National Laboratory; Brad Boyce, Sandia National Laboratories; Jennifer Carter, Case Western Reserve University; Anthony Rollett, Carnegie Mellon University; Jonathan Zimmerman, Sandia National Laboratories

Monday AM  
March 4, 2013

Room: 211  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Michael Demkowicz, MIT; Thomas Bieler, Michigan State University

### 8:30 AM Invited

**Atomistic Modeling of Deformation Mechanisms and Crack Initiation at Grain Boundaries:** Diana Farkas<sup>1</sup>; Laura Smith<sup>1</sup>; <sup>1</sup>Virginia Tech

#### 9:00 AM

**Characterization of Heterogeneous Deformation and Slip System Activation Along Grain Boundaries in Pure Tantalum:** Thomas Bieler<sup>1</sup>; Scott Sutton<sup>1</sup>; Martin Crimp<sup>1</sup>; Brad Boyce<sup>2</sup>; <sup>1</sup>Michigan State University; <sup>2</sup>Sandia National Laboratories

#### 9:20 AM

**High-Resolution Image Correlation, EBSD-Based Characterization and Simulation of Crack Tip and Grain Boundary Deformation in Al-Cu Alloys:** Vipul Gupta<sup>1</sup>; Jacob Hochhalter<sup>2</sup>; Erik Saether<sup>2</sup>; Scott Willard<sup>3</sup>; Ashley Spear<sup>4</sup>; Terryl Wallace<sup>2</sup>; Stephen Smith<sup>2</sup>; Edward Glaesgen<sup>2</sup>; <sup>1</sup>National Institute of Aerospace; <sup>2</sup>NASA Langley Research Center; <sup>3</sup>Science & Technology Corp.; <sup>4</sup>Cornell University

#### 9:40 AM Invited

**Combined Experimental and Computational Study of the Evolution of Local Slip Activity during Heterogeneous Deformation of Polycrystalline Ta, Ti, and Ti Alloys:** Thomas Bieler<sup>1</sup>; Chen Zhang<sup>1</sup>; Hongmei Li<sup>1</sup>; Yang Su<sup>1</sup>; Scott Sutton<sup>1</sup>; Philip Eisenlohr<sup>2</sup>; Claudio Zambaldi<sup>2</sup>; Martin Crimp<sup>1</sup>; Carl Boehlert<sup>1</sup>; Brad Boyce<sup>3</sup>; <sup>1</sup>Michigan State University; <sup>2</sup>Max-Planck-Institut für Eisenforschung; <sup>3</sup>Sandia National Laboratories

#### 10:10 AM Break

#### 10:20 AM

**Influence of Grain Boundary Properties on Spall Strength:** Saryu Fensin<sup>1</sup>; Steve Valone<sup>1</sup>; Ellen Cerreta<sup>1</sup>; George Gray<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

#### 10:40 AM Invited

**Healing of Nanocracks by Disclinations:** Michael Demkowicz<sup>1</sup>; Guoqiang Xu<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology

11:10 AM

**In-Situ TEM Study of Interfacial Faceting of Cu-Nb Nano-Lamellae during Indentation:** *Shijian Zheng*<sup>1</sup>; Jian Wang<sup>1</sup>; John Carpenter<sup>1</sup>; Robert Dickerson<sup>1</sup>; Irene Beyerlein<sup>1</sup>; Nathan Mara<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

11:30 AM Invited

**Exploring the Evolution and Deformation of Twinned Nanocrystalline Metals with Microscale Kinematic Metrics and Molecular Dynamics Simulations:** *Garritt Tucker*<sup>1</sup>; Stephen Foiles<sup>1</sup>; Henry Padilla<sup>1</sup>; Brad Boyce<sup>1</sup>; <sup>1</sup>Sandia National Laboratories

12:00 PM

**Quantifying the Relationship between Strain Mode, Anisotropy, and Surface Morphology in Deformed Aluminum Sheet:** *Mark Stoudt*<sup>1</sup>; Joseph Hubbard<sup>1</sup>; Lyle Levine<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

## Modeling of Multi-Scale Phenomena in Materials Processing - III: Microstructure Evolution I

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS/ASM: Computational Materials Science and Engineering Committee, TMS: Process Technology and Modeling Committee, TMS: Integrated Computational Materials Engineering Committee  
*Program Organizers:* Adrian Sabau, Oak Ridge National Laboratory; Anthony Rollett, Carnegie Mellon University; Laurentiu Nastac, The University of Alabama; Jonathan Madison, Sandia National Laboratories; Mei Li, Ford Motor Company

Monday AM  
March 4, 2013

Room: 216  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Laurentiu Nastac, University of Alabama - Tuscaloosa; Andrew Mullis, University of Leeds

8:30 AM Introductory Comments

8:35 AM Invited

**Application of a Modified Cellular Automaton Model to Simulating Solidification-Related Phenomena in Steels:** *Sebastian Micheli*<sup>1</sup>; Christian Bernhard<sup>2</sup>; <sup>1</sup>Montanuniversitaet Leoben / INTECO Special Melting Technologies; <sup>2</sup>Montanuniversitaet Leoben

9:20 AM

**Numerical Simulation of Solute Diffusion -Controlled Dendritic Growth with Cellular Automaton Method:** *Sen Luo*<sup>1</sup>; Miao-yong Zhu<sup>1</sup>; <sup>1</sup>Northeastern University

9:45 AM Break

10:15 AM Invited

**Multi-Scale Modelling Using 3-Dimensional Adaptive Meshing with an Implicit, Multigrid Solver: A Crystallization Example:** *Andrew Mullis*<sup>1</sup>; Christopher Goodyer<sup>1</sup>; Peter Bollada<sup>1</sup>; Peter Jimack<sup>1</sup>; <sup>1</sup>University of Leeds

11:00 AM

**A Multi Scale Method for Predicting Microstructure Changes from an External Magnetic Field:** *Andrew Kao*<sup>1</sup>; *Koulis Pericleous*<sup>1</sup>; <sup>1</sup>University of Greenwich

## Nanostructured Materials for Lithium Ion Batteries and for Supercapacitors:

### Nanostructured Materials for Lithium Ion Batteries and for Supercapacitors Session I

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Energy Conversion and Storage Committee  
*Program Organizer:* David Mitlin, University of Alberta and NINT NRC

Monday AM  
March 4, 2013

Room: 007B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* David Mitlin, University of Alberta and NINT NRC; Reza Shahbazian-Yassar, Michigan Technological University; Peter Kalisvaart, University of Alberta and NINT NRC; Zhi Li, University of Alberta and NINT NRC

8:30 AM Invited

**Silicon Anode Materials for All-Solid-State Lithium-ion Microbatteries:** *Peter Notten*<sup>1</sup>; <sup>1</sup>Eindhoven University

8:50 AM Invited

**3D Nanostructured Bicontinuous Electrodes: Path to Ultra-High Power and Energy Density Batteries:** *Paul Braun*<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign

9:10 AM Invited

**Engineering Electrochemically Active Nano-Scale Silicon Based Hetero-Structures:** *Prashant Kuma*<sup>1</sup>; <sup>1</sup>University of Pittsburgh

9:30 AM Invited

**Silicon Nanowire Core Aluminum Shell Coaxial Nanocomposites for Lithium Ion Battery Anodes Grown with and without a TiN Interlayer:** *Elmira Memarzadeh*<sup>1</sup>; *Peter Kalisvaart*<sup>2</sup>; Alireza Kohandehghan<sup>1</sup>; Benjamin Zehri<sup>1</sup>; Christopher Holt<sup>1</sup>; David Mitlin<sup>1</sup>; <sup>1</sup>University of Alberta; <sup>2</sup>University of Alberta

9:50 AM Invited

**Using in Situ Thin Film Stress Measurements to Understand Fundamental Lithiation Mechanisms in Battery Electrode Materials:** *Brian Sheldon*<sup>1</sup>; Anton Tokranov<sup>1</sup>; Amartya Mukhopadhyay<sup>1</sup>; Sumit Soni<sup>1</sup>; Peng Lu<sup>2</sup>; Xingcheng Xiao<sup>2</sup>; Yue Qi<sup>2</sup>; Dawei Liu<sup>1</sup>; Hamed Haft-Baradaran<sup>1</sup>; Huajian Gao<sup>1</sup>; <sup>1</sup>Brown University; <sup>2</sup>General Motors

10:10 AM Break

10:30 AM Invited

**Characterization of Battery Cycling by In-Situ Microscopy:** *Shen Dillon*<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign

10:50 AM Invited

**In-Situ Studies of Nanoscale Transport and Alloying Phenomena:** *Jeffrey Urban*<sup>1</sup>; <sup>1</sup>LBNL

11:10 AM Invited

**Electrochemical Lithiation of Silicon Clathrate Materials:** *Rahul Raghavan*<sup>1</sup>; Nicholas Wagner<sup>1</sup>; Ran Zhao<sup>1</sup>; Wuwei Liang<sup>2</sup>; Kwai Chan<sup>2</sup>; *Candace Chan*<sup>1</sup>; <sup>1</sup>Arizona State University; <sup>2</sup>Southwest Research Institute

11:30 AM Invited

**Li-Ion Nanobattery: Lessons from In-Situ Electron Microscopy:** *Reza Shahbazian-Yassar*<sup>1</sup>; <sup>1</sup>Michigan Technological University

11:50 AM Invited

**Carbon-Sulfur Nanocomposite Cathode Materials for Lithium-Sulfur Batteries:** *Yuegang Zhang*<sup>1</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory

**12:10 PM Invited**

**Spatially Resolved Porous Electrode Theory for Rechargeable Lithium-Ion Battery Electrodes:** *R. Edwin Garcia*<sup>1</sup>; <sup>1</sup>Purdue University

**Neutron and X-ray Studies of Advanced Materials VI: Centennial and Beyond: Diffraction: 100 Years and Beyond**

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

*Program Organizers:* Rozaliya Barabash, Oak Ridge National Laboratory; Xun-Li Wang, City University of Hong Kong; Jaimie Tile, US Air Force Research Laboratory; Gernot Kosterz, ETH Zurich; Brent Fultz, California Institute of Technology; Peter Liaw, University of Tennessee

Monday AM  
March 4, 2013

Room: 209  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Gernot Kosterz, ETH; Wolfgang Pantleon, Risoe National Laboratory and DTU

**8:30 AM Introductory Comments**

**8:35 AM Keynote**

**Materials Science Enabled by the Advanced Photon Source Upgrade:** *Gregory Stephenson*<sup>1</sup>; <sup>1</sup>Argonne National Laboratory

**9:00 AM Invited**

**One Hundred Years (Almost) of Diffuse X-Ray Scattering:** *Richard Welberry*<sup>1</sup>; <sup>1</sup>Research School of Chemistry

**9:20 AM Invited**

**Neutron and X-Ray Scattering Studies of Solid Sorbents for Carbon Capture:** *Andrew Allen*<sup>1</sup>; *Laura Espinal*<sup>1</sup>; *Winnie Wong-Ng*<sup>1</sup>; *Martin Green*<sup>1</sup>; <sup>1</sup>NIST

**9:40 AM Invited**

**X-ray and Neutron Studies of Fluids in Confinement:** *Oskar Paris*<sup>1</sup>; <sup>1</sup>Montanuniversitaet Leoben

**10:00 AM Break**

**10:10 AM Invited**

**A Detecting Strain Distributions in Nanoelectronics Using X-Ray Diffraction:** *Conal Murray*<sup>1</sup>; <sup>1</sup>IBM T.J. Watson Research Center

**10:30 AM Invited**

**Novel Approach to Generate Magnetic Fields Using Vortices in High-T<sub>c</sub> Superconductors for X-Ray Scattering Studies with Unrestricted Optical Access:** *Zahirul Islam*<sup>1</sup>; *R. Das*<sup>1</sup>; *J. Ruff*<sup>1</sup>; *R. Weinstein*<sup>2</sup>; *R. Sawh*<sup>2</sup>; *P. Canfield*<sup>3</sup>; *J.-W. Kim*<sup>1</sup>; *J. Lang*<sup>1</sup>; <sup>1</sup>Advanced Photon Source, Argonne National Laboratory; <sup>2</sup>Texas Center for Superconductivity, University of Houston; <sup>3</sup>Ames Laboratory, Iowa State University

**10:50 AM Keynote**

**Recrystallization Characterized by Synchrotron X-Rays:** *Dorte Jensen*<sup>1</sup>; <sup>1</sup>DTU

**11:10 AM**

**In-Situ Mesoscale Study of Twin Boundary Motion in NiMnGa Alloys under External Fields:** *Rozaliya Barabash*<sup>1</sup>; *Christoph Kirchlechner*<sup>2</sup>; *Odile Robach*<sup>3</sup>; *Ruqing Xu*<sup>4</sup>; *Martin Kunz*<sup>5</sup>; *Nobumichi Tamura*<sup>5</sup>; *Oleg Barabash*<sup>6</sup>; *Alexei Sozinov*<sup>7</sup>; <sup>1</sup>Oak Ridge National Laboratory; <sup>2</sup>University of Leoben; <sup>3</sup>ESRF; <sup>4</sup>APS; <sup>5</sup>ALS; <sup>6</sup>University of Tennessee; <sup>7</sup>AdaptaMat

**11:25 AM Invited**

**A New Methodology for Determining Residual Stress Distributions Using Finite Elements and Synchrotron X-Ray Diffraction:** *Matthew Miller*<sup>1</sup>; *Paul Dawson*<sup>1</sup>; <sup>1</sup>Cornell University

**11:45 AM Invited**

**Mechanics of Nanostructures Probed In-Situ by Coherent X-Ray Diffraction during Mechanical Loading with a Dedicated AFM:** *Olivier Thomas*<sup>1</sup>; *Thomas Cornelius*<sup>1</sup>; *Stéphane Labat*<sup>1</sup>; *Marie-Ingrid Richard*<sup>1</sup>; *Francesca Mastropietro*<sup>1</sup>; *Marc Gailhanou*<sup>1</sup>; *Jean-Marc Roussel*<sup>1</sup>; *Guillaume Beutier*<sup>2</sup>; *Marc Verdier*<sup>2</sup>; *Bruno Gilles*<sup>2</sup>; *Guillaume Parry*<sup>2</sup>; *Marc de Boissieu*<sup>2</sup>; *Frederic Livet*<sup>2</sup>; *Vincent Jacques*<sup>3</sup>; *Gerardina Carbone*<sup>3</sup>; *Tobias Schüll*<sup>3</sup>; <sup>1</sup>Aix-Marseille Université; <sup>2</sup>Grenoble-INP; <sup>3</sup>ESRF

**12:05 PM Invited**

**Opportunities for Studies of Complex Materials Using High-Energy X-Rays:** *Jonathan Almer*<sup>1</sup>; *Peter Kenesei*<sup>1</sup>; *John Okasinski*<sup>1</sup>; <sup>1</sup>Argonne National Laboratory

**Ni-Co 2013: Plenary**

*Sponsored by:* The Minerals, Metals and Materials Society, Metallurgical Society of the Canadian Institute of Mining Metallurgy and Petroleum, Chinese Society for Metals, GDMB Society for Mining, Metallurgy, Resource and Environmental Technology, Society for Mining Metallurgy and Exploration, Mining and Materials Processing Institute of Japan, Associacao Brasileira de Metalurgia, Materiais e Mineracao, Southern African Institute of Mining and Metallurgy (SAIMM), Minerals Engineering International Online, Cobalt Development Institute, Societe Francaise de Metallurgie et de Materiaux, TMS Extraction and Processing Division, TMS: Hydrometallurgy and Electrometallurgy Committee, TMS: Pyrometallurgy Committee  
*Program Organizer:* Thomas Battle, Midrex Technologies

Monday AM  
March 4, 2013

Room: 007D  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* Thomas Battle, Midrex Technologies

**9:00 AM Joint Lecture**

Attendees are encouraged to attend the Extraction and Processing Division Distinguished Lecturer Presentation in Room 006D at 9:00 AM.

**Towards Sustainable Metal Production by Molten Oxide Electrolysis:** *Antoine Allanore*<sup>1</sup> on behalf of *Donald Sadoway*<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology

**10:00 AM**

**Laterites - Still a Frontier of Nickel Process Development:** *Alan Taylor*<sup>1</sup>; <sup>1</sup>ALTA Metallurgical Services

**10:30 AM**

**Nickel and Stainless Steels: 100 Years of Working Together:** *Gary Coates*<sup>1</sup>; <sup>1</sup>Nickel Institute



11:00 AM

**Cobalt - The Technology Enabler:** *David Weight*<sup>1</sup>; <sup>1</sup>Cobalt Development Institute

11:30 AM

**The Recycling of Cobalt from Alloy Scrap, Spent Batteries or Catalysts and Metallurgical Residues- An Overview:** *Joe Ferron*<sup>1</sup>; <sup>1</sup>Other

## Novel Synthesis and Consolidation of Powder Materials : Activated Sintering, Spark Plasma Sintering and High Voltage Electric Discharge Consolidation

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS: Powder Materials Committee  
*Program Organizers:* Ma Qian, The University of Queensland; Iver Anderson, The Ames Laboratory

Monday AM  
March 4, 2013

Room: Lone Star Salon C  
Location: Grand Hyatt

*Session Chairs:* Ma Qian, The University of Queensland ; Katsuyoshi Kondoh, Osaka University

8:30 AM

**Activated Sintering for the Manufacture of Bi-Layered AgC Electrical Contacts:** *Daudi Waryoba*<sup>1</sup>; Jeffery Johnson<sup>2</sup>; Craig Stringer<sup>1</sup>; <sup>1</sup>Penn State University, DuBois; <sup>2</sup>Contact Technologies, Inc.

8:50 AM

**Fabrication of High Performance Commercial Titanium Alloys by Spark Plasma Sintering:** *Ya-Feng Yang*<sup>1</sup>; K Kondoh<sup>2</sup>; Ma Qian<sup>1</sup>; <sup>1</sup>University of Queensland; <sup>2</sup>Osaka University

9:10 AM Invited

**Inter-Particle Contact Phenomena in Spark-Plasma Sintering (SPS) and High Voltage Electric Discharge Consolidation (HVDC):** *Eugene Olevsky*<sup>1</sup>; Elena Aleksandrova<sup>2</sup>; Andrey Kuzmov<sup>2</sup>; Evgeny Grigoryev<sup>2</sup>; <sup>1</sup>San Diego State University; <sup>2</sup>Moscow Engineering Physics University

9:40 AM

**Spark Plasma Sintering of Metal-Carbon Nanocomposites:** *Thomas Hutsch*<sup>1</sup>; Thomas Schubert<sup>1</sup>; Thomas Weißgärber<sup>1</sup>; Bernd Kieback<sup>1</sup>; <sup>1</sup>Fraunhofer IFAM Dresden

10:00 AM Break

10:20 AM Invited

**Thermo-Mechanical Properties of ZrO<sub>2</sub>/Ti Functionally Graded Materials Fabricated by Spark Plasma Sintering:** *Hideaki Tsukamoto*<sup>1</sup>; Yoshiki Komiya<sup>1</sup>; Hisashi Sato<sup>1</sup>; Yoshimi Watanabe<sup>1</sup>; <sup>1</sup>Nagoya Institute of Technology

10:50 AM

**A Comparative Study of Lead-Free (Na,K,Li) (Ta,Nb)O<sub>3</sub> Ferroelectric Ceramics Fabricated by Pressureless and Spark Plasma Sintering:** *Seema Sharma*<sup>1</sup>; Kim Vanmeensel<sup>2</sup>; Jef Vleugels<sup>2</sup>; <sup>1</sup>Magadh University; <sup>2</sup>K U Leuven

11:10 AM

**Influence of Spark Plasma Sintering on the Mechanical Behavior of Micro and Nano AA2124 Powders:** Ahmed Sayed<sup>1</sup>; Yasmine Ibrahim<sup>1</sup>; Hanadi Salem<sup>1</sup>; Mats Johnsson<sup>2</sup>; <sup>1</sup>American University in Cairo; <sup>2</sup>Stockholm University

11:30 AM

**High Voltage Electric Discharge Consolidation of Tantalum Powders:** *Evgeny Grigoryev*<sup>1</sup>; Eugene Olevsky<sup>1</sup>; Vera Demenyuk<sup>1</sup>; Maria Yurlova<sup>1</sup>; <sup>1</sup>MEPHI

11:50 AM

**Effect of Alloying Elements and Pulsed Electric Current Sintering Parameters on Nano-Dispersion Formation in Nanostructured Ferritic Steels:** *Somayeh Pasebani*<sup>1</sup>; Indrajit Charit<sup>1</sup>; Kerry Allahar<sup>2</sup>; James Cole<sup>3</sup>; Darryl Butt<sup>2</sup>; <sup>1</sup>University of Idaho; <sup>2</sup>Boise State University; <sup>3</sup>Idaho National Laboratory

## Pb-free Solders and Emerging Interconnect and Packaging Technologies: Solidification

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Electronic Packaging and Interconnection Materials Committee

*Program Organizers:* Nikhilesh Chawla, Arizona State University; Srinivas Chada, Whirlpool; Darrel Frear, Freescale Semiconductor; John Elmer, LNL; Tae-Kyu Lee, Cisco Systems; Yan Li, Intel; Laura Turbini, Research In Motion; Kwang-Lung Lin, National Cheng Kung University; Sohoon Yoo, Korea Institute of Industrial Technology

Monday AM  
March 4, 2013

Room: 217B  
Location: Henry B. Gonzalez Convention Center

*Session Chair:* To Be Announced

8:30 AM

**Liquidus Projection and Solidification of Sn-rich Sn-In-Ag-Zn Alloys:** *Sinn-wen Chen*<sup>1</sup>; Jui-shen Chang<sup>1</sup>; Chia-Ming Hsu<sup>1</sup>; Wan-ting Chiu<sup>1</sup>; Che-wei Hsu<sup>1</sup>; Ru-bo Chang<sup>1</sup>; <sup>1</sup>National Tsing Hua University

8:50 AM

**In-Situ Observation of Solidification in Micro-Alloyed Sn-0.7Cu Solder Alloys:** *Guang Zeng*<sup>1</sup>; Stuart McDonald<sup>1</sup>; Jonathan Read<sup>1</sup>; Christopher Gourlay<sup>2</sup>; Hideyuki Yasuda<sup>3</sup>; Kazuhiro Nogita<sup>1</sup>; <sup>1</sup>The University of Queensland; <sup>2</sup>Imperial College London; <sup>3</sup>Osaka University

9:10 AM

**Modified Hypereutectic Sn-Cu Pb-Free Solder for High Temperature Applications:** *Keith Sweatman*<sup>1</sup>; Motanori Miyaoka<sup>1</sup>; Takatoshi Nishimura<sup>1</sup>; Xuan Quy Tran<sup>2</sup>; Stuart McDonald<sup>2</sup>; Kazuhiro Nogita<sup>2</sup>; <sup>1</sup>Nihon Superior Co., Ltd.; <sup>2</sup>University of Queensland

9:30 AM

**Solidification of Sn-0.7Cu-0.05Ni Solder:** *Christopher Gourlay*<sup>1</sup>; Sergey Belyakov<sup>1</sup>; Guang Zeng<sup>2</sup>; Hideyuki Yasuda<sup>3</sup>; Kazuhiro Nogita<sup>2</sup>; <sup>1</sup>Imperial College London; <sup>2</sup>University of Queensland; <sup>3</sup>Osaka University

9:50 AM Break

10:10 AM

**New Bi-Containing No or Low Ag Solder Alloys with Reduced Melting Temperatures:** *Polina Snugovsky*<sup>1</sup>; Simin Bagheri<sup>2</sup>; Eva Kosiba<sup>2</sup>; Zohreh Bagheri<sup>2</sup>; Marianne Romansky<sup>2</sup>; Doug Perovic<sup>3</sup>; Leonid Snugovsky<sup>3</sup>; <sup>1</sup>Celestica ; <sup>2</sup>Celestica; <sup>3</sup>University of Toronto

10:30 AM

**The Redistribution of Ag, Sn Phase of Pb-Free Solder in a Temperature Gradient:** *Yu-Ping Su*<sup>1</sup>; Fan-Yi Ouyang<sup>1</sup>; <sup>1</sup>National Tsing Hua university

10:50 AM

**Microstructure Investigation of Mixed Solder Joints with Eutectic SnPb and Sn-3.0Ag-0.5Cu Solders:** *Won Sik Hong*<sup>1</sup>; Chulmin Oh<sup>1</sup>; <sup>1</sup>Korea Electronics Technology Institute(KETI)

11:10 AM

**Conductive Anodic Filament Formation Studies in Fine-Pitch through-Vias in Thin Organic Package Substrates:** *Koushik Ramachandran*<sup>1</sup>; Fuhan Liu<sup>1</sup>; Raj Pulugurtha<sup>1</sup>; Venky Sundaram<sup>1</sup>; Rao Tummala<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

## Phase Stability, Phase Transformations, and Reactive Phase Formation in Electronic Materials XII: Solder-related Reliability Issues

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Alloy Phases Committee

*Program Organizers:* Chao-hong Wang, National Chung Cheng University; Chih-Ming Chen, National Chung Hsing University; Jae-Ho Lee, Hongik University; Ikuo Ohnuma, Tohoku University; Clemens Schmetterer, TU Bergakademie Freiberg; Yee-Wen Yen, National Taiwan University of Science and Technology; Shien-Ping Feng, The University of Hong Kong; Shih-Kang Lin, National Cheng Kung University

Monday AM  
March 4, 2013

Room: 203B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Chao-Hong Wang, National Chung Cheng University; Yee-Wen Yen, National Taiwan University of Science & Technology

8:30 AM Invited

**Study of the Microstructural Evolution of the Sn-9 wt.% Zn/Cu Joints:** *Chih-Ming Chen*<sup>1</sup>; <sup>1</sup>National Chung Hsing University

8:50 AM

**Comparison of Cu Pad Consumption between Sn Solder and Sn<sub>3.5</sub>Ag:** *Chia-yu Chen*<sup>1</sup>; <sup>1</sup>National Central University

9:05 AM

**Electromigration Failure Mechanism in Package Solders:** *Liangshan Chen*<sup>1</sup>; Huili Xu<sup>1</sup>; Patricia Rodriguez<sup>2</sup>; Choongun Kim<sup>1</sup>; <sup>1</sup>MSE at UT Arlington

9:20 AM

**Supersaturation and Phase Stability of Pb-Sn Alloys under Current Stressing:** *Chao-kuei Yeh*<sup>1</sup>; Shih-kang Lin<sup>1</sup>; <sup>1</sup>National Cheng Kung University

9:35 AM

**Grain Rotation Induced by Thermomigration in the Pb-Free Solders:** *Wei-Neng Hsu*<sup>1</sup>; Fan-Yi Ouyang<sup>1</sup>; <sup>1</sup>National Tsing Hua University

9:50 AM

**Interfacial Reactions between Pb-Free Solders and Alloy 42 Substrates:** *Yee-Wen Yen*<sup>1</sup>; Yi-Pin Wu<sup>1</sup>; Yu-Ping Hsieh<sup>1</sup>; Ruo-Syun Syu<sup>1</sup>; <sup>1</sup>National Taiwan University of Science & Technology

10:05 AM Break

10:20 AM Invited

**Effects of Levelers in Pulse Current Electroplating on SiP Copper Via Filling:** *Ki-Tae Kim*<sup>1</sup>; Myung-Won Jung<sup>1</sup>; *Jae-Ho Lee*<sup>1</sup>; <sup>1</sup>Hongik University

10:40 AM

**Electromigration Induced Interface Reaction in Au-Wire/Al Film Diffusion Couple:** *Patricia Rodriguez*<sup>1</sup>; Liangshan Chen<sup>1</sup>; Choong-Un Kim<sup>1</sup>; <sup>1</sup>University of Texas at Arlington

10:55 AM

**Microstructural Evolution of Cu Wedge Bonding on the Al Metallization under a High Current Density:** *Zong-Han Yang*<sup>1</sup>; Fan-Yi Ouyang<sup>1</sup>; <sup>1</sup>Department of Engineering and System Science, National Tsing Hua University

11:10 AM

**Investigation of Sn Whisker Growth in Electroplated Sn and Sn-Ag as a Function of Plating Variables and Aging Conditions:** *Jaewon Chang*<sup>1</sup>; Sung Kang<sup>2</sup>; Jaeho Lee<sup>3</sup>; Keun-Soo Kim<sup>4</sup>; Hyuck Mo Lee<sup>1</sup>; <sup>1</sup>KAIST; <sup>2</sup>IBM T.J. Watson Research Center; <sup>3</sup>Hongik University; <sup>4</sup>Hoseo University

11:25 AM

**Electromigration in SAC305/Bismuth Telluride Thermoelectric System:** *Po-Yin Chien*<sup>1</sup>; Albert T. Wu<sup>2</sup>; <sup>1</sup>National Central University; <sup>2</sup>National Central University

11:40 AM

**Sn Grain Orientation Effect on the Formation of Highly Serrated Cathode Interface in Solder Joints under Electromigration:** *Ting-Li Yang*<sup>1</sup>; Ting-Chia Huang<sup>1</sup>; Jia-Hong Ke<sup>1</sup>; C. Robert Kao<sup>1</sup>; <sup>1</sup>National Taiwan University

11:55 AM

**Correlation between Microstructure Evolution and Mechanical Strength in Sn-3.0Ag-0.5Cu/ENEPIG Solder Joint:** *Chien-Fu Tseng*<sup>1</sup>; Jenq-Gong Duh<sup>1</sup>; <sup>1</sup>National Tsing Hua University, Hsinchu, Taiwan

## Phase Transformation and Microstructural Evolution: MPMD Distinguished Scientist/Engineer Award Symposium for J.E. Morral

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS/ASM: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS/ASM: Phase Transformations Committee, TMS: Process Technology and Modeling Committee, ASM: Alloy Phase Diagrams Committee

*Program Organizers:* Amy Clarke, Los Alamos National Laboratory; Sudarsanam Suresh Babu, Ohio State University; Rajarshi Banerjee, University of North Texas; John Morral, Ohio State University; Brian Gleeson, University of Pittsburgh; Carelyn Campbell, National Institute of Standards & Technology; Yongho Sohn, University of Central Florida; Yunzhi Wang, Ohio State University

Monday AM  
March 4, 2013

Room: 204B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Carelyn Campbell, NIST; Yongho Sohn, University of Central Florida

8:30 AM Invited

**Simulation of Surface Treating Processes: Models and Database Needs:** *Richard Sisson*<sup>1</sup>; Mei Yang<sup>1</sup>; Yingying Wei<sup>1</sup>; Danielle Belsito<sup>1</sup>; Lei Zhang<sup>1</sup>; <sup>1</sup>Worcester Polytechnic Institute, Center for Heat Treating Excellence

9:00 AM Invited

**Experimental Observations and Analyses from Diffusion Studies for U-Mo Nuclear Fuel Alloys:** *Yongho Sohn*<sup>1</sup>; Ke Huang<sup>1</sup>; Emmanuel Perez<sup>2</sup>; Ashley Ewh<sup>1</sup>; Dennis Keiser<sup>2</sup>; <sup>1</sup>University of Central Florida; <sup>2</sup>Idaho National Laboratory

9:30 AM

**Interdiffusion Microstructure Maps in Multi-Component and Multi-Phase Dual-Alloy Systems:** *Xiaoqin Ke*<sup>1</sup>; John Morral<sup>1</sup>; Yunzhi Wang<sup>1</sup>; <sup>1</sup>The Ohio State University

9:50 AM Break

**10:10 AM Invited**

**Role of Multicomponent Diffusion in Microstructure Evolution during Additive Manufacturing of Structural Alloys:** *Sudarsanam Babu*<sup>1</sup>; <sup>1</sup>The Ohio State University

**10:40 AM Invited**

**File and Data Repositories for CALPHAD and Beyond:** *Ursula Kattner*<sup>1</sup>; Carelyn Campbell<sup>1</sup>; Laura Bartolo<sup>2</sup>; Alden Dima<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology; <sup>2</sup>Kent State University

**11:10 AM Invited**

**Reference Self Diffusion Mobility Data for CALPHAD and Beyond:** *Carelyn Campbell*<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

**11:40 AM Invited**

**Derived Uncertainties and the Evaluation of Multicomponent Interdiffusion Data:** *Jeffrey LaCombe*<sup>1</sup>; Alonso Jaques<sup>2</sup>; <sup>1</sup>University of Nevada, Reno; <sup>2</sup>Universidad Técnica Federico Santa María

**12:10 PM**

**The RMS Error of 3-Component Diffusivities Measured from One Diffusion Couple:** *John Morral*<sup>1</sup>; <sup>1</sup>The Ohio State University

**Physical and Mechanical Metallurgy of Shape Memory Alloys: In-situ Microstructural Characterization**

*Sponsored by:* TMS/ASM: Phase Transformations Committee  
*Program Organizers:* Haluk Karaca, University of Kentucky; Ibrahim Karaman, Texas A&M University; Othmane Benafan, NASA Glenn Research Center; Ryosuke Kainuma, Tohoku University; Hans Jurgen Maier, University of Paderborn

Monday AM

March 4, 2013

Room: Lone Star Salon B

Location: Grand Hyatt

*Session Chairs:* Petr Sittner, Institute of Physics, Academy of Sciences of the Czech Republic; Minoru Nishida, Kyushu University

**8:30 AM**

**Formation Process of Self-Accommodation Morphology of B19' Martensite in Ti-Ni Alloys:** *Minoru Nishida*<sup>1</sup>; Yohei Soejima<sup>1</sup>; Shinsaku Shibuta<sup>1</sup>; Shunichi Motomura<sup>1</sup>; Mastoshi Mitsuhara<sup>1</sup>; Tomonari Inamura<sup>2</sup>; <sup>1</sup>Kyushu University; <sup>2</sup>Tokyo Institute of Technology

**9:00 AM**

**In Situ Neutron and Synchrotron X-Ray Diffraction Studies of NiTi-Based High Temperature Shape Memory Alloys:** *Othmane Benafan*<sup>1</sup>; Ronald Noebe<sup>1</sup>; Santo Padula<sup>1</sup>; Glen Bigelow<sup>1</sup>; Darrell Gaydos<sup>2</sup>; Anita Garg<sup>3</sup>; Raj Vaidyanathan<sup>4</sup>; Bjorn Clausen<sup>5</sup>; Norbert Schell<sup>6</sup>; <sup>1</sup>NASA Glenn Research Center; <sup>2</sup>Ohio Aerospace Institute; <sup>3</sup>University of Toledo; <sup>4</sup>University of Central Florida; <sup>5</sup>Los Alamos National Laboratory; <sup>6</sup>GKSS Research Center Geesthacht

**9:20 AM**

**Deformation Mechanics of Shape-Memory NiTi Martensite:** *Aaron Stebner*<sup>1</sup>; <sup>1</sup>Caltech

**9:40 AM**

**Asymmetry and Control Mode Effects in Polycrystalline NiTi:** *Douglas Nicholson*<sup>1</sup>; Othmane Benafan<sup>2</sup>; Santo Padula<sup>2</sup>; Ron Noebe<sup>2</sup>; Raj Vaidyanathan<sup>1</sup>; <sup>1</sup>University of Central Florida; <sup>2</sup>NASA Glenn Research Center

**10:00 AM Break**

**10:20 AM**

**Heat Treatment, Shape Setting and Actuation Instability of NiTi:** *Petr Sittner*<sup>1</sup>; Jan Pilch<sup>1</sup>; Ludek Heller<sup>1</sup>; Pavel Sedmák<sup>1</sup>; Carolina Curfús<sup>1</sup>; <sup>1</sup>Institute of Physics ASCR

**10:50 AM**

**In Situ Scanning Electron Microscopy Studies of Superelastic Cu-Zn-Al Microwires:** *Stian Ueland*<sup>1</sup>; Christopher Schuh<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology

**11:10 AM**

**In Situ, Elevated Temperature Micro-Compression of NiTiPd:** *Jeffrey Wheeler*<sup>1</sup>; Rejin Raghavan<sup>1</sup>; Mark Weaver<sup>2</sup>; Greg Thompson<sup>2</sup>; Johann Michler<sup>1</sup>; <sup>1</sup>EMPA; <sup>2</sup>The University of Alabama

**11:30 AM**

**Twinning during Shape Memory and Post-Shape Memory Deformation in U-14at.%Nb:** *Robert Field*<sup>1</sup>; Amy Clarke<sup>1</sup>; Rodney McCabe<sup>1</sup>; Donald Brown<sup>1</sup>; Bjorn Clausen<sup>1</sup>; Catherine Tupper<sup>2</sup>; John Swadener<sup>3</sup>; Carl Cady<sup>1</sup>; Dan Thoma<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory; <sup>2</sup>Northwestern University; <sup>3</sup>Aston University

**11:50 AM**

**Full Field Mapping of Microstructural Strain Accommodation during Superelastic Deformation in Nickel Titanium:** *Michael Kimiecik*<sup>1</sup>; J. Jones<sup>1</sup>; Samantha Daly<sup>1</sup>; <sup>1</sup>University of Michigan

**12:10 PM**

**In Situ Macroscopic Investigation on Lüders-Like Bands Evolution during Cycle Loading with Different Strain Rates in NiTi Alloys:** *Hongfei Du*<sup>1</sup>; Pan Zeng<sup>1</sup>; Liping Lei<sup>1</sup>; Gang Fang<sup>1</sup>; <sup>1</sup>Tsinghua University

**Recent Developments in Biological, Electronic, and Functional Thin Films and Coatings: Biological, Electronic, and Functional Thin Films and Coatings I**

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Thin Films and Interfaces Committee  
*Program Organizers:* R. Narayan, UNC/NCSSU Joint Department of Biomedical Engineering; Choong-Un Kim, University of Texas at Arlington; Jian Luo, Clemson University; Nancy Michael, University of Texas at Arlington; Nuggehalli Ravindra, New Jersey Institute of Technology; Adele Carradò, IPCMS

Monday AM

March 4, 2013

Room: 214D

Location: Henry B. Gonzalez Convention Center

*Session Chair:* Diego Mantovani, Laval University

**8:30 AM Invited**

**Graphene: The Thinnest Known Coating for Corrosion Protection:** *RK Singh Raman*<sup>1</sup>; <sup>1</sup>Monash University

**9:10 AM Invited**

**Coating Effect on the Physico-Chemical Properties of Nanometric Iron Oxide:** *Geneviève Pourroy*<sup>1</sup>; Julien Jouhannaud<sup>1</sup>; Antonio Garofalo<sup>1</sup>; Delphine Felder-Flesch<sup>1</sup>; Franklin Tellier<sup>1</sup>; Patrick Poulet<sup>1</sup>; Jerome Steibel<sup>1</sup>; <sup>1</sup>CNRS University of Strasbourg-IPCMS

**9:30 AM**

**Corrosion Resistance of Cerium-Based Conversion Coated Ti-6Al-4V Alloy:** *Surender Maddela*<sup>1</sup>; Matt Ruder<sup>1</sup>; Matthew O'Keefe<sup>1</sup>; <sup>1</sup>Missouri University of Science and Technology

**9:50 AM**

**CVD of Protective Mullite Coatings on Single Crystal Silicon Substrates:** *JiaPeng Xu*<sup>1</sup>; *Daniel Erickson*<sup>1</sup>; Sudesna Roy<sup>1</sup>; Vinod Sarin<sup>1</sup>; <sup>1</sup>Boston University

**10:10 AM Break**



10:30 AM

**Characterization of High Temperature Mechanical Properties of Two Unique Experimental Coatings:** *Amit Pandey*<sup>1</sup>; Kevin Hemker<sup>2</sup>; Vladimir Tolpygoc<sup>3</sup>; <sup>1</sup>ORNL; <sup>2</sup>The Johns Hopkins University; <sup>3</sup>Honeywell

10:50 AM

**Structural, Optical and Electronic Properties of CdS<sub>x</sub>Se<sub>1-x</sub>:** *Yan Liu*<sup>1</sup>; Dongguo Chen<sup>1</sup>; Nuggehalli Ravindra<sup>1</sup>; <sup>1</sup>New Jersey Institute of Technology

11:10 AM

**Eclipse Active and Passive Solar Control Coatings:** *Hulya Demiryont*<sup>1</sup>; Kenneth Shannon<sup>1</sup>; Matthew Bratcher<sup>2</sup>; <sup>1</sup>Eclipse Energy Systems, Inc.; <sup>2</sup>US. Army

11:30 AM

**Effect of Chemical Structure Change on Thermo-Mechanical Instability of Porous Low-k Thin Films:** *Yoonki Sa*<sup>1</sup>; Todd Ryan<sup>2</sup>; Sean King<sup>3</sup>; Choong-Un Kim<sup>1</sup>; <sup>1</sup>University of Texas at Arlington; <sup>2</sup>Globalfoundries; <sup>3</sup>Intel Co.

11:50 AM

**Fabrication and Characterization of Chitin-Carbon Nanotube Composites:** *Sujeily Soto*<sup>1</sup>; Deborah Marty<sup>1</sup>; O. Marcelo Suarez<sup>1</sup>; <sup>1</sup>University of Puerto Rico

12:10 PM

**Separation and Conductivity Measurements of Living Cells Using Microfluidics:** *Faiza Javed*<sup>1</sup>; Naila Javed<sup>1</sup>; Arshad Bhatti<sup>2</sup>; <sup>1</sup>MS Student; <sup>2</sup>Supervisor

## Recent Developments in the Processing, Characterization, Properties, Performance and Applications of Metal Matrix Composites: Innovative and Nano-composite Materials

*Sponsored by:* TMS Structural Materials Division, TMS/ASM: Composite Materials Committee

*Program Organizers:* Martin Pech-Canul, Centro de Investigacion y de Estudios Avanzados del Instituto Politecnico Nacional; Zariff Chaudhury, Materion Coporation; Golam Newaz, Wayne State University

Monday AM  
March 4, 2013

Room: Bowie A  
Location: Grand Hyatt

*Session Chairs:* Zariff Chaudhury, Materion Corporation; Martin Pech-Canul, CINVESTAV IPN SALTILLO

8:30 AM

**Three Dimensional (3D) Microstructure Visualization and Modeling of Deformation in Metal Matrix Composites by In Situ X-ray Synchrotron Tomography:** Jason Williams<sup>1</sup>; Jonathan Silva<sup>1</sup>; *Nikhilesh Chawla*<sup>1</sup>; Francesco De Carlo<sup>2</sup>; Xianghui Xiao<sup>2</sup>; <sup>1</sup>Arizona State University; <sup>2</sup>Advanced Photon Source, Argonne National Laboratory

8:50 AM

**Characterization of Nanoparticle Reinforced Mg-Based Composites Processed by Electromagnetic Acoustic Transduction:** *Hunter Henderson*<sup>1</sup>; Zachary Bryan<sup>1</sup>; Orlando Rios<sup>2</sup>; Alexander Melin<sup>2</sup>; Gerard Ludtka<sup>2</sup>; Gail Ludtka<sup>2</sup>; Michele Manuel<sup>1</sup>; <sup>1</sup>University of Florida; <sup>2</sup>Oak Ridge National Laboratory

9:10 AM

**In-Situ Formed Al-TiB<sub>2</sub> Metal Matrix Composites as a Feed Stock for Semi-Solid Metal Processing:** *Vijay Nimbalkar*<sup>1</sup>; <sup>1</sup>NMRL

9:30 AM

**Influence of Substrate Bias on Structure and Properties of TiZrN Prepared by Sputtering System:** Yu-Wei Lin<sup>1</sup>; Fong-Zhi Chen<sup>1</sup>; Jia-Hong Huang<sup>2</sup>; Ge-Ping Yu<sup>2</sup>; <sup>1</sup>National Applied Research Laboratories; <sup>2</sup>National Tsing Hua University

9:50 AM

**Development, Processing and Applications for Bulk Metallic Glass Matrix Composites:** *Douglas Hofmann*<sup>1</sup>; <sup>1</sup>NASA JPL/Caltech

10:10 AM

**A Disintegrable Metal Matrix Composite:** *Zhiyue Xu*<sup>1</sup>; <sup>1</sup>Baker Hughes

10:30 AM

**Application of External Fields to Technology of Metal-Matrix Composite Materials:** Nadendla Hari Babu<sup>1</sup>; Zhongyun Fan<sup>1</sup>; *Dmitry Eskin*<sup>1</sup>; <sup>1</sup>Brunel University

10:50 AM

**Microstructure and Mechanical Properties of Bulk Ultrafine Structured Al-5vol.%Al<sub>2</sub>O<sub>3</sub> and Cu-5vol.%Al<sub>2</sub>O<sub>3</sub> Nanocomposite Produced by a Combination of High Energy Mechanical Milling and Powder Consolidation:** *Deliang Zhang*<sup>1</sup>; Amro Gazawi<sup>1</sup>; Dengshan Zhou<sup>1</sup>; Charlie Kong<sup>2</sup>; Paul Munroe<sup>2</sup>; <sup>1</sup>The University of Waikato; <sup>2</sup>University of New South Wales, Australia

11:10 AM

**Determination of Nanostructural Evolution during Wear of Multifunctional Adaptive Composites Coatings:** *Hamidreza Mohseni*<sup>1</sup>; Jon-Erik Mogonye<sup>1</sup>; Sundeep Gopagani<sup>1</sup>; Junyeon Hwang<sup>1</sup>; Peter Collins<sup>1</sup>; Jaimie Tiley<sup>2</sup>; Rajarshi Banerjee<sup>1</sup>; Thomas Scharf<sup>1</sup>; <sup>1</sup>University of North Texas; <sup>2</sup>Air Force Research Laboratory

11:30 AM

**In-Situ Formation of Novel Al-AlN Composites by Gas-Melt Reaction:** *Je In Lee*<sup>1</sup>; Eun Soo Park<sup>1</sup>; <sup>1</sup>Seoul National University

11:50 AM

**Thermal Property Characterization for a Steel Fibre Reinforced Aluminum Metal Matrix Composite (AIMMC):** *Scott Kenningley*<sup>1</sup>; Simon Barnes<sup>2</sup>; Philip Withers<sup>2</sup>; <sup>1</sup>Federal Mogul; <sup>2</sup>University of Manchester

## Refractory Metals 2013: Refractory Metal-based Materials I

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

*Program Organizers:* David Honecker, Climax Molybdenum; Omer Dogan, DOE National Energy Technology Laboratory

Monday AM  
March 4, 2013

Room: Mission A  
Location: Grand Hyatt

*Session Chairs:* David Honecker, Climax Molybdenum Technology Center; James Ciulik, Element Materials Technology

8:30 AM **Introductory Comments**

8:35 AM

**Response of Two Nb-Cr-Mo-Si-B Alloys to Static Oxidation:** *Kathryn Thomas*<sup>1</sup>; Shailendra Varma<sup>1</sup>; <sup>1</sup>The University of Texas at El Paso

8:55 AM **Question and Answer Period**

9:00 AM

**How Can One Improve the Oxidation Resistance of Nb Silicide Based Alloys?:** *Panayiotis Tsakopoulos*<sup>1</sup>; <sup>1</sup>The University of Sheffield

9:20 AM Question and Answer Period

9:25 AM

**Molybdenum Composites of Mo<sub>2</sub>B, T<sub>2</sub>, and Silica:** *William Daloz*<sup>1</sup>; Peter Marshall<sup>1</sup>; Joe Cochran<sup>1</sup>; <sup>1</sup>GA Tech

9:45 AM Question and Answer Period

9:50 AM

**The Creep Behavior of Molybdenum and Other Commercial-Purity Refractory Metals:** *James Ciulik*<sup>1</sup>; <sup>1</sup>Element Materials Technology

10:10 AM Question and Answer Period

10:15 AM Break

10:35 AM

**Microstructural Observations of Texture Gradient Effects on Dynamic Abnormal Grain Growth in Mo:** *Philip Noell*<sup>1</sup>; Nicholas Pedrazas<sup>1</sup>; Daniel Worthington<sup>1</sup>; Thomas Buchheit<sup>2</sup>; Elizabeth Holm<sup>2</sup>; Eric Taleff<sup>2</sup>; <sup>1</sup>University of Texas at Austin, Dept of Mechanical Engrg; <sup>2</sup>Sandia National Laboratory, New Mexico

10:55 AM Question and Answer Period

11:00 AM

**Enhancement of Tantalum Carbide Oxidation Resistance in a High Temperature Plasma Flow by Addition of Graphene NanoPlatelets:** *Andy Nieto*<sup>1</sup>; Debrupa Lahiri<sup>1</sup>; Cheng Zhang<sup>1</sup>; Arvind Agarwal<sup>1</sup>; <sup>1</sup>Florida International University

11:20 AM Question and Answer Period

11:25 AM

**Microstructure Development in Seamless Nb Tube:** *Shreyas Balachandran*<sup>1</sup>; Roston Elwell<sup>2</sup>; Di Kang<sup>3</sup>; Thomas Bieler<sup>3</sup>; Karl Hartwig<sup>1</sup>; <sup>1</sup>Texas A&M University; <sup>2</sup>Shearform Inc; <sup>3</sup>Michigan State University

11:45 AM Question and Answer Period

11:50 AM Concluding Comments

**Synergies of Computational and Experimental Materials Science II: Materials for Energy and Electronic Applications**

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

*Program Organizers:* Katsuyo Thornton, University of Michigan; Thomas Buchheit, Sandia National Laboratories; Anthony Rollett, Carnegie Mellon University; David Rowenhorst, Naval Research Lab

Monday AM  
March 4, 2013

Room: 217A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Katsuyo Thornton, University of Michigan; Scott Barnett, Northwestern University

8:30 AM Introductory Comments

8:35 AM Invited

**Three-Dimensional Measurements and Simulations of Electrode Microstructure: Correlation with Electrochemical Performance and Degradation:** *Scott Barnett*<sup>1</sup>; Scott Cronin<sup>1</sup>; Kyle Yakal-Kremski<sup>1</sup>; David Kennouche<sup>1</sup>; <sup>1</sup>Northwestern University

9:05 AM Invited

**3D Analysis and Modeling of Solid Oxide Fuel Cell Cathodes:** *Ellen Ivers-Tiffée*<sup>1</sup>; <sup>1</sup>KIT

9:35 AM

**FIB/SEM Reconstruction and 3D Simulations of SOFC Electrodes:** *Jochen Joos*<sup>1</sup>; Thomas Carraro<sup>2</sup>; Moses Ender<sup>1</sup>; André Weber<sup>1</sup>; Ellen Ivers-Tiffée<sup>1</sup>; <sup>1</sup>Karlsruhe Institute of Technology (KIT); <sup>2</sup>University of Heidelberg

9:55 AM

**Investigation of Interactions between Lithium Iron Phosphate Nanoparticles Using 6Li and 7Li Isotopes:** *Bernardo Orvananos*<sup>1</sup>; Hui-Chia Yu<sup>1</sup>; Hao Liu<sup>2</sup>; Rahul Malik<sup>3</sup>; Gerbrand Ceder<sup>3</sup>; Clare Grey<sup>2</sup>; Katsuyo Thornton<sup>1</sup>; <sup>1</sup>University of Michigan; <sup>2</sup>University of Cambridge; <sup>3</sup>Massachusetts Institute of Technology

10:15 AM Break

10:30 AM Invited

**Addressing the Materials Genome Initiative through the AFLOWLIB.ORG Consortium: Thermoelectric Properties of Sintered Compounds with High-Throughput Ab-Initio Calculations:** *Stefano Curtarolo*<sup>1</sup>; <sup>1</sup>Duke University

11:00 AM Invited

**The Composition and Growth of Nanowires:** Kevin Yoon<sup>1</sup>; Andrew Gamalski<sup>2</sup>; Justin Connell<sup>1</sup>; R. Sharma<sup>3</sup>; C. Ducati<sup>2</sup>; Lincoln Lauhon<sup>1</sup>; Stefan Hofman<sup>2</sup>; *Peter Voorhees*<sup>1</sup>; <sup>1</sup>Northwestern University; <sup>2</sup>Cambridge University; <sup>3</sup>National Institute for Standards and Technology

11:30 AM

**Role of Oxygen Vacancies on Wettability and Evaporation Rate of Water on ZnO Surfaces:** Han Hu<sup>1</sup>; *Ying Sun*<sup>1</sup>; <sup>1</sup>Drexel University

11:50 AM

**Experimental Measurement of Coupled Thermo Mechanics in Silicon with an Account of Length Scale, Stresses, and Quantum Scale Thermodynamics:** Ming Gan<sup>1</sup>; *Vikas Tomar*<sup>1</sup>; <sup>1</sup>Purdue University

12:10 PM

**Influence of Tb<sup>3+</sup> Concentration on Luminescence Properties of Gd<sub>2</sub>O<sub>3</sub>:Tb Nanophosphor:** *Fei Wang*<sup>1</sup>; <sup>1</sup>Kunming University of Science and Technology

**Three-Dimensional Materials Science VII: Novel Techniques in Three-Dimensional Materials Science**

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

*Program Organizers:* Jonathan Madison, Sandia National Laboratories; Nikhilesh Chawla, Arizona State University; Michael Groeber, Air Force Research Laboratory

Monday AM  
March 4, 2013

Room: 212A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Jonathan Madison, Sandia National Laboratories; Christopher Szczepanski, AFRL, Wright Patterson AFB

8:30 AM Invited

**An Automated 3D Serial Sectioning System for Characterizing Microstructural Features in Large Volumes (> 1 mm<sup>3</sup>) Using Multi-Modal Data Streams:** *Megha Shah*<sup>1</sup>; Michael Uchic<sup>2</sup>; Michael Groeber<sup>2</sup>; Patrick Callahan<sup>3</sup>; David Rowenhorst<sup>4</sup>; Adam Shiveley<sup>1</sup>; Jonathan Spowart<sup>2</sup>; <sup>1</sup>UES/Air Force Research Laboratory; <sup>2</sup>Air Force Research Laboratory; <sup>3</sup>Carnegie Mellon University/Air Force Research Laboratory; <sup>4</sup>Naval Research Lab

**9:00 AM Invited**

**Acquisition of 3-D Datasets Via Tri-Beam Tomography:** *Tresa Pollock*<sup>1</sup>; McLean Echlin<sup>1</sup>; Alessandro Mottura<sup>1</sup>; <sup>1</sup>University of California Santa Barbara

**9:30 AM**

**Combined FIB Lift Out – EBSD Specimen Preparation for Atom Probe Tomography – Application to Steels:** *Frederic Danoix*<sup>1</sup>; Fabien Cuvilly<sup>1</sup>; Grant Thomas<sup>2</sup>; Jacques Lacaze<sup>3</sup>; Dominique Mangelinck<sup>4</sup>; John Speer<sup>2</sup>; <sup>1</sup>CNRS - Université de Rouen; <sup>2</sup>Colorado School of Mines; <sup>3</sup>CIRIMAT ENCIACET Toulouse; <sup>4</sup>IM2NP CNRS

**9:50 AM Break**

**10:05 AM**

**Fatigue Crack Closure and Corrosion Fatigue in Al 7075 Alloy Using In Situ X-Ray Synchrotron Tomography:** *Sudhanshu Singh*<sup>1</sup>; Jason Williams<sup>1</sup>; Xianghui Xiao<sup>2</sup>; Francesco De Carlo<sup>2</sup>; Nikhilesh Chawla<sup>1</sup>; <sup>1</sup>Arizona State University; <sup>2</sup>Advanced Photon Source, Argonne National Laboratory

**10:25 AM**

**Measurement of Materials Performance during In-Situ Experiments Using X-ray Tomography:** *Brian Patterson*<sup>1</sup>; Kevin Henderson<sup>1</sup>; Zach Smith<sup>1</sup>; Duan Zhang<sup>1</sup>; Paul Giguere<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

**10:45 AM**

**Optimizing Tilt-Series Data Acquisition in Dislocation Tomography Observations: Methods and Applications:** *Satoshi Hata*<sup>1</sup>; Ryutaro Akiyoshi<sup>1</sup>; Makoto Shimizu<sup>1</sup>; Masatoshi Mitsuhashi<sup>1</sup>; Ken-ichi Ikeda<sup>1</sup>; Hideharu Nakashima<sup>1</sup>; <sup>1</sup>Kyushu University

**11:05 AM**

**3D Orientation Contrast Microscopy Characterization of Thermo-Mechanical Fatigue Crack Morphology in Compacted Graphite Iron:** Sepideh Ghodrati<sup>1</sup>; *Hadi Pirgazi*<sup>2</sup>; Leo Kestens<sup>2</sup>; <sup>1</sup>Delft University of Technology (TUDelft); <sup>2</sup>Ghent University

**11:25 AM**

**In-Situ Monitoring of Dynamic Phenomena during Solidification:** *Amy Clarke*<sup>1</sup>; Paul Gibbs<sup>1</sup>; Seth Imhoff<sup>1</sup>; Jason Cooley<sup>1</sup>; Brian Patterson<sup>1</sup>; Wah-Keat Lee<sup>2</sup>; Kamel Fezzaa<sup>3</sup>; Christopher Morris<sup>1</sup>; Frank Merrill<sup>1</sup>; Brian Hollander<sup>1</sup>; Kester Clarke<sup>1</sup>; Robert Field<sup>1</sup>; David Teter<sup>1</sup>; Dan Thoma<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory; <sup>2</sup>Brookhaven National Laboratory; <sup>3</sup>Argonne National Laboratory

**11:45 AM**

**3D Orientation Imaging with Transmission Electron Microscopy:** *Søren Schmidt*<sup>1</sup>; Haihua Liu<sup>2</sup>; Andy Godfrey<sup>3</sup>; Henning Poulsen<sup>1</sup>; Xiaoxu Huang<sup>1</sup>; <sup>1</sup>Technical University of Denmark; <sup>2</sup>Caltech; <sup>3</sup>Tsinghua University

**12:05 PM**

**3D Mapping of Amorphization Zone in Boron Carbide Using Raman Spectroscopy:** *Ghatu Subhash*<sup>1</sup>; Dipankar Ghosh<sup>1</sup>; Jutin Blabber<sup>2</sup>; <sup>1</sup>University of Florida; <sup>2</sup>Georgia Institute of Technology

**2013 and Beyond: Flexible Electronics: Semiconductor Advances in Flexible Electronics Systems**

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Biomaterials Committee, TMS: Nanomaterials Committee

*Program Organizer:* Walter Voit, UT Dallas

Monday PM  
March 4, 2013

Room: 204A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* To Be Announced

**2:00 PM**

**Flexible Organic Transistors on Shape Memory Polymer Substrates for Conformable Biointegrated Interfaces:** *Jonathan Reeder*<sup>1</sup>; Taylor Ware<sup>1</sup>; Dustin Simon<sup>1</sup>; Naoji Matsuhisa<sup>2</sup>; Tsuyoshi Sekitani<sup>2</sup>; Takao Someya<sup>2</sup>; Walter Voit<sup>1</sup>; <sup>1</sup>University of Texas at Dallas; <sup>2</sup>University of Tokyo

**2:20 PM Question and Answer Period**

**2:30 PM**

**Flexible, Large-Area Sensor Circuits Fabricated by Additive Printing:** *Tse Nga Ng*<sup>1</sup>; David Schwartz<sup>1</sup>; Gregory Whiting<sup>1</sup>; Robert Street<sup>1</sup>; Janos Veres<sup>1</sup>; <sup>1</sup>Palo Alto Research Center

**2:50 PM Question and Answer Period**

**3:00 PM**

**Flexible Organic Thin Film Transistors for Neural Interfaces:** *Adrian Avendano*<sup>1</sup>; Taylor Ware<sup>1</sup>; Dustin Simon<sup>1</sup>; David Arreaga-Salas<sup>1</sup>; Walter Voit<sup>1</sup>; <sup>1</sup>University of Texas at Dallas

**3:20 PM Question and Answer Period**

**3:30 PM Break**

**3:45 PM**

**High-Performance Flexible Organic Photovoltaic Cells with Amorphous ZITO Electrode:** *Nanjia Zhou*<sup>1</sup>; D. Bruce Buchholz<sup>1</sup>; Tobin Marks<sup>1</sup>; Robert Chang<sup>1</sup>; <sup>1</sup>Northwestern University

**4:05 PM Question and Answer Period**

**4:15 PM**

**Growth Time Performance Dependence of Vertically Aligned Carbon Nanotube Supercapacitors Grown on Aluminum Substrates:** JJ Nguyen<sup>1</sup>; Jud Ready<sup>1</sup>; *Radu Reit*<sup>2</sup>; <sup>1</sup>Georgia Institute of Technology; <sup>2</sup>UT Dallas

**4:35 PM Question and Answer Period**

**4:45 PM Break**

**5:00 PM**

**Electrochemical Gating and Oxide Field-effect Transistors: Switching Speed and Device Stability Issues:** Subho Dasgupta<sup>1</sup>; Ganna Stoesser<sup>1</sup>; Babak Nasr<sup>1</sup>; Robert Kruk<sup>1</sup>; *Horst Hahn*<sup>1</sup>; <sup>1</sup>Karlsruhe Institute of Technology

**5:20 PM Question and Answer Period**

**5:30 PM**

**Fabricating High-Strain Capacity Conductors on Shape Memory Polymers in Metastable States to Accommodate Large Shape Changes in Flexible Electronic Devices:** *Abhishek Raj*<sup>1</sup>; Wenzhe Cao<sup>1</sup>; Sigurd Wagner<sup>2</sup>; Walter Voit<sup>1</sup>; <sup>1</sup>UT Dallas; <sup>2</sup>Princeton University

**5:50 PM Question and Answer Period**



## 2013 Functional Nanomaterials: Synthesis, Properties and Applications: Carbon Nanomaterials

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Nanomaterials Committee

*Program Organizers:* Seong Jin Koh, University of Texas at Arlington; Nitin Chopra, University of Alabama; Jiyoung Kim, University of Texas at Dallas; Yuanbing Mao, University of Texas-Pan American; Ashwin Ramasubramaniam, University of Massachusetts; Gregory Thompson, University of Alabama

Monday PM  
March 4, 2013

Room: 201  
Location: Henry B. Gonzalez  
Convention Center

*Funding support provided by:* Qualcomm, Inc.

*Session Chairs:* Jiyoung Kim, University of Texas; Ashwin Ramasubramaniam, University of Massachusetts Amherst

### 2:00 PM Invited

**Graphene-Based and Graphene-Derived Materials:** Rod Ruoff<sup>1</sup>; *Ariel Ismach*<sup>1</sup>; <sup>1</sup>The University of Texas at Austin

### 2:35 PM Invited

**Not a Molecule, Not a Polymer, Not a Substrate: The Many Faces of Graphene as Chemical Platform:** *Vincenzo Palermo*<sup>1</sup>; <sup>1</sup>CNR - National Research Council of Italy

### 3:10 PM

**Seeded Growth of Single Crystal Bilayer Graphene Arrays:** *Wei Wu*<sup>1</sup>; Sirui Xing<sup>1</sup>; Shin-Shem Pei<sup>1</sup>; <sup>1</sup>University of Houston

### 3:30 PM Break

### 3:50 PM

**High Performance of Transparent and Flexible Graphene Field-Effect Transistors on Plastic Substrates:** *Sangchul Lee*<sup>1</sup>; Srikanth Janhyala<sup>2</sup>; David Iyore<sup>2</sup>; Saungeun Park<sup>2</sup>; Byoung Hun Lee<sup>1</sup>; Jiyoung Kim<sup>2</sup>; <sup>1</sup>Gwangju Institute of Science & Technology; <sup>2</sup>The University of Texas at Dallas

### 4:10 PM

**Reduced Graphene Sheets Decorated with ZnO Flowers by Hydrothermal Process:** *Hem Pant*<sup>1</sup>; Chan Park<sup>1</sup>; Han Kim<sup>1</sup>; Cheol Kim<sup>1</sup>; <sup>1</sup>Chonbuk National University, South Korea

### 4:30 PM

**Rectangular Graphene Domains Grown at Low-Temperature from Toluene on Electropolished Copper Foils:** *Bin Zhang*<sup>1</sup>; Rodney Ruoff<sup>2</sup>; <sup>1</sup>Key Laboratory for Anisotropy and Texture of Materials of Ministry of Education, Northeastern University, China; <sup>2</sup>Department of Mechanical Engineering and the Materials Science and Engineering Program, The University of Texas at Austin, USA

### 4:50 PM

**Oxidation Kinetics of Gold Nanoparticles for Growth of Graphene Shells:** *Nitin Chopra*<sup>1</sup>; Junchi Wu<sup>1</sup>; Wenwu Shi<sup>1</sup>; <sup>1</sup>The University of Alabama

## 4th International Symposium on High-Temperature Metallurgical Processing: Fundamental Research of Metallurgical Process

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

*Program Organizers:* Tao Jiang, Central South University; Jiann-Yang Hwang, Michigan Technological University; Phillip Mackey, Consultant; Onuralp Yücel, ITU; Guifeng Zhou, Wuhan Iron and Steel

Monday PM  
March 4, 2013

Room: 008B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* Bing Xie, Chongqing University

### 2:00 PM Introductory Comments

### 2:25 PM Keynote

**Reaction Mechanisms and Product Morphologies on Gaseous Reduction of Metal Compounds -- Extractive Metallurgy Meets Materials Science:** *Peter Hayes*<sup>1</sup>; <sup>1</sup>University of Queensland

### 2:40 PM

**Research on the Slag Phase Type of Vanadium-Titanium Magnetite in PreReduction/Electric Furnace Smelting Processing:** Yufeng Guo<sup>1</sup>; Minjun Tang<sup>1</sup>; Tao Jiang<sup>1</sup>; Guanzhou Qiu<sup>1</sup>; Jianfeng Zhou<sup>1</sup>; Linjiang Qing<sup>1</sup>; *Xiaolei Song*<sup>1</sup>; <sup>1</sup>Center South University

### 2:55 PM

**On Dependence of High Temperature Rheological Behaviour of Blast Furnace Slag on Its Network Structure:** *Swatantra Prakash*<sup>1</sup>; <sup>1</sup>National Metallurgical Laboratory

### 3:10 PM

**Density of CaO-5%MgO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> Slag with Low Silica:** Jianchao Li<sup>1</sup>; *Tao Zeng*<sup>1</sup>; Jifang Xu<sup>2</sup>; Chang Jie<sup>1</sup>; Jieyu Zhang<sup>1</sup>; Kuochih Chou<sup>1</sup>; <sup>1</sup>Shanghai University; <sup>2</sup>Soochow University

### 3:25 PM

**Study on the Magnetic Roasting Kinetic of Oolitic Hematite:** Yufeng Guo<sup>1</sup>; Linjiang Qing<sup>1</sup>; *Tao Jiang*<sup>1</sup>; Lin Yang<sup>1</sup>; Shuishi Liu<sup>1</sup>; MingJun Tan<sup>1</sup>; Xiaolei Song<sup>1</sup>; Jiangfeng Zhou<sup>1</sup>; <sup>1</sup>Central South University in China

### 3:40 PM Break

### 3:50 PM

**Basic Research on External Desulfurization of Hot Iron by Dolomite:** *Ren Xiaodong*<sup>1</sup>; Zhang Ting'an<sup>1</sup>; Liu Yan<sup>1</sup>; Dou Zhihe<sup>1</sup>; Lv Guozhi<sup>1</sup>; <sup>1</sup>Northeastern University

### 4:05 PM

**Experimental Investigations of Dynamic Strain Ageing in Austenitic Stainless Steel 316:** *Syed Hussaini*<sup>1</sup>; Gupta AK<sup>1</sup>; Singh SK<sup>2</sup>; <sup>1</sup>BITS-Pilani-Hyderabad Campus; <sup>2</sup>GRIET

### 4:15 PM

**Iron-Carbon Nuggets Coalescence: Influence of Slag's Liquidus Temperatures:** *Alberto Eloy Nogueira*<sup>1</sup>; Adolfo Zambrano<sup>2</sup>; Cyro Takano<sup>1</sup>; Marcelo Mourão<sup>1</sup>; <sup>1</sup>Universidade de São Paulo; <sup>2</sup>Pontificia Universidad Catolica del Peru

### 4:30 PM

**Effect of Mixed Charge of Ore and Lump Coal on The Softening-Melting Property of Burden:** Guo Hongwei<sup>1</sup>; *Yang Guangqing*<sup>1</sup>; Zhang Jianliang<sup>1</sup>; Shao Jiugang<sup>1</sup>; Fu Yuandi<sup>1</sup>; Wang Dan<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing

4:45 PM

**The Thermal Balance in the Melted Material Zone of the Electrical Furnace in Drenas:** *Ahmet Haxhiaj<sup>1</sup>; Bajram Haxhiaj<sup>1</sup>; <sup>1</sup>University of Prishtina*

5:00 PM

**Effects of Oxygen Content And Roasting Temperature on the Sintering Mineralization Properties of Different Iron Ores:** *Xiaoming Mao<sup>1</sup>; Zhixiong You<sup>1</sup>; Yuanbo Zhang<sup>1</sup>; Zhenyu Fan<sup>1</sup>; Tao Jiang<sup>1</sup>; <sup>1</sup>Central South University*

5:15 PM

**Analysis on Wear Mechanism of Refractories Used in Hot Air Pipeline for Large Scal Blast Furnaces:** *Guotao Xu<sup>1</sup>; <sup>1</sup>Wuhan Iron and Steel Group Company*

5:30 PM

**Research on Velocity Field of Liquid Steel in RH:** *Minren Xu<sup>1</sup>; Qingcai Liu<sup>2</sup>; Jian Yang<sup>2</sup>; Dongran Ma<sup>2</sup>; <sup>1</sup>Chongqing University; <sup>2</sup>Chongqing University*

## Advanced Materials and Reservoir Engineering for Extreme Oil & Gas Environments: Nanocrystalline Metals II

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Nanomaterials Committee

*Program Organizers:* Indranil Roy, Schlumberger; Brajendra Mishra, Colorado School of Mines; Manuel Marya, Schlumberger Technology Corporation; Kuo-Chiang Chen, Schlumberger; Partha Ganguly, Schlumberger; Richard Lewis, Schlumberger; Suveen Mathaudhu, U.S. Army Research Office; Nitin Chopra, The University of Alabama; Xinghang Zhang, Texas A&M University; Greg Kusinski, Chevron; John Meng, BP America Inc.; Jefferson Rodrigues, Petrobras; Justin Cheney, Scoperta

Monday PM  
March 4, 2013

Room: Lone Star Salon A  
Location: Grand Hyatt

*Session Chairs:* Xinghang Zhang, Texas A&M University; Suveen Mathaudhu, U.S. Army Research Office

**2:00 PM Introductory Comments Kuo-Chiang Chen - Mechanical and Materials Technology Manager, Schlumberger**

**2:05 PM Keynote**

**Asphaltene Nano-science for Reservoir Characterization:** *Oliver Mullins<sup>1</sup>; <sup>1</sup>Reservoir Characterization Group*

**2:35 PM Keynote**

**Nanotechnology and Future Directions in Petrobras Brazil:** *Gabriel Sotomayor<sup>1</sup>; <sup>1</sup>Petrobras*

**3:05 PM Invited**

**Enhancing Mechanical & Functional Properties Of Bulk Nanostructured Materials:** *Michael Zehetbauer<sup>1</sup>; <sup>1</sup>University of Vienna*

**3:25 PM**

**Thermal Stability of Carbon Nanostructures:** *Nitin Chopra<sup>1</sup>; Wenwu Shi<sup>1</sup>; Yuan Li<sup>1</sup>; <sup>1</sup>The University of Alabama*

**3:45 PM Break**

**4:00 PM Invited**

**Austenitic Steels Strengthened by Nano-Twinned Austenitic Grains:** *K. Lu<sup>1</sup>; <sup>1</sup>Shenyang National Laboratory for Materials Science, Institute of Metal research, Chinese Academy of Sciences*

4:30 PM

**A Study of the Characteristics of Passive Film on UFG Al<sub>50</sub>83 by Synchrotron Radiation:** *Varshni Singh<sup>1</sup>; Indranil Roy; Manuel Marya; Xinghang Zhang; Enrique Laverna; <sup>1</sup>TMS*

4:50 PM

**Enhanced Fatigue Property of a Martensitic Steel with a Gradient Nano-Grained Surface Layer:** *H.W. Huang<sup>1</sup>; Z.B. Wang<sup>1</sup>; X.P. Yong<sup>2</sup>; K. Lu<sup>1</sup>; <sup>1</sup>Institute of Metal Research, Chinese Academy of Sciences; <sup>2</sup>Shenyang Blower Works Group Co. Ltd.*

5:10 PM

**Property Enhancement of Oilfield Alloys through Ultrasonic Treatment:** *Virendra Singh<sup>1</sup>; Indranil Roy<sup>1</sup>; Manuel Marya<sup>1</sup>; <sup>1</sup>Schlumberger*

5:30 PM

**Strengthening Mechanisms of Highly Textured Cu/Ni Multilayers with Extremely Fine Nanotwins:** *Yue Liu<sup>1</sup>; Haiyan Wang<sup>1</sup>; Xinghang Zhang<sup>1</sup>; <sup>1</sup>Texas A&M University*

**5:45 PM Day 1 Wrap Up:** *Oliver Mullins, Science Advisor, RCG, Schlumberger*

## Advances in Surface Engineering: Alloyed and Composite Coatings II: Functional Coatings II

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

*Program Organizers:* Srinivasa Bakshi, Indian Institute of Technology Madras; Graham McCartney, University of Nottingham; Arvind Agarwal, Florida International University; Sandip Harimkar, Oklahoma State University

Monday PM  
March 4, 2013

Room: Bowie B  
Location: Grand Hyatt

*Funding support provided by:* Bulk Nanostructured Materials Programs, Office of Naval Research

*Session Chair:* To Be Announced

**2:00 PM Invited**

**Recent Advanced in Surface Engineering for Friction and Wear Control:** *Ali Erdemir<sup>1</sup>; <sup>1</sup>Argonne National Laboratory*

**2:20 PM Invited**

**Transparent Composite Electrodes for Future Flexible Photovoltaic Applications:** *Terry Alford<sup>1</sup>; <sup>1</sup>Arizona State University*

**2:40 PM Invited**

**High Temperature Oxidation Behavior of Sputtered Nanostructured Coatings:** *Jayaganthan R<sup>1</sup>; Atikur Rahman<sup>1</sup>; Ramesh Chandra<sup>1</sup>; <sup>1</sup>IIT Roorkee*

**3:00 PM**

**Gold Sputtering on Titanium:** *Yoshitaka Shibuya<sup>1</sup>; Atsushi Kodama<sup>1</sup>; Norio Yuki<sup>1</sup>; Kazuhiko Fukamachi<sup>1</sup>; <sup>1</sup>JX Nippon Mining & Metals Corporation*

**3:15 PM**

**Microstructural Property Relationships in CrNiN Thin Film Coatings:** *P.C. Wo<sup>1</sup>; Zonghan Xie<sup>1</sup>; Paul Munroe<sup>1</sup>; <sup>1</sup>Materials Science and Engineering*

**3:30 PM Break**

**3:45 PM**

**Nanocrystalline Porous Coatings:** *Guglya Aleksey<sup>1</sup>; <sup>1</sup>NSC Kharkov Institute of Physics and Technology*

4:00 PM

**Grain Boundary Diffusion Process in Nd-Fe-B Magnets by Dipping and EPD:** Marko Soderžnik<sup>1</sup>; Paul McGuinness<sup>1</sup>; Kristina Žužek-Rožman<sup>1</sup>; Zoran Samardžija<sup>1</sup>; *Spomenka Kobe*<sup>1</sup>; <sup>1</sup>Jožef Stefan Institute

4:15 PM

**Effect of Electroplating Parameters on Internal Stress in Ni-MoS<sub>2</sub> Composite Plating:** *Ebru Saraloglu Guler*<sup>1</sup>; Ishak Karakaya<sup>1</sup>; Erkan Konca<sup>2</sup>; <sup>1</sup>Middle East Technical University; <sup>2</sup>Atilim University

4:30 PM

**The Preparation of Alloy Coating with Special Properties:** *Li Naijun*; Li Meimei; Science College of Shenyang University

4:45 PM

**A Novel Porous Hydroxyapatite Scaffold Coated with Nanostructured Forsterite for Bone Tissue Engineering:** *Adel Sheikhhosseini*<sup>1</sup>; <sup>1</sup>UT

## Alloys and Compounds for Thermoelectric and Solar Cell Applications: Thermoelectric II

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Alloy Phases Committee, TMS: Energy Conversion and Storage Committee

*Program Organizers:* Sinn-wen Chen, National Tsing Hua University; Yoshisato Kimura, Tokyo Institute of Technology; Chih-Huang Lai, National Tsing-Hua University; CW Nan, Tsinghua University; G. Jeffrey Snyder, California Institute of Technology; Hubert Scherrer, Ecole des Mines

Monday PM  
March 4, 2013

Room: 007C  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Ce-Wen Nan, Tsinghua University; Yoshisato Kimura, Tokyo Institute of Technology

2:00 PM Invited

**Thermoelectric Properties of Environmental Friendly Thermoelectric Materials: Zintl Compounds:** *Yoshiki Takagiwa*<sup>1</sup>; Alex Zevalkink<sup>2</sup>; Koichi Kitahara<sup>1</sup>; Kaoru Kimura<sup>1</sup>; Jeffrey Snyder<sup>2</sup>; <sup>1</sup>The University of Tokyo; <sup>2</sup>California Institute of Technology

2:25 PM

**Improving Thermoelectric Properties of Bulk Mg<sub>2</sub>(Si,Sn) Solid Solutions by Incorporating Nanostructures:** *Abdullah Tazebay*<sup>1</sup>; Choongho Yu<sup>1</sup>; <sup>1</sup>Texas A&M University

2:45 PM

**Defects and the Control of Carrier Concentration in Zintl Thermoelectric Phases:** *Gregory Pomrehn*<sup>1</sup>; G. Jeffery Synder<sup>1</sup>; Axel van de Walle<sup>2</sup>; <sup>1</sup>California Institute of Technology; <sup>2</sup>Brown University

3:05 PM

**Microstructure Formation Based on Phase Separation Between Half-Heusler ZrNiSn and Heusler Zr(Ni,Co)<sub>2</sub>Sn:** *Kentaro Yoshioka*<sup>1</sup>; Yaw Wang Chai<sup>1</sup>; Yoshisato Kimura<sup>1</sup>; <sup>1</sup>Tokyo Institute of Technology

3:25 PM

**The Evolution of Nanoprecipitate Microstructure in Half-Heusler TiNiSn Alloys:** *Yaw Wang Chai*<sup>1</sup>; Yoshisato Kimura<sup>1</sup>; <sup>1</sup>Tokyo Institute of Technology

3:45 PM Break

4:00 PM Invited

**High Performance Oxides-Based Thermoelectric Ceramics for Energy Conversion:** *Yuanhua Lin*<sup>1</sup>; Jinle Lan<sup>1</sup>; Ce-Wen Nan<sup>1</sup>; <sup>1</sup>Tsinghua University

4:25 PM

**Phase Stability of Half Heusler Titanium Nickel Material:** *Jean Claude Tedenac*<sup>1</sup>; Philippe Jund<sup>1</sup>; Catherine Colinet<sup>1</sup>; <sup>1</sup>University of Montpellier

4:45 PM

**Mg<sub>2</sub>(Si,Sn) by Design: Nanoprecipitation, Nanostructure Stability and Thermoelectric Properties:** *Philippe Bellanger*<sup>1</sup>; Stéphane Gorsse<sup>1</sup>; Claude Delmas<sup>1</sup>; Christelle Navone<sup>2</sup>; <sup>1</sup>CNRS, Université de Bordeaux, ICMCB; <sup>2</sup>CEA-LITEN

5:05 PM

**Interplay Between Mismatch Strain, Buckling, and Topological Defects in Graphene-Boron Nitride Superlattice: Continuum and Atomistic Descriptions:** *Dinkar Nandwana*<sup>1</sup>; Elif Ertekin<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana Champaign

## Alumina and Bauxite: Digestion

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

*Program Organizer:* Pat Clement, Alcoa

Monday PM  
March 4, 2013

Room: 212B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* Chris Phillips, Alcoa Point Comfort Operations

2:00 PM Introductory Comments

2:10 PM

**Implementation of Logic Control by DCS to Measure the Caustic Concentration in Spent Liquor:** *Ayana Oliveira*<sup>1</sup>; Aécio Carvalho<sup>1</sup>; Bruno Urakawa<sup>1</sup>; Antonio Santos<sup>1</sup>; Milton Maciel<sup>1</sup>; <sup>1</sup>Hydro Alunorte

2:30 PM

**Study of Influences on the Alumina/Caustic (A/C) Ratio and Discharge Digestion (DBO) Caustic of Through Design of Experiments (DOE) Statistic Tool:** Bruno Urakawa<sup>1</sup>; Américo Borges<sup>1</sup>; Arthur Monteiro<sup>1</sup>; *Ayana Oliveira*<sup>1</sup>; Joel Miranda<sup>1</sup>; Dauton Silva<sup>1</sup>; <sup>1</sup>Hydro Alunorte

2:50 PM

**Particle Size Distribution Model for Leaching Kinetics of Alumina:** Li Bao<sup>1</sup>; *Ting-an Zhang*<sup>2</sup>; Weimin Long<sup>1</sup>; Anh V Nguyen<sup>3</sup>; Guozhi Lv<sup>2</sup>; Jia Ma<sup>1</sup>; Yan Liu<sup>2</sup>; <sup>1</sup>State Key Laboratory of Advanced Brazing Filler Metals and Technology, Zhengzhou Research Institute of Mechanical Engineering; <sup>2</sup>School of Materials and Metallurgy, Northeastern University; <sup>3</sup>University of Queensland

3:10 PM

**Fractal Kinetic Model for Digesting Alumina:** Li Bao<sup>1</sup>; *Ting-an Zhang*<sup>2</sup>; Anh V Nguyen<sup>3</sup>; Weimin Long<sup>1</sup>; Jia Ma<sup>1</sup>; Zhihe Dou<sup>2</sup>; Guozhi Lv<sup>2</sup>; <sup>1</sup>State Key Laboratory of Advanced Brazing Filler Metals and Technology, Zhengzhou Research Institute of Mechanical Engineering; <sup>2</sup>School of Materials and Metallurgy, Northeastern University; <sup>3</sup>University of Queensland

3:30 PM

**MAX HT® Bayer Sodalite Scale Inhibitor: A Green Solution To Energy Consumption:** *Morris Lewellyn*<sup>1</sup>; Alan Rothenberg<sup>1</sup>; Calvin Franz<sup>1</sup>; Frank Ballentine<sup>1</sup>; Frank Kula<sup>1</sup>; Luis Soliz<sup>1</sup>; Qi Dai<sup>1</sup>; Scott Moffatt<sup>1</sup>; <sup>1</sup>Cytec Industries Inc

3:50 PM Concluding Comments



## Aluminum Alloys: Fabrication, Characterization and Applications: Development and Application

*Sponsored by:* TMS Light Metals Division, TMS: Aluminum Processing Committee  
*Program Organizers:* Zhengdong Long, Kaiser Aluminum; Subodh Das, Phinix LLC; Tongguang Zhai, University of Kentucky; William Golumbskie, Naval Surface Warfare Center

Monday PM  
 March 4, 2013

Room: 213A  
 Location: Henry B. Gonzalez Convention Center

*Session Chair:* Zhengdong Long, Kaiser Aluminum

### 2:00 PM

**Hemming of Aluminum Alloy Sheets by Electromagnetic Forming:** *Jianhui Shang*<sup>1</sup>; Steve Hatkevich<sup>1</sup>; Larry Wilkerson<sup>1</sup>; <sup>1</sup>American Trim LLC

### 2:20 PM

**Mechanical Properties of Al-Zn-Mg-Cu Alloys Processed with High-pressure Torsion:** *Shigeru Kuramoto*<sup>1</sup>; Ichiro Aoi<sup>1</sup>; Tadahiko Furuta<sup>1</sup>; <sup>1</sup>Toyota Central R&D Labs., Inc.

### 2:40 PM

**High-Performance Be-Al Casting Alloys:** *Charles Pokross*<sup>1</sup>; Gary Schuster<sup>1</sup>; <sup>1</sup>Materion

### 3:00 PM

**Effect of Solute Additions on the Thermal Stability of Grain Size in Aluminum Alloys:** *Andrew Baker*<sup>1</sup>; Stephen Kampel<sup>1</sup>; <sup>1</sup>Michigan Tech

### 3:20 PM Break

### 3:40 PM

**Phase Diagram Determination in Aluminum Rich Al-Sc-Zr Alloys and Interdiffusion Coefficients of Scandium and Zirconium in Aluminum:** Kyle Deane<sup>1</sup>; Marcel Kerkove<sup>1</sup>; Paul Sanders<sup>1</sup>; Douglas Swenson<sup>1</sup>; Thomas Wood<sup>1</sup>; <sup>1</sup>Michigan Technological University

### 4:00 PM

**The Effect of Temperature on Compressive Strength of Al-Si-Cu-Mg Cast Alloy with Zr, V and Ti Additions:** *Sugrib Shah*<sup>1</sup>; Wojciech Kasprzak<sup>2</sup>; Frank Czerwinski<sup>2</sup>; Daolun Chen<sup>1</sup>; <sup>1</sup>Ryerson University; <sup>2</sup>CanmetMATERIALS, Natural Resources Canada

### 4:20 PM

**The Influence of Sc Additions on the Microstructure and Mechanical Properties of an Ultrafine Grained Al-Mg Alloy:** *Tammy Harrell*<sup>1</sup>; Troy Topping<sup>1</sup>; Tao Hu<sup>1</sup>; Julie Schoenung<sup>1</sup>; Enrique Lavernia<sup>1</sup>; <sup>1</sup>University of California, Davis

### 4:40 PM

**Multi-Axial Deformation Behavior of Al6061 Subjected to Fire Damage:** *Dayakar Penumadu*<sup>1</sup>; Akawat Siriruk<sup>1</sup>; Stephen Pupilampu<sup>1</sup>; Brian Lattimer<sup>2</sup>; Patrick Summers<sup>2</sup>; <sup>1</sup>University of Tennessee; <sup>2</sup>Virginia Tech

### 5:00 PM

**Structure Optimization of Al-Si-Type Alloys for Thermal and Mechanical High Loaded Components:** Marcel Rosefort<sup>1</sup>; *Andreas Kleine*<sup>1</sup>; Ansgar Pithan<sup>2</sup>; Christiane Matthies<sup>1</sup>; Hubert Koch<sup>1</sup>; <sup>1</sup>TRIMET ALUMINIUM AG; <sup>2</sup>Martinrea Honsel Germany GmbH

### 5:20 PM

**Development of High Strength Aluminium Alloys at BALCO:** *Narasimharaghavan Puliur Krishnaswamy*<sup>1</sup>; Mousumi Kar<sup>1</sup>; Sachin Prasad<sup>1</sup>; <sup>1</sup>Bharat Aluminium Co. Ltd., (A Unit of Vedanta Resources Plc.), BALCO Nagar, Korba

## Aluminum Reduction Technology: Cell Design and Performance

*Sponsored by:* TMS Light Metals Division, TMS: Aluminum Committee  
*Program Organizer:* Mark Cooksey, CSIRO

Monday PM  
 March 4, 2013

Room: Grand Ballroom C1  
 Location: Henry B. Gonzalez Convention Center

*Session Chair:* Songqing Gu, Chinalco

### 2:00 PM Introductory Comments

### 2:05 PM

**In Depth Analysis of Energy-Saving and Current Efficiency Improvement of Aluminum Reduction Cells:** Jianfei Zhou<sup>1</sup>; *Marc Dupuis*<sup>2</sup>; Feiya Yan<sup>1</sup>; Shaoyong Ruan<sup>1</sup>; <sup>1</sup>Guiyang Aluminum Magnesium Design and Research Institute; <sup>2</sup>GéniSim Inc

### 2:30 PM

**Rio Tinto Alcan AP4X Low Energy Cell Development:** Pascal Thibeault<sup>1</sup>; *Alexandre Blais*<sup>1</sup>; Sébastien Becasse<sup>1</sup>; Patrice Côté<sup>1</sup>; Laurent Fiot<sup>1</sup>; François Laflamme<sup>2</sup>; <sup>1</sup>RioTinto Alcan; <sup>2</sup>Aluminerie Alouette Inc.

### 2:55 PM

**Energy Reduction Technology for Aluminum Electrolysis: Choice of the Cell Voltage:** *Feng Naixiang*<sup>1</sup>; Peng Jianping<sup>1</sup>; Wang Yaowu<sup>1</sup>; <sup>1</sup>Northeastern University

### 3:20 PM

**Advancements of Dubal High Amperage Reduction Cell Technologies:** *Michel Reverdy*<sup>1</sup>; Abdalla Zarouni<sup>1</sup>; Jean-Luc Faudou<sup>1</sup>; Qassim Galadari<sup>1</sup>; Ali Al Zarouni<sup>1</sup>; Sergey Akhmetov<sup>1</sup>; Kamel Al Aswad<sup>1</sup>; Maryam Al-Jallaf<sup>1</sup>; Walid Al Sayed<sup>2</sup>; Vinko Potocnik<sup>1</sup>; <sup>1</sup>DUBAL; <sup>2</sup>Emirates Aluminium Company (EMAL)

### 3:45 PM Break

### 3:55 PM

**Development of Low-Voltage Energy-Saving Aluminum Reduction Technology:** Li Jie<sup>1</sup>; Lv Xiaojun<sup>1</sup>; *Zhang Hongliang*<sup>2</sup>; Liu Yexiang<sup>1</sup>; <sup>1</sup>School of Metallurgical Science and Engineering, Central South University; <sup>2</sup>School of Metallurgical Science and Engineering, Central South University,

### 4:20 PM

**D18+: Potline Modernisation at DUBAL:** *Sergey Akhmetov*<sup>1</sup>; Daniel Whitfield<sup>1</sup>; Maryam Al-Jallaf<sup>1</sup>; Ali Al Zarouni<sup>1</sup>; Alexander Arkhipov<sup>1</sup>; Amer Al Redhwan<sup>1</sup>; Wael Abou Sidou<sup>1</sup>; <sup>1</sup>Dubai Aluminium

### 4:45 PM

**Industry Test of Perforation Anode In Aluminium Electrolysis Technology:** *Yingfu Tian*<sup>1</sup>; Hesong Li<sup>2</sup>; Longhe Wei<sup>2</sup>; Xi Cao<sup>2</sup>; Jianguo Yin<sup>3</sup>; <sup>1</sup>Chongqing Tiantai Aluminum Industry Co., Ltd; <sup>2</sup>Central South University; <sup>3</sup>Chongqing University of Science and Technology

### 5:10 PM

**The First Results of the Industrial Application of the EcoSoderberg Technology at the Krasnoyarsk Aluminium Smelter:** *Victor Buzunov*<sup>1</sup>; Victor Mann<sup>2</sup>; Evgeniy Chichuk<sup>1</sup>; Vladimir Frizorger<sup>1</sup>; Andrey Pinaev<sup>1</sup>; Evgeniy Nikitin<sup>3</sup>; <sup>1</sup>RUSAL ETC; <sup>2</sup>UC RUSAL; <sup>3</sup>RUSAL - Krasnoyarsk

## Aluminum Reduction Technology: Fundamentals: Modelling

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

Program Organizer: Mark Cooksey, CSIRO

Monday PM  
March 4, 2013

Room: Grand Ballroom C2  
Location: Henry B. Gonzalez Convention Center

Session Chair: Christian Droste, Hydro Aluminium

### 2:00 PM Introductory Comments

#### 2:05 PM

**Unsteady MHD Modelling Applied to Cell Stability:** *Renaudier Steeve*<sup>1</sup>; Bardet Benoit<sup>1</sup>; Steiner Gilles<sup>2</sup>; Pedcenko Alex<sup>3</sup>; Rappaz Jacques<sup>4</sup>; Molokov Sergei<sup>3</sup>; Masserey Alexandre<sup>2</sup>; <sup>1</sup>Rio Tinto Alcan; <sup>2</sup>Ycoor Systems SA; <sup>3</sup>Coventry University; <sup>4</sup>EPFL

#### 2:30 PM

**Impact of Magnetohydrodynamic and Bubbles Driving Forces on the Alumina Concentration in the Bath of an Hall-Héroult Cell:** *René von Kaenel*<sup>1</sup>; <sup>1</sup>KAN-NAK SA

#### 2:55 PM

**Investigation of Electrolytic Bubble Behaviour in Aluminium Smelting Cell:** Morshed Alam<sup>1</sup>; Yos Morsi<sup>1</sup>; William Yang<sup>2</sup>; Krishna Mohanarangam<sup>2</sup>; *Geoffrey Brooks*<sup>1</sup>; John Chen<sup>3</sup>; <sup>1</sup>Swinburne University of Technology; <sup>2</sup>CSIRO; <sup>3</sup>University of Auckland

#### 3:20 PM

**Mathematical Model Validation of Aluminium Electrolysis Cells at DUBAL:** Abdalla Zarouni<sup>1</sup>; *Lalit Mishra*<sup>1</sup>; Marwan Bastaki<sup>1</sup>; Amal Al Jasmi<sup>1</sup>; Alexander Arkhipov<sup>1</sup>; Vinko Potocnik<sup>2</sup>; <sup>1</sup>DUBAL; <sup>2</sup>Consultant

#### 3:45 PM Break

#### 3:55 PM

**Production Application Study on Magneto-Hydro-Dynamic Stability of a Large Prebaked Anode Aluminum Reduction Cell:** Shaoyong Ruan<sup>1</sup>; Feiya Yan<sup>1</sup>; *Marc Dupuis*<sup>2</sup>; Valdis Bojarevics<sup>3</sup>; Jianfei Zhou<sup>1</sup>; <sup>1</sup>Guiyang Aluminum Magnesium Design and Research Institute; <sup>2</sup>GéniSim Inc; <sup>3</sup>School of Computing and Mathematics, Greenwich University

#### 4:20 PM

**MHD of Aluminium Cells with the Effect of Channels and Cathode Perturbation Elements:** *Valdis Bojarevics*<sup>1</sup>; <sup>1</sup>University of Greenwich

#### 4:45 PM

**Magnetohydrodynamic Model Coupling Multiphase Flow in Aluminum Reduction Cell with Innovative Cathode Protrusion:** *Qiang Wang*<sup>1</sup>; Baokuan Li<sup>1</sup>; Fang Wang<sup>1</sup>; Naixiang Feng<sup>1</sup>; <sup>1</sup>Northeastern University of China

#### 5:10 PM

**Optimization of the Cathode Collector Bar with a Copper Insert Using Finite Element Method:** *Mathieu Gagnon*<sup>1</sup>; Patrice Goulet<sup>1</sup>; Richard Beeler<sup>2</sup>; Donald Ziegler<sup>3</sup>; Mario Fafard<sup>1</sup>; <sup>1</sup>Université Laval; <sup>2</sup>Alcoa Technical Center; <sup>3</sup>Alcoa Canada

#### 5:35 PM

**Energy Savings in Aluminum Electrolysis Cells: Effect of the Cathode Design:** Mathieu Blais<sup>1</sup>; *Martin Désilets*<sup>1</sup>; Marcel Lacroix<sup>1</sup>; <sup>1</sup>Sherbrooke University

## Biological Materials Science Symposium: Mechanical Behavior of Biological Materials II: Natural Materials

Sponsored by: TMS Electronic, Magnetic, and Photonic Materials Division, TMS Structural Materials Division, TMS: Biomaterials Committee

Program Organizers: Candan Tamerler, University of Washington; Molly Gentleman, Texas A & M University; Po-Yu Chen, National Tsing Hua University; Kajal Mallick, University of Warwick; Rajendra Kumar Kasinath, University of Montana; Paul G. Allison, US Army Corp of Engineers

Monday PM  
March 4, 2013

Room: 214C  
Location: Henry B. Gonzalez Convention Center

Funding support provided by: Biomaterials Program, National Science Foundation

Session Chairs: John Nychka, University of Alberta; Po-Yu Chen, National Tsing Hua University

### 2:00 PM Invited

**Phase Transitions in CaCO<sub>3</sub> Biominerals Mapped with 20-nm Resolution:** *P.U.P.A. Gilbert*<sup>1</sup>; <sup>1</sup>University of Wisconsin

#### 2:30 PM

**Structure and Fracture Resistance of Armored Fish Scales:** *Wen Yang*<sup>1</sup>; Bernd Gludovatz<sup>2</sup>; Elizabeth Zimmermann<sup>2</sup>; Robert Ritchie<sup>3</sup>; Marc Meyers<sup>1</sup>; <sup>1</sup>University of California, San Diego; <sup>2</sup>Lawrence Berkeley National Laboratory; <sup>3</sup>University of California, Berkeley

#### 2:50 PM

**On the Structural and Mechanical Design of Cuttlebone:** Yao-Tien Ku<sup>1</sup>; Yi-Hsin Lee<sup>1</sup>; Chuan-Chin Chiao<sup>1</sup>; *Po-Yu Chen*<sup>1</sup>; <sup>1</sup>National Tsing Hua University

#### 3:10 PM

**Microstructure and Mechanical Behaviour of Megalops Atlanticus Scales:** *Santiago Gil*<sup>1</sup>; Alex Ossa<sup>1</sup>; <sup>1</sup>Eafit University

#### 3:30 PM

**On the Changes in Mechanical Behavior of Fish Scales by Polar Solvents:** Guihua Li<sup>1</sup>; *Mobin Yahyazadehfar*<sup>2</sup>; Adriana Garrano<sup>3</sup>; Alex Ossa<sup>4</sup>; Dwayne Arola<sup>2</sup>; <sup>1</sup>Anhui University; <sup>2</sup>University of Maryland Baltimore County; <sup>3</sup>University of Catania; <sup>4</sup>Eafit University

#### 3:50 PM Break

#### 4:00 PM Invited

**Toughness Amplification in Natural Composites:** *Francois Barthelat*<sup>1</sup>; Reza Rabiei<sup>1</sup>; Ahmad Khayer Dastjerdi<sup>1</sup>; <sup>1</sup>McGill University

#### 4:30 PM

**Cavitation Induced Structural and Neuronal Damage in Brain Tissue:** *Ghatu Subhash*<sup>1</sup>; Malisa Samtinoranan<sup>1</sup>; Michael King<sup>1</sup>; Yu Hong<sup>1</sup>; <sup>1</sup>University of Florida

#### 4:50 PM

**Unusual Deformation Mechanisms in the Prehensile Tails of Seahorses and Pipefish:** *Michael Porter*<sup>1</sup>; Ana Bertha Castro-Cesena<sup>1</sup>; Ekaterina Novitskaya<sup>1</sup>; Zherrina Manilay<sup>1</sup>; Marc Meyers<sup>1</sup>; Joanna McKittrick<sup>1</sup>; <sup>1</sup>University of California San Diego

#### 5:05 PM

**Investigation of Material Property Variation in Red-Eared Slider Turtle Shell Bone Using Microindentation and Nanoindentation:** Nicole Diamantides<sup>1</sup>; Aylin Dincer<sup>1</sup>; C. Tristan Stayton<sup>1</sup>; *Donna Ebnstein*<sup>1</sup>; <sup>1</sup>Bucknell University

5:25 PM

**'Mesolayers': A Contribution to Toughness in Abalone Nacre?:** *Maria Lopez<sup>1</sup>; Pedro Meza-Martinez<sup>1</sup>; Marc Meyers<sup>1</sup>; <sup>1</sup>UCSD*

5:40 PM

**Structural Characterization and Mechanical Performance of Durophagous Fish: A Comparative Study:** *Hao-Jen Fang<sup>1</sup>; Yu-Chen Chan<sup>1</sup>; Tzu-Chin Tseng<sup>2</sup>; Jyh-Wei Lee<sup>2</sup>; Jeng-Gong Duh<sup>1</sup>; Po-Yu Chen<sup>1</sup>; <sup>1</sup>National Tsing Hua University; <sup>2</sup>Ming Chi University of Technology*

6:00 PM

**The Effect of Tungsten Exposure on the Structure-Property Relationships of Herbivorous Gastropod (Snail) Shells and Rat Femurs:** *R.R. McCullough<sup>1</sup>; P. G. Allison<sup>2</sup>; J.M. Seiter<sup>3</sup>; J.H. Lindsay<sup>3</sup>; B.A. Williams<sup>3</sup>; D.R. Johnson<sup>3</sup>; A.J. Kennedy<sup>3</sup>; <sup>1</sup>University of Alabama; <sup>2</sup>US Army Engineer Research & Development Center ; <sup>3</sup>US Army Engineer Research & Development Center*

6:15 PM Invited

**Property - Processing Relationships of Natural Reinforcing Fibers:** *Nicole Robertson<sup>1</sup>; John Nychka<sup>1</sup>; John Wolodko<sup>2</sup>; <sup>1</sup>University of Alberta; <sup>2</sup>Alberta Innovates Technology Futures*

## Bulk Metallic Glasses X: Alloy Development and Application II

*Sponsored by:* TMS Structural Materials Division, TMS/ASM: Mechanical Behavior of Materials Committee  
*Program Organizers:* Peter Liaw, The University of Tennessee; Hahn Choo, The University of Tennessee; Yanfei Gao, The University of Tennessee; Gongyao Wang, The University of Tennessee

Monday PM  
March 4, 2013

Room: Lone Star Salon D  
Location: Grand Hyatt

*Funding support provided by:* Materials Processing and Manufacturing Division, National Science Foundation

*Session Chairs:* C. T. Liu, Hong Kong Polytechnic University; Ke-Fu Yao, Tsinghua University

2:00 PM Keynote

**Phase Selection in Multi-Component Alloys with Equiatomic and Close-to-Equiatomic Compositions:** *Sheng Guo<sup>1</sup>; C. T. Liu<sup>1</sup>; Qiang Hu<sup>2</sup>; <sup>1</sup>City University of Hong Kong; <sup>2</sup>Nortwestern Polytechnic University*

2:30 PM

**Replication of Surface Detail in Bulk Metallic Glass Casting:** *Sven Bossuyt<sup>1</sup>; Erno Soinila<sup>1</sup>; Tuomas Pihlajamäki<sup>1</sup>; Hannu Hänninen<sup>1</sup>; <sup>1</sup>Aalto University*

2:45 PM Invited

**Metallic Glass Nanowire by Gas Atomization:** *Koji Nakayama<sup>1</sup>; Yoshihiko Yokoyama<sup>1</sup>; Takeshi Wada<sup>1</sup>; Na Chen<sup>1</sup>; <sup>1</sup>Tohoku University*

3:05 PM

**Development of Work Hardenable Ti-based Bulk Metallic Glass Matrix Composites:** *Wook Ha Ryu<sup>1</sup>; Hye Jeong Chang<sup>2</sup>; Wan Chuck Woo<sup>3</sup>; Eun Soo Park<sup>1</sup>; <sup>1</sup>Seoul National University; <sup>2</sup>Korea Institute of Science and Technology; <sup>3</sup>Korea Atomic Energy Research Institute*

3:20 PM Invited

**Structure, Fragility and Glass Formation:** *Ken Kelton<sup>1</sup>; James Bendert<sup>1</sup>; Anup Gangopadhyay<sup>1</sup>; Mark Johnson<sup>1</sup>; Nicholas Mauro<sup>1</sup>; Adam Vogt<sup>1</sup>; <sup>1</sup>Washington University*

3:40 PM

**Development of Zr-Based Bulk Metallic Glass Composites with In-Situ Formed ZrN Secondary Phases:** *Je In Lee<sup>1</sup>; Eun Soo Park<sup>1</sup>; <sup>1</sup>Seoul National University*

3:55 PM Break

4:10 PM

**Identifying Bulk Metallic Glass Compositions Through Combinatorial Strategies:** *Jan Schroers<sup>1</sup>; Shiyang Ding<sup>1</sup>; Yanhui Liu<sup>1</sup>; Yanglin Li<sup>1</sup>; <sup>1</sup>Yale University*

4:30 PM Invited

**Research on the Glass-Forming Ability of Low Density Ti-Based Bulk Metallic Glasses:** *Ke-Fu Yao<sup>1</sup>; Pan Gong<sup>1</sup>; <sup>1</sup>Tsinghua University*

4:50 PM

**Thermodynamic Basis for Glass Formation in Cu-Zr Rich Ternary Systems and Their Synthesis by Mechanical Alloying:** *S. Vincent<sup>1</sup>; Jatin Bhatt<sup>1</sup>; B. S. Murty<sup>2</sup>; <sup>1</sup>Visvesvaraya National Institute of Technology, Nagpur; <sup>2</sup>Indian Institute of Technology Madras*

5:05 PM

**In-Situ and Ex-Situ Composites of Zr-Based Bulk Metallic Glass:** *Dongchun Qiao<sup>1</sup>; Atakan Peker<sup>1</sup>; <sup>1</sup>Washington State University*

5:20 PM Invited

**Interfacial Free Energy and Local Order of Metallic Liquids from Elements to Alloys:** *Geun Woo Lee<sup>1</sup>; Dong-Hee Kang<sup>1</sup>; Byeongchan Lee<sup>1</sup>; Sangho Jeon<sup>1</sup>; Soo Heyong Lee<sup>1</sup>; <sup>1</sup>Korea Research Institute of Standards and Science*

5:40 PM

**Study on the Glass-Forming Ability of Binary Cu-Zr Bulk Metallic Glasses:** *Dong-Hee Kang<sup>1</sup>; Sangho Jeon<sup>2</sup>; Soo Heyong Lee<sup>1</sup>; Hyun Hwi Lee<sup>3</sup>; Geun Woo Lee<sup>1</sup>; <sup>1</sup>Korea Research Institute of Standards and Science; <sup>2</sup>University of Science and Technology; <sup>3</sup>Pohang Accelerator Laboratory*

5:55 PM

**Synthesis of Porous Bulk Metallic Glass Composite Fabricated by Spark Plasma Sintering Method Depending on the Type of Dissolution Phase:** *Bo-Kyeong Guem<sup>1</sup>; Song Yi Kim<sup>1</sup>; Do Hyang Kim<sup>2</sup>; Bum Sung Kim<sup>1</sup>; Min Ha Lee<sup>1</sup>; <sup>1</sup>Korea Institute of Industrial Technology, Yonsei university; <sup>2</sup>Yonsei University*

## Cast Shop for Aluminum Production: Aluminum Cast Shop I

*Sponsored by:* TMS Light Metals Division, TMS: Aluminum Committee  
*Program Organizer:* Gyan Jha, Tri-Arrows Aluminum

Monday PM  
March 4, 2013

Room: 210A  
Location: Henry B. Gonzalez Convention Center

*Session Chair:* Gyan Jha, Tri-Arrows Aluminum

2:00 PM Introductory Comments

2:10 PM

**Very High Purity Ingot – An Endangered Species?:** *Stephen Lindsay<sup>1</sup>; <sup>1</sup>Alcoa, Inc.*



2:30 PM

**Innovations and Trends in the Modern Smelter Casthouse:** *Mike Unitl*<sup>1</sup>; Graham Guest<sup>1</sup>; Fabienne Virieux<sup>2</sup>; <sup>1</sup>Solios Thermal; <sup>2</sup>Fives Solios

2:50 PM

**Degassing Processing and Its Effect on Aluminum Metal Quality:** *Eulogio Velasco*<sup>1</sup>; Enrique Resendiz<sup>1</sup>; Alejandra Rodriguez<sup>1</sup>; <sup>1</sup>NEMAK

3:10 PM

**Permanent Magnet Stirred Round-Top Melting Furnace:** *Shridas Ningileri*<sup>1</sup>; Randall Bowers<sup>2</sup>; Xiaoxuan Li<sup>2</sup>; Gyan Jha<sup>3</sup>; <sup>1</sup>University of Kentucky; <sup>2</sup>Secat, Inc.; <sup>3</sup>Tri-Arrows Aluminum

3:30 PM Break

3:50 PM

**Energy Control in Primary Aluminium Casthouse Furnaces:** *Inge Johansen*<sup>1</sup>; Sverre Ivar Strømhaug<sup>2</sup>; <sup>1</sup>Hydro Aluminium, Research & Technology Development; <sup>2</sup>Hydro Aluminium, R&D, Casthouse Support

4:10 PM

**Metal Contamination Associated with Dross Processing:** *Ray Peterson*<sup>1</sup>; <sup>1</sup>Aleris International Inc

4:30 PM

**Modeling of Molten Metal Flow through a Baffled Closed Loop Furnace:** *Randall Bowers*<sup>1</sup>; Shridas Ningileri<sup>2</sup>; Xiaoxuan Li<sup>1</sup>; <sup>1</sup>Secat, Inc.; <sup>2</sup>University of Kentucky

## Characterization of Materials through High Resolution Coherent Imaging: X-ray Based Techniques II

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

*Program Organizers:* John Carpenter, Los Alamos National Laboratory; Ross Harder, Argonne National Laboratory; Richard Sandberg, Los Alamos National Laboratory

Monday PM  
March 4, 2013

Room: 206B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Ross Harder, Argonne National Laboratory; Richard Sandberg, Los Alamos National Laboratory

2:00 PM Keynote

**Quantitative Characterisation of the Strain Fields Associated with Individual Dislocations:** *Brian Abbey*<sup>1</sup>; Harry Quiney<sup>2</sup>; Ruben Dilanian<sup>2</sup>; Andrew Peele<sup>3</sup>; <sup>1</sup>La Trobe University; <sup>2</sup>The University of Melbourne; <sup>3</sup>The Australian Synchrotron

2:30 PM Invited

**Core-Shell Strain Structure of Zeolite Microcrystals:** *Wonsuk Cha*<sup>1</sup>; Sanghoon Song<sup>1</sup>; Nak Cheon Jeong<sup>1</sup>; Hyun-jun Park<sup>1</sup>; Tung Cao Thanh Pham<sup>1</sup>; Ross Harder<sup>1</sup>; Gang Xiong<sup>1</sup>; Ian McNulty<sup>1</sup>; Kyung Byung Yoon<sup>1</sup>; Ian Robinson<sup>1</sup>; *Hyunjung Kim*<sup>1</sup>; <sup>1</sup>Sogang University

2:50 PM Invited

**Ptychographic Reconstructions Using Shared Data Sets:** Martin Dierolf<sup>1</sup>; Pierre Thibault<sup>2</sup>; *Irene Zanette*<sup>3</sup>; Bjoern Enders<sup>3</sup>; Andreas Menzel<sup>4</sup>; Oliver Bunk<sup>4</sup>; Franz Pfeiffer<sup>1</sup>; <sup>1</sup>Technische Universitaet Muenchen & Paul Scherrer Institute & Ecole Polytechnique Federale de Lausanne; <sup>2</sup>Technische Universitaet Muenchen & Paul Scherrer Institute; <sup>3</sup>Technische Universitaet Muenchen; <sup>4</sup>Paul Scherrer Institute

3:10 PM Invited

**Nanometer Scale Materials Studies with Tabletop Soft X-Ray Coherent Imaging:** *Richard Sandberg*<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

3:30 PM Break

3:50 PM Keynote

**Opportunities for X-Ray Coherence in the Dynamics of Complex Oxide Materials:** *Paul Evans*<sup>1</sup>; <sup>1</sup>University of Wisconsin

4:20 PM Invited

**Applications of X-Ray Bragg Projections Ptychography:** *Stephan Hruszkewycz*<sup>1</sup>; Martin Holt<sup>1</sup>; Conal Murray<sup>2</sup>; Dongjin Kim<sup>1</sup>; Matthew Highland<sup>1</sup>; Chad Folkman<sup>1</sup>; Seungbum Hong<sup>1</sup>; Paul Fuoss<sup>1</sup>; <sup>1</sup>Argonne National Laboratory; <sup>2</sup>IBM T.J. Watson Research Center

4:40 PM

**Elemental Imaging Using Micro, Confocal and Doubly Curved Crystal-Based X-Ray Fluorescence Instrumentation for Materials Characterization:** *George Havrilla*<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

## Characterization of Minerals, Metals and Materials 2013: Characterization of Ferrous Metals II

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

*Program Organizers:* Jiann-Yang Hwang, Michigan Technological University; Chen-Guang Bai, Chongqing University; John Carpenter, DOE LANL; Shadia Ikhamayies, Al Isra University; Bowen Li, Michigan Technological University; Mingming Zhang, ArcelorMittal Global R&D; Sergio Monteiro, State University of North Rio de Janeiro; Zhiwei Peng, Michigan Technological University

Monday PM  
March 4, 2013

Room: 206A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Donato Firrao, Politecnico di Torino; Anchao Ren, Wuhan University of Science and Technology

2:00 PM

**High-Cycle Fatigue Behavior of Three Ferrite Stainless Steels at 800°C:** *Tianlong Liu*<sup>1</sup>; Lijia Chen<sup>1</sup>; Hongyun Bi<sup>2</sup>; Xin Che<sup>1</sup>; <sup>1</sup>Shenyang University of Technology; <sup>2</sup>Baoshan Iron & Steel Co., Ltd.

2:20 PM

**Inclusions Removal by Gas Bubbles in Steel Continuous Casting Tundish:** *Ming-Mei Zhu*<sup>1</sup>; Fei Xiong<sup>1</sup>; Guang-Hua Wen<sup>1</sup>; Sheng-Jian Cao<sup>1</sup>; Jian Li<sup>1</sup>; <sup>1</sup>Chongqing University

2:40 PM

**Precipitation of Cu<sub>x</sub> Inclusions in Steel during Rapid Solidification:** *Zhao Dan*<sup>1</sup>; <sup>1</sup>Shanghai University

3:00 PM

**Strength and Ductility of Ultrafine Grained 304SS Prepared by Accumulative Rolling and Annealing:** W.Y. Xue<sup>1</sup>; *Yongfeng Shen*<sup>1</sup>; D.F. Liu<sup>1</sup>; Z.Y. Liu<sup>1</sup>; Y.D. Wang<sup>1</sup>; <sup>1</sup>Northeastern University

3:20 PM

**Thermo-Mechanical Behavior of the Cast Iron Connector in the "Anode Block - Steel Stub" Assembly after Casting and during Operation of the Hall-Héroult Process:** Rimma Zhelateleva<sup>1</sup>; Dmitry Lukovnikov<sup>1</sup>; <sup>1</sup>University Research Centre on Aluminium (CURAL) - University of Québec at Chicoutimi

3:40 PM

**Thermographic Characterization of Tensile Behavior in Railway Bogie Materials:** *Jeongguk Kim*<sup>1</sup>; Sung Cheol Yoon<sup>1</sup>; <sup>1</sup>Korea Railroad Research Institute

## Computational Discovery of Novel Materials: Electrochemical Energy Storage and Conversion

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Integrated Computational Materials Engineering Committee  
*Program Organizers:* Richard Hennig, Cornell University; Dallas Trinkle, University of Illinois at Urbana-Champaign

Monday PM  
March 4, 2013

Room: 207B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* Richard Hennig, Cornell University

### 2:00 PM Invited

**Design and Discovery of Novel Energy Materials:** *Stephan Lany*<sup>1</sup>; <sup>1</sup>NREL

### 2:35 PM Invited

**Extending the Concept of Semiconductor Defect Chemistry to Electrochemistry:** *Mira Todorova*<sup>1</sup>; Joerg Neugebauer<sup>1</sup>; <sup>1</sup>Max-Planck-Institut fuer Eisenforschung GmbH

### 3:10 PM Invited

**Ab Initio Scanning of Chemical Trends for H Solubility, Diffusivity and Interaction with Defects in Metals:** *Roman Nazarov*<sup>1</sup>; Ugur Aydin<sup>1</sup>; Tilmann Hickel<sup>1</sup>; Joerg Neugebauer<sup>1</sup>; <sup>1</sup>Max-Planck-Institut fuer Eisenforschung

### 3:45 PM Break

### 4:00 PM

**Computational Design of Nanosegregated Catalysts:** *Guofeng Wang*<sup>1</sup>; Zhiyao Duan<sup>1</sup>; <sup>1</sup>University of Pittsburgh

### 4:20 PM

**Computational Design of Novel Photocatalysts through Surface Disorder Engineering:** Kulbir Ghuman<sup>1</sup>; *Chandra Veer Singh*<sup>1</sup>; <sup>1</sup>University of Toronto

### 4:40 PM Invited

**Simulation of Electrochemical Processes: Application to Novel Battery Material Design:** Hui-Chia Yu<sup>1</sup>; Chen Ling<sup>1</sup>; Jishnu Bhattacharya<sup>1</sup>; Anton Van der Ven<sup>1</sup>; *Katsuyo Thornton*<sup>1</sup>; <sup>1</sup>Department of Materials Science & Engineering, University of Michigan, Ann Arbor

### 5:15 PM

**First-Principles Studies of Lithiation, Delithiation and Pulverization Processes in Si Anodes in Li-Ion Batteries:** *Kwai Chan*<sup>1</sup>; Wuwei Liang<sup>1</sup>; Candace Chan<sup>2</sup>; <sup>1</sup>Southwest Research Institute; <sup>2</sup>Arizona State University

### 5:35 PM

**First Principles Studies of Fullerene-Like Silicon Clathrates as Anode Materials in Li-ion Batteries:** *Kwai Chan*<sup>1</sup>; Wuwei Liang<sup>1</sup>; Candace Chan<sup>2</sup>; <sup>1</sup>Southwest Research Institute; <sup>2</sup>Arizona State University

## Computational Thermodynamics and Kinetics: First-principles and Multi-scale

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS Materials Processing and Manufacturing Division, TMS: Alloy Phases Committee, TMS: Chemistry and Physics of Materials Committee, TMS/ASM: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS/ASM: Phase Transformations Committee, TMS: Process Technology and Modeling Committee

*Program Organizers:* Joerg Neugebauer, Max-Planck-Institut fuer Eisenforschung GmbH; Carelyn Campbell, NIST; Dongwon Shin, Oakridge National Lab; Zi Kui Liu, Penn State; Michael Demkowicz, Massachusetts Institute of Technology; Raymundo Arroyave, Texas A & M University; Shenyang Hu, Pacific Northwest National Laboratory

Monday PM  
March 4, 2013

Room: 207A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Micheal Short, MIT; Carelyn Campbell, NIST

### 2:00 PM Invited

**Substitutional Solid-State Diffusion in Ni Alloys from First Principles:** *Anton Van der Ven*<sup>1</sup>; <sup>1</sup>University of Michigan

### 2:25 PM

**Diffusion in L12 Structures: A Comparison of Ni<sub>3</sub>Al, Ni<sub>3</sub>Ga and Ni<sub>3</sub>Ge:** Priya Gopal<sup>1</sup>; *Srinivasan Srivilliputhur*<sup>1</sup>; <sup>1</sup>University of North Texas, Denton

### 2:40 PM

**Non-Dilute Defect Calculations in Thermoelectric Zintl Phases:** *Gregory Pomrehn*<sup>1</sup>; G. Jeffery Synder<sup>1</sup>; Axel van de Walle<sup>2</sup>; <sup>1</sup>California Institute of Technology; <sup>2</sup>Brown University

### 2:55 PM

**Pseudomorphic Growth in Mg/Nb Multi-layered Thin Films:** *Anchalee Junkaew*<sup>1</sup>; Byoungsoo Ham<sup>1</sup>; Xinghang Zhang<sup>1</sup>; Raymundo Arroyave<sup>1</sup>; <sup>1</sup>Texas A&M University

### 3:10 PM

**First-Principles Investigation of Mechanical Properties of Dilute Si in BCC-Fe:** *Ying Chen*<sup>1</sup>; Arkapol Saengdeejing<sup>1</sup>; Ken Suzuki<sup>1</sup>; Hideo Miura<sup>1</sup>; Tetsuo Mohri<sup>2</sup>; <sup>1</sup>Tohoku University; <sup>2</sup>Hokkaido University

### 3:25 PM

**New Bond-Order Potentials for Study of Crystal Defects in BCC Transition Metals:** *Vaclav Vitek*<sup>1</sup>; Yi-Shen Lin<sup>1</sup>; Matous Mrovec<sup>2</sup>; <sup>1</sup>University of Pennsylvania; <sup>2</sup>Fraunhofer Institute for Mechanics of Materials

### 3:40 PM Break

### 4:00 PM Invited

**Coupling Effects Between Multiphysical Phenomena, Thermodynamics, and Length Scales in 3D Modeling of PWR CRUD Deposits:** *Michael Short*<sup>1</sup>; David Andersson<sup>2</sup>; Theodore Besmann<sup>3</sup>; Chris Stanek<sup>2</sup>; Dennis Hussey<sup>4</sup>; Brian Kendrick<sup>2</sup>; Sidney Yip<sup>1</sup>; <sup>1</sup>MIT; <sup>2</sup>Los Alamos National Laboratory; <sup>3</sup>Oak Ridge National Laboratory; <sup>4</sup>Electric Power Research Institute

### 4:25 PM Invited

**Phase Field Modeling of Diffusion-Controlled Deformation Processes:** Cheng Feng<sup>1</sup>; Ning Zhou<sup>1</sup>; Hallee Deutchman<sup>1</sup>; Mike Mills<sup>1</sup>; *Yunzhi Wang*<sup>1</sup>; <sup>1</sup>Ohio State University

4:50 PM

**AKMC Simulations of Complex Phase Interfaces in Molybdenum:** *Ari Harjunmaa*<sup>1</sup>; Jutta Rogal<sup>1</sup>; Ralf Drautz<sup>1</sup>; <sup>1</sup>Ruhr University Bochum

5:05 PM

**An Atomistic Perspective on Dynamic Solute-Interface Interactions:** *Tegar Wicaksono*<sup>1</sup>; Chad Sinclair<sup>1</sup>; Matthias Militzer<sup>1</sup>; <sup>1</sup>UBC

### Cost Affordable Titanium IV: Low Cost: Additive Manufacturing and Metal Injection Molding

*Sponsored by:* TMS Structural Materials Division, TMS: Titanium Committee

*Program Organizers:* M. Ashraf Imam, Naval Research Lab; Sam Froes, University of Idaho (Retired); Ramana Reddy, The University of Alabama

Monday PM  
March 4, 2013

Room: 217C  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* F.H. (Sam) Froes, University of Idaho; Sami El-Soudani, The Boeing Company

2:00 PM Invited

**Powder Metallurgy and Additive Manufacturing of Titanium Powders:** *William Peter*<sup>1</sup>; Thomas Muth<sup>1</sup>; Ryan Dehoff<sup>1</sup>; Steve Nunn<sup>1</sup>; Yukinori Yamamoto<sup>1</sup>; Wei Chen<sup>1</sup>; Adrian Sabau<sup>1</sup>; Alan Liby<sup>1</sup>; Craig Blue<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

2:20 PM

**Microstructure, Mechanical Properties, and Failure Mechanisms in Parts Made by Additive Manufacturing:** *Yuwei Zhai*<sup>1</sup>; Diana Lados<sup>1</sup>; <sup>1</sup>WPI

2:40 PM

**Microstructural Analysis of Ti-6Al-4V Components Made by Electron Beam Additive Manufacturing:** *Rashadd Coleman*<sup>1</sup>; Kevin Chou<sup>1</sup>; Viola Acoff<sup>1</sup>; <sup>1</sup>The University of Alabama

3:00 PM

**Links between Melt Pool Geometry and Microstructure in Electron Beam Additive Manufacturing:** *Joy Gockel*<sup>1</sup>; *Jack Beuth*<sup>1</sup>; Nathan Klingbeil<sup>2</sup>; Karen Taminger<sup>3</sup>; <sup>1</sup>Carnegie Mellon University; <sup>2</sup>Wright State University; <sup>3</sup>NASA Langley Research Center

3:20 PM

**Low Cost Titanium Powder Development for Additive Manufacturing in an Electron Beam Melting System:** *Francisco Medina*<sup>1</sup>; Sara Gaytan<sup>1</sup>; Edwin Martinez<sup>1</sup>; Larry Murr<sup>1</sup>; Ryan Wicker<sup>1</sup>; <sup>1</sup>University of Texas at El Paso

3:40 PM Break

4:20 PM

**The Effect of Laser Metal Deposition Operating Parameters on the Microstructure of Ti-5Al-5Mo-5V-3Cr:** *Dacian Tomus*<sup>1</sup>; Guillaume Leclerc<sup>1</sup>; Colleen Bettles<sup>1</sup>; Tom Jarvis<sup>1</sup>; Junfa Mei<sup>1</sup>; Xinhua Wu<sup>1</sup>; <sup>1</sup>Monash University

4:00 PM

**Rheological Properties of Feedstock Composed of Titanium Alloy Powder and Polyethylene Glycol Based Binder System for Metal Injection Moulding:** *Gnanavinthan Thavanayagam*<sup>1</sup>; Deliang Zhang<sup>1</sup>; Kim Pickering<sup>1</sup>; <sup>1</sup>The University of Waikato

4:40 PM

**Microstructure and Texture Development in Ti-5Al-5Mo-5V-3Cr Alloy during Cold Rolling and Annealing:** *Alireza Ghaderi*<sup>1</sup>; Peter Hodgson<sup>1</sup>; Matthew Barnett<sup>1</sup>; <sup>1</sup>Deakin University

### Deformation, Damage, and Fracture of Light Metals and Alloys: Deformation, Damage, and Fracture of Light Metals and Alloys Session I

*Sponsored by:* TMS Light Metals Division, TMS/ASM: Mechanical Behavior of Materials Committee

*Program Organizers:* Ke An, Oak Ridge National Laboratory; Qizhen Li, University of Nevada, Reno

Monday PM  
March 4, 2013

Room: 210B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* Carl Boehlert, Michigan State University

2:00 PM

**Atomic Level Observations of Fatigue Structures in Lamellar Ti-45Al-8Nb-0.2C (TNB-V2):** *Fritz Appel*<sup>1</sup>; Ali El-Chaikh<sup>2</sup>; Hans-Jürgen Christ<sup>2</sup>; <sup>1</sup>Helmholtz Zentrum Geesthacht; <sup>2</sup>Universität Siegen

2:20 PM

**Mechanical Properties and Dislocation Structure Evolution in Ti<sub>4</sub>Al<sub>3</sub>Nb Alloy Processed by High Pressure Torsion:** *Miloš Janeček*<sup>1</sup>; Jakub Čížek<sup>1</sup>; Josef Stráský<sup>1</sup>; Kristína Václavová<sup>1</sup>; Irina Semenova<sup>2</sup>; <sup>1</sup>Charles University; <sup>2</sup>USATU

2:40 PM

**Microstructural Characterization and Mechanical Properties of Boron Modified Ti-6Al-4V Alloy in Different Environments:** *Gaurav Singh*<sup>1</sup>; Upadrasta Ramamurthy<sup>1</sup>; <sup>1</sup>Indian Institute of Science Bangalore

2:55 PM

**Quasi-static Tension and Dynamic Compression Properties of As-Cast Ti-6Al-4V Alloy by Trace Boron Addition:** *Yang YU*<sup>1</sup>; Songxiao HUI<sup>1</sup>; Wenjun YE<sup>1</sup>; Xiaoyun SONG<sup>1</sup>; Rui LIU<sup>1</sup>; Yanyan Fu<sup>1</sup>; <sup>1</sup>General Research Institute for Nonferrous Metals, Beijing, China

3:10 PM

**Plastic Behaviour of Ti-6Al-4V from RT to 600°C:** *Martin Surand*<sup>1</sup>; Bernard Viguier<sup>2</sup>; Emilie Herny<sup>1</sup>; <sup>1</sup>MICROTURBO; <sup>2</sup>Institut Carnot CIRIMAT, INP-ENSIACET, Université de Toulouse

3:25 PM

**Microstructure and Crystallographic Texture Evolution during Hot Deformation of Ti-6Al-2Sn-4Zr-6Mo Titanium Alloy:** *Abdlaziz Elarbi*<sup>1</sup>; <sup>1</sup>University of Sheffield

3:40 PM Break

3:50 PM

**Atomistic Simulation of Deformation Mechanisms of Nanostructured Titanium:** *G.P. Zheng*<sup>1</sup>; <sup>1</sup>Hong Kong Polytechnic University

4:10 PM

**The Influence of Heating Rate on Phase Transformations in Ti-6.8Mo-4.5Fe-1.5Al:** *Herbert Boeckels*<sup>1</sup>; Henry Rack<sup>1</sup>; <sup>1</sup>Clemson University

4:25 PM

**Characterization and Bayesian Neural Network Modeling of Microstructure-Tensile Properties Correlations in Beta-Processed Ti-5111 Alloy:** *Vikas Dixit*<sup>1</sup>; Brian Welk<sup>1</sup>; S.H. Mills<sup>1</sup>; P. Collins<sup>2</sup>; Hamish Fraser<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>University of North Texas

4:40 PM

**Solidification Behaviour and Microstructure Characteristics during Double Directional Solidification Technique of Ti-46Al-5Nb Alloy:** *Liwei Zhang*<sup>1</sup>; X.F. Ding<sup>1</sup>; J.P. Lin<sup>1</sup>; <sup>1</sup>University of Science & Technology Beijing(USTB)



4:55 PM

**Effect of Post-Weld Heat Treatment on Microstructure and Mechanical Properties of Laser Beam Welded TiAl-Based Alloy:** *Jie Liu<sup>1</sup>*; Volker Ventzke<sup>1</sup>; Peter Staron<sup>1</sup>; Norbert Schell<sup>1</sup>; Nikolai Kashaev<sup>1</sup>; Norbert Huber<sup>1</sup>; <sup>1</sup>Helmholtz-Zentrum Geesthacht, Germany

5:10 PM

**Design and Microstructural Characterization of High Performance  $\beta$ -Metastable Titanium Alloys Presenting Simultaneous TRIP and TWIP Effects:** *Matthieu Marteleur<sup>1</sup>*; Pascal Jacques<sup>1</sup>; Frédéric Prima<sup>2</sup>; <sup>1</sup>Université Catholique de Louvain; <sup>2</sup>Ecole Nationale Supérieure de Chimie de Paris

## Electrode Technology for Aluminium Production: Anode Raw Materials

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

*Program Organizers:* Les Edwards, Rain CII Carbon; Hans Darmstadt, Rio Tinto Alcan; Sunil Bhajun, Qatalum; Juraj Chmelar, Hydro; Matvey Golubev, Rusal; Pretesh Patel, Light Metals Research Centre; Elaine Sum, Rio Tinto Alcan; Marc Gagnon, Aluminerie Alouette

Monday PM  
March 4, 2013

Room: 213B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* Hans Darmstadt, Rio Tinto Alcan

## 2:00 PM Introductory Comments

2:05 PM

**Review of Different Techniques to Study the Interaction Between Coke and Pitch in Anode Manufacturing:** *Duygu Kocaefe<sup>1</sup>*; Arunima Sarkar<sup>1</sup>; Shipan Das<sup>1</sup>; Salah Amrani<sup>1</sup>; Dipankar Bhattacharyay<sup>1</sup>; Dilip Sarkar<sup>1</sup>; Yasar Kocaefe<sup>1</sup>; Brigitte Morais<sup>2</sup>; Marc Gagnon<sup>2</sup>; <sup>1</sup>University of Quebec at Chicoutimi; <sup>2</sup>Aluminerie Alouette inc.

2:30 PM

**Observations on the Coke Air Reactivity Test:** Les Edwards<sup>1</sup>; Jim Marino<sup>1</sup>; *Keith Neyrey<sup>1</sup>*; <sup>1</sup>Rain CII Carbon

2:55 PM

**Impurity Removal from Petroleum Coke:** Alexandre Gagnon<sup>1</sup>; *Hans Darmstadt<sup>1</sup>*; Nigel Backhouse<sup>1</sup>; Esme Ryan<sup>2</sup>; Laurence Dyer<sup>3</sup>; David Dixon<sup>3</sup>; <sup>1</sup>Rio Tinto Alcan; <sup>2</sup>Rio Tinto Technology & Innovation; <sup>3</sup>University of British Columbia,

3:20 PM

**Calcined Coke Round Robin 19 and the Precision of Bulk Density Tests:** *Marvin Lubin<sup>1</sup>*; Les Edwards<sup>1</sup>; Lorentz Petter Lossius<sup>2</sup>; <sup>1</sup>Rain CII Carbon; <sup>2</sup>Hydro Aluminium

3:45 PM Break

3:55 PM

**A Method for the Rapid Characterisation of Petroleum Coke Microstructure Using Polarised Light Microscopy:** *Andris Innus<sup>1</sup>*; Alain Jomphe<sup>1</sup>; Hans Darmstadt<sup>1</sup>; <sup>1</sup>Rio Tinto Alcan

4:20 PM

**Improvements of Vibrated Bulk Density Analysis at VM-CBA and Petrocoque S.A:** *Jean Pardo<sup>1</sup>*; Edinaldo da Silva<sup>2</sup>; <sup>1</sup>Votorantim Metals - CBA; <sup>2</sup>Votorantim Metais - CBA

4:45 PM

**Influence of GPC Properties on the CPC Quality:** *Jingli Zhao<sup>1</sup>*; Qingcai Zhao<sup>1</sup>; Qingbo Zhao<sup>1</sup>; Lei Yu<sup>1</sup>; Pusheng Yu<sup>1</sup>; <sup>1</sup>Jinan Aohai Carbon Products Corporation Ltd.

5:10 PM

**Quality of Calcined Petroleum Coke and It's Influence on Aluminium Smelting:** *José Subero<sup>1</sup>*; <sup>1</sup>CVG Venalum

## Fatigue and Fracture of Thin Films and Nanomaterials: Fracture of Thin Films and Nanomaterials

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS/ASM: Mechanical Behavior of Materials Committee, TMS: Nanomechanical Materials Behavior Committee

*Program Organizers:* Megan Cordill, Erich Schmid Institute of Materials Science; Daniel Kiener, Montanuniversitaet Leoben; Xinghang Zhang, Texas A & M University; Daniel Gianola, University of Pennsylvania; Corinne Packard, Colorado School of Mines

Monday PM  
March 4, 2013

Room: Bowie C  
Location: Grand Hyatt

*Funding support provided by:* Hysitron, Inc., and Nanomechanics, Inc.

*Session Chairs:* Corinne Packard, Colorado School of Mines; Neville Moody, Sandia National Laboratories

2:00 PM Invited

**Brittleness Criteria as Affected by Size and Constraint:** William Gerberich<sup>1</sup>; Eric Hintsala<sup>1</sup>; Douglas Stauffer<sup>2</sup>; <sup>1</sup>University of Minnesota; <sup>2</sup>Hysitron, Inc

2:30 PM

**Experiments Investigating Strength Size Effects in Polysilicon and the Existence of a Threshold Strength:** Mohamed Saleh<sup>1</sup>; *Jack Beuth<sup>1</sup>*; Maarten de Boer<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

2:50 PM

**Experimental Determination of the Fracture Toughness Via Scratch Tests:** *Nicholas Randall<sup>1</sup>*; Bo Zhou<sup>1</sup>; Gregory Favaro<sup>1</sup>; <sup>1</sup>CSM Instruments

3:10 PM

**Fracture Characteristics of Severely Plastically Deformed Metals:** *Anton Hohenwarter<sup>1</sup>*; <sup>1</sup>Department of Materials Physics, Montanuniversität Leoben, Austria

3:30 PM Break

3:50 PM Invited

**Probing Materials' Properties and Reliability at the Micron- and Nanoscale and the Need for Novel Experiments:** *Chris Eberl<sup>1</sup>*; <sup>1</sup>KIT

4:20 PM

**Size and Rate Dependent Plastic Localization in Thin Metallic Films:** *Thomas Pardoen<sup>1</sup>*; Michael Coulombier<sup>1</sup>; Hosni Idrissi<sup>1</sup>; Nick Schryvers<sup>2</sup>; Frédéric Mompou<sup>3</sup>; Marc Legros<sup>3</sup>; Jean-Pierre Raskin<sup>1</sup>; <sup>1</sup>UCL; <sup>2</sup>University of Antwerp; <sup>3</sup>CNRS & U. Toulouse

4:40 PM

**Mechanical Behavior and Fracture Properties in Scandium Deuteride Films and Pillars:** *Neville Moody<sup>1</sup>*; Eric Hintsala<sup>2</sup>; Clare Teresi<sup>2</sup>; David Adams<sup>1</sup>; Daniel Kammler<sup>1</sup>; E. David Reedy<sup>1</sup>; Nancy Yang<sup>1</sup>; Marian Kennedy<sup>3</sup>; William Gerberich<sup>2</sup>; <sup>1</sup>Sandia National Laboratories; <sup>2</sup>University of Minnesota; <sup>3</sup>Clemson University

5:00 PM

**Fracture Toughness of SPD-Deformed Nanostructured Rail Steels and Its Implications on the In-Service Behaviour:** *Christoph Kammerhofer*<sup>1</sup>; Anton Hohenwarter<sup>1</sup>; Stephan Scheriau<sup>2</sup>; Reinhard Pippan<sup>1</sup>; <sup>1</sup>Erich Schmid Institute of Materials Science - Austrian Academy of Sciences; <sup>2</sup>voestalpine Schienen GmbH

5:20 PM

**Atomistic Deformation and Fracture Mechanisms in Gradient Nano-Grained Metals:** *Ting Zhu*<sup>1</sup>; Zhi Zeng<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

## Friction Stir Welding and Processing VII: Friction Stir Welding and Processing: Modeling and Controls

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS: Shaping and Forming Committee  
*Program Organizers:* Rajiv Mishra, University of North Texas; Murray Mahoney, Retired from Rockwell Scientific; Yutaka Sato, Tohoku University; Yuri Hovanski, Pacific Northwest National Laboratory; Ravi Verma, General Motors

Monday PM  
March 4, 2013

Room: Grand Ballroom C3  
Location: Henry B. Gonzalez Convention Center

*Session Chairs:* Murray Mahoney, Retired from Rockwell Scientific; Terry McNeley, Naval Postgraduate School; Michael Miles, BYU

2:00 PM Keynote

**Three-Dimensional Visualization of Metallic Flow and Control of FSW Joint Properties Using New FSP Technique:** *Hidetoshi Fujii*<sup>1</sup>; Yoshiaki Morisada<sup>1</sup>; Takuya Imaizumi<sup>1</sup>; <sup>1</sup>Osaka University

2:25 PM Invited

**System Parameter Identification for Friction Stir Processing:** *Carl Sorensen*<sup>1</sup>; Dustin Marshall<sup>1</sup>; <sup>1</sup>Brigham Young University

2:45 PM Invited

**Advances in Temperature Control of FSP:** *Kenneth Ross*<sup>1</sup>; Carl Sorensen<sup>2</sup>; <sup>1</sup>Manufacturing Technology, Inc.; <sup>2</sup>Brigham Young University

3:05 PM Invited

**Analysis of Tool Feedback Forces and Material Flow during Friction Stir Welding:** *Enkhsaikhan Boldsaikhan*<sup>1</sup>; Michael McCoy<sup>1</sup>; <sup>1</sup>Wichita State University

3:25 PM

**Paradigm Shift in Control of the Spindle Axis:** *Kenneth Ross*<sup>1</sup>; Carl Sorensen<sup>2</sup>; <sup>1</sup>Manufacturing Technology, Inc; <sup>2</sup>Brigham Young University

3:45 PM Break

3:55 PM

**A Coupled Thermal/Material Flow Model of Friction Stir Welding Applied to Sc-Modified Aluminum Alloys:** *Carter Hamilton*<sup>1</sup>; Mateusz Kopyscianski<sup>2</sup>; Stanislaw Dymek<sup>2</sup>; Oleg Senkov<sup>3</sup>; <sup>1</sup>Miami University; <sup>2</sup>AGH University Of Science And Technology; <sup>3</sup>UES, Inc

4:15 PM Invited

**Finite Element Modeling of High Speed Friction Stir Spot Welding:** *Michael Miles*<sup>1</sup>; Utsab Karki<sup>1</sup>; Yuri Hovanski<sup>2</sup>; <sup>1</sup>BYU; <sup>2</sup>Pacific Northwest National Lab

4:35 PM Invited

**Microstructure Refinement and Homogenization of Non-deforming Constituent Distributions During FSW/P:** *Terry McNeley*<sup>1</sup>; Sarath Menon<sup>1</sup>; Jeffrey Woertz<sup>1</sup>; <sup>1</sup>Naval Postgraduate School

4:55 PM

**Defect Identification in FSWs Using Data Analysis Techniques:** *Haley Doude*<sup>1</sup>; Judy Schneider<sup>1</sup>; <sup>1</sup>Mississippi State University

5:10 PM

**Modeling the Effects of Tool Geometries on the Temperature Distributions and Material Flow of Friction Stirred AA 7039 Welds:** *Manas Mahapatra*<sup>1</sup>; D Venkateswarlu<sup>1</sup>; H.K. Mohanty<sup>1</sup>; S. P. Harsh<sup>1</sup>; N.R. Mandal<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Roorkee

5:30 PM

**Application of Acoustic Emission Technique to Monitor FSW Process to Produce Defect Free Welds:** *B M Rajaprakash*<sup>1</sup>; Suresha C N<sup>1</sup>; Sarala Upadhy<sup>1</sup>; <sup>1</sup>University Visvesvaraya College of Engineering

5:50 PM

**Finite Element Evaluation of Residual Stresses Developed in Friction Stir Welded Tube-Tubesheet Joint:** *Fadi Al-Badour*<sup>1</sup>; Nesar Merah<sup>1</sup>; Abdelrahman Shuaib<sup>1</sup>; Abdelaziz Bazoune<sup>1</sup>; <sup>1</sup>King Fahd University of Petroleum and Minerals

## Frontiers in Solidification Science: Industrial Aspects of Solidification

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS: Solidification Committee  
*Program Organizers:* Andre Phillion, University of British Columbia; Silvere Akamatsu, Institut des Nanosciences de Paris; Christoph Beckermann, The University of Iowa; Michel Rappaz, Ecole Polytechnique Federale de Lausanne

Monday PM  
March 4, 2013

Room: Lone Star Salon F  
Location: Grand Hyatt

*Funding support provided by:* Materials Processing and Manufacturing Division, National Science Foundation

*Session Chairs:* Andre Phillion, University of British Columbia; Steven Cockcroft, University of British Columbia

2:00 PM Invited

**Advances in Investment Cast Aerospace Components:** *Boyd Mueller*<sup>1</sup>; <sup>1</sup>Alcoa Power and Propulsion

2:30 PM Invited

**Constellium Point of View on Solidification Issues Relevant to the Industry of Aluminium Alloys Processing:** *Philippe Jarry*<sup>1</sup>; <sup>1</sup>Constellium

3:00 PM

**Numerical and Experimental Studies of the Grain Morphological Transitions and Macrosegregation in the Sedimentation Cone of an Industrial Steel Ingot:** *Lerich Nicolas*<sup>1</sup>; Kumar Arvind<sup>2</sup>; Combeau Herve<sup>1</sup>; Zoloznik Miha<sup>1</sup>; Demurger Joelle<sup>3</sup>; Wendenbaum Jean<sup>3</sup>; Gandin Charles-André<sup>4</sup>; <sup>1</sup>Institut Jean Lamour; <sup>2</sup>Indian Institute of Technology Kanpur; <sup>3</sup>Ascometal; <sup>4</sup>MINES ParisTech, CEMEF UMR CNRS 7635

3:20 PM

**Texture Control During Laser Deposition of FCC Alloys:** *Guru Dindal*<sup>1</sup>; Jyoti Mazumder<sup>2</sup>; Douglas Grant<sup>1</sup>; Robert Ruokolainen<sup>1</sup>; Ashish Dasgupta<sup>1</sup>; <sup>1</sup>Focus: HOPE; <sup>2</sup>University of Michigan

3:40 PM Break

3:55 PM Invited

**Commercial Production of Thin-Strip by Twin-Roll Strip Casting - CASTRIP® Process:** *Rama Mahapatra*<sup>1</sup>; Hisahiko Fukase<sup>2</sup>; Mark Schlichting<sup>3</sup>; Neal Ross<sup>4</sup>; Peter Woodberry<sup>1</sup>; Walter Blejdel<sup>1</sup>; <sup>1</sup>Castrip LLC; <sup>2</sup>IHI MetalTech Co; <sup>3</sup>Nucor Steel; <sup>4</sup>Nucor Castrip Arkansas LLC

4:25 PM

**Microstructure Modification by Nanoparticles during Solidification of Aluminum Alloys:** Yi Sun<sup>1</sup>; Hongseok Choi<sup>1</sup>; Hiromi Konishi<sup>1</sup>; Xiaochun Li<sup>1</sup>; <sup>1</sup>University of Wisconsin Madison

4:45 PM

**Crystallization of Intermetallic Phases Fe-Zn during Hot-Dip Galvanizing Process:** *Dariusz Kopycinski*<sup>1</sup>; <sup>1</sup>AGH University of Science and Technology

## High Temperature Electrochemistry: High Temperature Metals and Materials

*Sponsored by:* TMS Extraction and Processing Division, TMS: Pyrometallurgy Committee

*Program Organizers:* Prabhat Tripathy, Idaho National Laboratory; Guy Fredrickson, Idaho National Laboratory

Monday PM  
March 4, 2013

Room: 006D  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Derek Fray, University of Cambridge; Vasant Kumar, University of Cambridge

2:00 PM

**Reduction of TiO<sub>2</sub> or TiCl<sub>3</sub> into Liquid Bi in Molten Salts:** *Yuya Kado*<sup>1</sup>; Sho Maruyama<sup>1</sup>; Akihiro Kishimoto<sup>1</sup>; Tetsuya Uda<sup>1</sup>; <sup>1</sup>Kyoto University

2:30 PM

**Cathodic Behavior of Silicon (IV) in BaF<sub>2</sub>-CaF<sub>2</sub>-SiO<sub>2</sub> Melts:** Yuejiao Hu<sup>1</sup>; *Shuqiang Jiao*<sup>1</sup>; Xin Wang<sup>1</sup>; Jiusan Xiao<sup>1</sup>; Hongmin Zhu<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing

3:00 PM

**Cyclic Voltammetry Investigation of Titanium Dioxide Reduction in Molten Oxide Electrolytes:** *Chanaka De Alwis*<sup>1</sup>; Donald Sadoway<sup>2</sup>; <sup>1</sup>UTRS Inc.; <sup>2</sup>Massachusetts Institute of Technology

3:30 PM Break

3:50 PM

**Electrorefining of Titanium from Bi-Ti Alloys in a NaCl-KCl Molten Salt:** *Akihiro Kishimoto*<sup>1</sup>; Yuya Kado<sup>1</sup>; Shuhei Arisawa<sup>1</sup>; Tetsuya Uda<sup>1</sup>; <sup>1</sup>Kyoto University

4:20 PM

**High Temperature Corrosion and Electrochemical Behavior of Weld Overlay Alloy 625 in Molten Salt Mixture of PbSO<sub>4</sub>Pb<sub>3</sub>O<sub>4</sub>PbC<sub>12</sub>-ZnO-CdO:** *E. Mohammadi Zahrani*<sup>1</sup>; A. Alfantazi<sup>1</sup>; <sup>1</sup>The University of British Columbia

4:50 PM

**Fundamental Study on Anodic Dissolution Behavior of Platinum Group Metals:** *Katsuhiro Nose*<sup>1</sup>; Toru Okabe<sup>1</sup>; <sup>1</sup>The Institute of Industrial Science, the University of Tokyo

## Hume-Rothery Award Symposium: Electronic Structure Theory of Stability and Bonding in Alloys: Alloy Theory I

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Alloy Phases Committee

*Program Organizer:* Chris Wolverton, Northwestern University

Monday PM  
March 4, 2013

Room: 205  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Barry Klein, University California Davis; Ralf Drautz, University of Oxford

2:00 PM Invited

**Extending the Lattice Stability Framework in Ab Initio Alloy Thermodynamics:** *Axel van de Walle*<sup>1</sup>; <sup>1</sup>Brown University

2:30 PM Invited

**First Principles Modeling of Planar Defects in Solid Solutions by the Special Quasirandom Structure Approach:** Maarten de Jong<sup>1</sup>; David Olmsted; Axel van de Walle<sup>2</sup>; *Mark Asta*<sup>1</sup>; <sup>1</sup>University of California, Berkeley; <sup>2</sup>Brown University

3:00 PM Invited

**Diffuse Interfaces, Gradient Energy and Their Kinetic and Thermodynamic Consequences:** *Alan Ardell*<sup>1</sup>; <sup>1</sup>University of California

3:30 PM Break

3:50 PM Invited

**Anharmonic Phonons and Thermodynamics:** *Brent Fultz*<sup>1</sup>; Chen Li<sup>1</sup>; Tian Lan<sup>1</sup>; <sup>1</sup>California Institute of Technology

4:20 PM Invited

**First Principles Phase Diagram Calculations for Octahedral Interstitial Ordering of Oxygen and Vacancies in hcp Ti, Zr, and Hf:** *Benjamin Burton*<sup>1</sup>; Axel van de Walle<sup>2</sup>; <sup>1</sup>NIST; <sup>2</sup>Brown University

## Hybrid and Hierarchical Composite Materials: Multifunctionality

*Sponsored by:* TMS Structural Materials Division, TMS/ASM: Composite Materials Committee

*Program Organizers:* Tomoko Sano, US Army Research Laboratory; Charles Randow, US Army Research Laboratory; Chang Soo Kim, University of Wisconsin -Milwaukee

Monday PM  
March 4, 2013

Room: 215  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* Meisha Shofner, Georgia Institute of Technology

2:00 PM

**Rate Dependent Mechanical Response of Epoxy Polymers:** *Joseph Lenhart*<sup>1</sup>; Daniel Knorr<sup>1</sup>; Jan Andzelm<sup>1</sup>; Adam Richardson<sup>1</sup>; Mark Hindenlang<sup>1</sup>; <sup>1</sup>US Army Research Laboratory

2:30 PM

**Sulfonated Poly(Fluorene Ether Ketone) (SPFEK)/a-Zirconium Phosphate (ZrP) Nanocomposite Membranes for Fuel Cell Applications:** *Fuchuan Ding*<sup>1</sup>; Hang Hu<sup>1</sup>; Matthew F. Milner<sup>1</sup>; Min Xiao<sup>2</sup>; Yuezhong Meng<sup>2</sup>; Luyi Sun<sup>2</sup>; <sup>1</sup>Texas State University-San Marcos; <sup>2</sup>Sun Yat-sen University



2:50 PM

**Manufacture of RF Absorptive Composites by Direct-Write:** *Garth Wilks<sup>1</sup>*; Gerard Simon<sup>1</sup>; Thomas Ekiert<sup>1</sup>; Gyaneshwar Tandon<sup>1</sup>; Zongwu Bai<sup>1</sup>; Max Alexander<sup>1</sup>; Ryan Justice<sup>1</sup>; <sup>1</sup>Air Force Research Laboratory

3:10 PM

**New Insight into Multi-Functional, Hierarchical Poly(Urethane Urea) Elastomers: From Molecules-by-Design to Multiscale Modeling:** *Alex Hsieh<sup>1</sup>*; Tanya Chantawansri<sup>1</sup>; <sup>1</sup>Army Research Laboratory

3:30 PM Break

3:45 PM

**Multifunctional Architected Materials for Electromagnetic Absorption:** Pierre Bollen<sup>1</sup>; Nicolas Quievy<sup>1</sup>; Isabelle Huynen<sup>1</sup>; Christian Bailly<sup>1</sup>; Christophe Detrembleur<sup>2</sup>; Jean-Michel Thomassin<sup>2</sup>; *Thomas Pardoen<sup>1</sup>*; <sup>1</sup>UCL; <sup>2</sup>ULg

4:05 PM

**High Thermal-Conductive Aluminum/Diamond Composites for Electronic Packaging:** *Xitao Wang<sup>1</sup>*; Yang Zhang<sup>1</sup>; Jianhua Wu<sup>1</sup>; Hailong Zhang<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing

4:25 PM

**Hierarchical Architected Metal-Elastomer Composites for Multifunctional Applications:** *Lorenzo Valdevit<sup>1</sup>*; <sup>1</sup>University of California, Irvine

4:45 PM

**Extrinsic Toughening of Shape Memory Alloy Embedded Composites:** *Fatmata Barrie<sup>1</sup>*; Michele Manuel<sup>1</sup>; <sup>1</sup>University of Florida

5:05 PM

**Morphology and Phase Evaluation in Shape Memory Alloy (SMA) – MAX Phase Interpenetrating Composites:** Liangfa Hu<sup>1</sup>; *Ankush Kothalkar<sup>1</sup>*; Miladin Radovic<sup>1</sup>; Ibrahim Karaman<sup>1</sup>; <sup>1</sup>Texas A&M University

## Integrated Computational Modeling of Materials for Nuclear Energy: Fuel Modeling II: Multiscale Modeling

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS/ASM: Computational Materials Science and Engineering Committee, TMS/ASM: Nuclear Materials Committee

*Program Organizers:* Remi Dingreville, Sandia National Laboratories; Koenraad Janssens, Paul Scherrer Institute; Timothy Bartel, Sandia National Laboratories

Monday PM  
March 4, 2013

Room: 202B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* To Be Announced

2:00 PM Invited

**Heterogeneity Effects on the Thermal Conductivity of UO<sub>2</sub>+x:** *Marius Stan<sup>1</sup>*; Bogdan Mihaila<sup>2</sup>; Di Yun<sup>1</sup>; Zhi-Gang Mei<sup>1</sup>; Petrica Cristea<sup>3</sup>; <sup>1</sup>Argonne National Laboratory; <sup>2</sup>Los Alamos National Laboratory; <sup>3</sup>University of Bucharest

2:30 PM Invited

**Mesoscale Model of Bubble/Grain Boundary Interaction in Irradiated Materials:** *Michael Tonks<sup>1</sup>*; Liangzhe Zhang<sup>1</sup>; Paul Millett<sup>1</sup>; Bulent Biner<sup>1</sup>; Yongfeng Zhang<sup>1</sup>; <sup>1</sup>Idaho National Laboratory

3:00 PM

**Multi-Physics Mechanical Response of Fuel Pin Swelling:** *Timothy J. Bartel<sup>1</sup>*; Remi Dingreville<sup>1</sup>; Josh Robbins<sup>1</sup>; <sup>1</sup>Sandia National Laboratories

3:20 PM Invited

**Development of the Mechanistic Fuel Performance and Safety Code SFPR Using the Multi-Scale Approach:** *Mikhail Veshchunov<sup>1</sup>*; A. Boldyrev<sup>1</sup>; V.D. Ozrin<sup>1</sup>; V. Shestak<sup>1</sup>; V. Tarasov<sup>1</sup>; G. Norman<sup>1</sup>; A. Kuksin<sup>1</sup>; V. Pisarev<sup>1</sup>; D. Smirnova<sup>1</sup>; V. Stegailov<sup>1</sup>; S. Starikov<sup>1</sup>; A. Yanilkin<sup>1</sup>; <sup>1</sup>Nuclear Safety Institute (IBRAE) of Russian Academy of Sciences

3:40 PM Break

4:00 PM Invited

**Continuum Theory of Defects and Materials Response to Irradiation:** *Anter El-Azab<sup>1</sup>*; <sup>1</sup>Purdue University

4:30 PM

**Phonon Thermal Transport in UO<sub>2</sub> Crystals with Defects:** *Ryan Deskins<sup>1</sup>*; Anter El-Azab<sup>1</sup>; <sup>1</sup>Purdue University

4:50 PM Invited

**Multiscale Computer Simulation of Fission Gas Release in Oxide Fuels:** *Paul Millett<sup>1</sup>*; Michael Tonks<sup>1</sup>; David Andersson<sup>2</sup>; Yongfeng Zhang<sup>1</sup>; Bulent Biner<sup>1</sup>; <sup>1</sup>Idaho National Laboratory; <sup>2</sup>Los Alamos National Laboratory

5:20 PM

**Multi-Scale Modeling of Intergranular Fracture in UO<sub>2</sub>:** *Yongfeng Zhang<sup>1</sup>*; Paul Millett<sup>1</sup>; Michael Tonks<sup>1</sup>; Bulent Biner<sup>1</sup>; <sup>1</sup>Idaho National Laboratory

## Magnesium Technology 2013: Primary Production and Casting

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

*Program Organizers:* Norbert Hort, Helmholtz-Zentrum Geesthacht; Suveen Mathaudu, US Army Research Office; Neale Neelameggham, IND LLC; Martyn Alderman, Magnesium Elektron

Monday PM  
March 4, 2013

Room: 214A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Neale Neelameggham, Ind LLC; Adam Powell, Metal Oxygen Separation Technologies

2:00 PM

**Doing Projects in a Foreign Language – Communications Management, Issues and Strategies:** *Deling Xian<sup>1</sup>*; <sup>1</sup>Hatch

2:20 PM

**Evolution of the Magnetherm Magnesium Reduction Process:** *James Sever<sup>1</sup>*; Marlyn Ballain<sup>2</sup>; <sup>1</sup>Alpha / Omega Engineering; <sup>2</sup>Ballain Consulting, Inc

2:40 PM

**Impact of Site Elevation on Mg Smelter Design:** *Phillip Baker<sup>1</sup>*; <sup>1</sup>Hatch Ltd.

3:00 PM

**Purification of Highly Contaminated Magnesium Melt:** *Byoung-Gi Moon<sup>1</sup>*; Do-Youn Kim<sup>2</sup>; Bong-Sun You<sup>1</sup>; Ki-Ho Koh<sup>3</sup>; <sup>1</sup>Korea Institute of Materials Science; <sup>2</sup>University of Science and Technology; <sup>3</sup>Inje University

3:20 PM

**Research on New Type Materials Preparation for Magnesium Production by Silicothermic Process:** *Wen Ming<sup>1</sup>*; Zhang Ting'an<sup>1</sup>; Dou Zhihe<sup>1</sup>; Zhang Rui<sup>1</sup>; Ren Xiaodong<sup>1</sup>; Zhou Lian<sup>2</sup>; <sup>1</sup>Northeastern University; <sup>2</sup>Northwest Insititute For Non-ferrous Metal Reasearch

3:40 PM Break

**4:00 PM**

**Selective Laser Melting of Magnesium and Magnesium Alloys:** *Matthias Gieseke*<sup>1</sup>; Christian Noelke<sup>1</sup>; Stefan Kaierle<sup>1</sup>; Volker Wesling<sup>1</sup>; Heinz Haferkamp<sup>1</sup>; <sup>1</sup>Laser Zentrum Hannover e.V.

**4:20 PM**

**Computational Multi-Scale Modeling of the Microstructure and Segregation of Cast Mg Alloys at Low Superheat:** *Laurentiu Nastac*<sup>1</sup>; Nagy El-Kaddah<sup>1</sup>; <sup>1</sup>University of Alabama

**4:40 PM**

**Effect of Casting Defects Distribution on the Beginning of Tensile Fracture in Semi-Solid Injected Magnesium AZ91D Alloy:** *Yuichiro Murakami*<sup>1</sup>; Kenji Miwa<sup>2</sup>; Naoyuki Kanetake<sup>3</sup>; Shuji Tada<sup>1</sup>; <sup>1</sup>Advanced Industrial Science and Technology; <sup>2</sup>Aichi Science and Technology Foundation; <sup>3</sup>Nagoya University

**5:00 PM**

**Effect of Inoculation Method of Refiner on the Grain Refinement of AZ91 Alloy:** *Jun Ho Bae*<sup>1</sup>; Young Min Kim<sup>1</sup>; Chang Dong Yim<sup>1</sup>; Ha-Sik Kim<sup>1</sup>; Bong Sun You<sup>1</sup>; <sup>1</sup>Korea Institute of Materials Science

## Magnetic Materials for Energy Applications -III: Rare Earth-free Permanent Magnets I

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Energy Committee, TMS: Energy Conversion and Storage Committee, TMS: Magnetic Materials Committee  
*Program Organizers:* Sivaraman Guruswamy, University of Utah; Thomas Woodcock, IFW Dresden; Yongmei Jin, Michigan Technological University; Raju Ramanujan, Nanyang Technological University; Frank Johnson, GE Global Research; Oliver Gutfleisch, Technische Universität Darmstadt

Monday PM  
March 4, 2013

Room: 217D  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Yongmei Jin, Michigan Tech; Thomas. Woodcock, IFW Dresden

**2:00 PM Invited**

**Rare-Earth Free Permanent Magnets:** *Yang-Ki Hong*<sup>1</sup>; <sup>1</sup>University of Alabama

**2:30 PM Invited**

**New Materials and Novel Anisotropies for Rare-Earth-Free Permanent Magnets:** *Laura Lewis*<sup>1</sup>; <sup>1</sup>Northeastern University

**3:00 PM Invited**

**Advances in Rare-earth Free Permanent Magnets:** David Sellmyer<sup>1</sup>; B Balamurugan; W. Zhang; R. Skomski; <sup>1</sup>University of Nebraska

**3:30 PM**

**Thermal Stabilization of Magnetic Hardness in Exchange-Biased Nanostructures for Advanced Permanent Magnets:** *Joshua Marion*<sup>1</sup>; Felix Jimenez-Villacorta<sup>1</sup>; Laura Lewis<sup>1</sup>; <sup>1</sup>Northeastern University

**3:50 PM Break****4:05 PM Invited**

**Novel High Energy Permanent Magnet without Critical Elements:** *R McCallum*<sup>1</sup>; <sup>1</sup>Ames Laboratory

**4:35 PM Invited**

**Non-Rare Earth Permanent Magnets: Nanocrystalline Mn-Al-C:** *Jeff Shield*<sup>1</sup>; Michael Lucis<sup>1</sup>; Timothy Prost<sup>1</sup>; Ralph Skomski<sup>1</sup>; <sup>1</sup>University of Nebraska

**5:05 PM**

**Tetrateaenite (FeNi)- A Potential Candidate For a Rare-Earth -Free Permanent Magnet:** *Arif Mubarak*<sup>1</sup>; Nina Bordeaux<sup>2</sup>; Joseph Goldstein<sup>1</sup>; Laura Lewis<sup>2</sup>; <sup>1</sup>University of Massachusetts; <sup>2</sup>Northeastern University

## Materials and Fuels for the Current and Advanced Nuclear Reactors II: Irradiation Studies

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

*Program Organizers:* Ramprashad Prabhakaran, Idaho National Laboratory; Dennis Keiser, Idaho National Laboratory; Raul Rebak, GE Global Research

Monday PM  
March 4, 2013

Room: 202A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* Raul Rebak, GE Global Research

**2:00 PM Invited**

**Development of Radiation Tolerant Cladding Materials for Fast Spectrum Reactors:** *Stuart Maloy*<sup>1</sup>; Osman Anderoglu<sup>1</sup>; Tarik Saleh<sup>1</sup>; Mychailo Toloczko<sup>2</sup>; James Cole<sup>3</sup>; Jian Gan<sup>3</sup>; Dave Hoelzer<sup>4</sup>; Thak-Sang Byun<sup>4</sup>; G. Robert Odette<sup>5</sup>; <sup>1</sup>Los Alamos National Laboratory; <sup>2</sup>PNNL; <sup>3</sup>INL; <sup>4</sup>ORNL; <sup>5</sup>UCSB

**2:40 PM**

**GENESIS : An Open Platform for the Study and Nano Analysis (Atom Probe, SEM Cross Beam Station and MET (In Situ Straining, Temperature, Tomography) of Irradiation Effects in Radioactive Materials for Nuclear Application:** *Philippe Pareige*<sup>1</sup>; <sup>1</sup>Rouen University

**3:00 PM**

**Irradiation Studies on Friction Stir Welded ODS Alloys:** *Ramprashad Prabhakaran*<sup>1</sup>; Jatu Burns<sup>2</sup>; James Cole<sup>1</sup>; Yaqiao Wu<sup>2</sup>; B Miller<sup>1</sup>; Indrajit Charit<sup>3</sup>; Rajiv Mishra<sup>4</sup>; K. Murty<sup>5</sup>; <sup>1</sup>Idaho National Laboratory; <sup>2</sup>CAES; <sup>3</sup>University of Idaho; <sup>4</sup>University of North Texas; <sup>5</sup>North Carolina State University

**3:20 PM**

**Understanding of the Microstructural Evolution of Austenitic Model Alloy and 316 Steel under Ion Irradiation by Coupling of TEM and APT Investigations - Part I: TEM:** Alexandre Volgin<sup>1</sup>; *Brigitte Decamps*<sup>2</sup>; Aurélie Gentils<sup>2</sup>; Franck Fortuna<sup>2</sup>; Bertrand Radiguet<sup>3</sup>; Philippe Pareige<sup>3</sup>; Cédric Pokor<sup>4</sup>; Abderrahim Al-Mazzouzi<sup>4</sup>; <sup>1</sup>EDF R&D; <sup>2</sup>CNRS/IN2P3; <sup>3</sup>GPM; <sup>4</sup>EDF R&D

**3:40 PM Break****4:00 PM**

**Understanding of the Microstructural Evolution of Austenitic Model Alloy and 316 Steel under Ion Irradiation by Coupling of TEM and APT Investigations – Part II: APT Results:** Alexandre Volgin<sup>1</sup>; *Bertrand Radiguet*<sup>2</sup>; Philippe Pareige<sup>2</sup>; Brigitte Decamps<sup>2</sup>; Aurélie Gentil<sup>3</sup>; Frank Fortuna<sup>3</sup>; Cedric Pokor<sup>1</sup>; <sup>1</sup>EDF R&D - MMC; <sup>2</sup>GPM UMR CNRS 6634 - Université et INSA de Rouen; <sup>3</sup>CSNSM - CNRS IN2P3 - Université Paris Sud

**4:20 PM**

**Point Defect Cluster Interactions with Grain Boundaries in Nanocrystalline Iron:** *Greg Vetterick*<sup>1</sup>; Chris Barr<sup>1</sup>; John Baldwin<sup>2</sup>; Pete Baldo<sup>3</sup>; Mark Kirk<sup>3</sup>; Amit Misra<sup>2</sup>; Mitra Taheri<sup>1</sup>; <sup>1</sup>Drexel University; <sup>2</sup>Los Alamos National Laboratory; <sup>3</sup>Argonne National Laboratory

4:40 PM

**Synergetic Effect of Ni and Cu in French Reactor Pressure Vessel Steels:** Hefei Huang<sup>1</sup>; *Bertrand Radigue*<sup>1</sup>; Patrick Todeschini<sup>2</sup>; François Clémendo<sup>3</sup>; Philippe Pareige<sup>1</sup>; <sup>1</sup>GPM UMR CNRS 6634 - Université et INSA de Rouen; <sup>2</sup>EDF R&D - MMC; <sup>3</sup>EDF Production and Engineering - CEIDRE/DLAB

5:00 PM

**Studies on the Ion Bombardment and LBE Corrosion Resistance Properties of Polycrystalline SiC:** *Jianrong Sun*<sup>1</sup>; Peng Song<sup>1</sup>; Tielong Shen<sup>1</sup>; Zhiguang Wang<sup>1</sup>; <sup>1</sup>Institute of Modern Physics, Chinese Academy of Sciences

## Materials in Clean Power Systems VIII: Durability of Materials : Alloy Development for Clean and Efficient Energy Technologies

*Sponsored by:* TMS Structural Materials Division, TMS/ASM: Corrosion and Environmental Effects Committee  
*Program Organizers:* Sebastien Dryepondt, ORNL; Kinga Unocic, ORNL; Jeffrey Fergus, Auburn University; Xingbo Liu, West Virginia University

Monday PM  
March 4, 2013

Room: 007A  
Location: Henry B. Gonzalez Convention Center

*Session Chairs:* Jeffrey Hawk, U.S. Department of Energy, National Energy Technology Laboratory; Amit Shyam, Oak Ridge National Laboratory

2:00 PM Invited

**Reduced Temperature Range for the Heat to Fuel Energy Conversion by Using Ceria Nanoparticles:** *Siu-wai Chan*<sup>1</sup>; Bin Wang<sup>1</sup>; William Robson<sup>1</sup>; Jacob Keith<sup>1</sup>; Prashant Mukhopadhyay<sup>1</sup>; Apisak Meesrisom<sup>1</sup>; Joan Raitano<sup>1</sup>; Hong-Ying Liang<sup>1</sup>; <sup>1</sup>Columbia University

2:30 PM

**Improved Processing Efficiency and Microstructure Control of ODS Ferritic Alloys:** *Joel Rieken*<sup>1</sup>; Iver Anderson<sup>1</sup>; Matthew Kramer<sup>1</sup>; Sebastien Dryepondt<sup>2</sup>; David Hoelzer<sup>2</sup>; <sup>1</sup>Ames Laboratory; <sup>2</sup>Oak Ridge National Laboratory

2:50 PM Invited

**Advanced Heat Resistant Austenitic Stainless Steel and Composite Tube Materials for High Efficient and Clean Energy Technology:** *Guocai Chai*<sup>1</sup>; <sup>1</sup>Sandvik Materials Technology

3:20 PM Break

3:40 PM Invited

**Recent Developments in Creep-Resistant, Alumina-Forming Austenitic Stainless Steels:** Yukinori Yamamoto<sup>1</sup>; *Govindarajan Muralidharan*<sup>1</sup>; Michael Brady<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

4:10 PM

**Homogenizing Castings to Improve the Mechanical Properties of Traditionally Wrought Ni-Based Superalloys for A-USC Steam Turbines:** *Paul Jablonski*<sup>1</sup>; Jeffrey Hawk<sup>1</sup>; Daniel Purdy<sup>2</sup>; Phillip Maziasz<sup>3</sup>; <sup>1</sup>US Department of Energy; <sup>2</sup>GE Energy; <sup>3</sup>Oak Ridge National Laboratory

## Materials Processing Fundamentals: Process Metallurgy of Steel

*Sponsored by:* TMS Extraction and Processing Division, TMS: Process Technology and Modeling Committee  
*Program Organizers:* Lifeng Zhang, University of Science and Technology Beijing; Antoine Allanore, Massachusetts Institute of Technology; Cong Wang, Saint-Gobain High Performance Materials; James Yurko, Materion Brush Beryllium and Composites; Justin Crapps, ExxonMobil

Monday PM  
March 4, 2013

Room: 008A  
Location: Henry B. Gonzalez Convention Center

*Session Chair:* Lifeng Zhang, University of Science and Technology Beijing

2:00 PM

**Evolution of Inclusions in Ti-Bearing Ultra-Low Carbon Steel during RH Refining Process:** Wen Yang<sup>1</sup>; *Lifeng Zhang*<sup>1</sup>; Xinhua Wang<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing

2:20 PM

**Mass Action Concentration Model of CaO-MgO-FeO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> Slag Systems and Its Application to the Formation Mechanism of MgO-Al<sub>2</sub>O<sub>3</sub> Spinel Type Inclusion in Casing Steel:** *Haiyan Tang*<sup>1</sup>; Jingshe Li<sup>1</sup>; Chuanbo Ji<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing

2:40 PM

**Effect of Casting Conditions Regarding to Macro-Segregation and Macro-Cleanliness of Fe-Mn-C-Al Steel Grades:** *Petrice von Schweinichen*<sup>1</sup>; Dieter Senk<sup>1</sup>; Hubert Weerts<sup>1</sup>; <sup>1</sup>RWTH Aachen University

3:00 PM

**Theory Analysis of Steel Cleanliness Control during Electroslag Remelting:** *Cheng-bin Shi*<sup>1</sup>; Xi-chun Chen<sup>2</sup>; Yi-wa Luo<sup>1</sup>; Han-jie Guo<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing; <sup>2</sup>Central Iron and Steel Research Institute

3:20 PM

**Formation and Drop of Metal Droplets in Slag Bath of Electroslag Remelting Processes:** *Baokuan Li*<sup>1</sup>; Ruinan Li<sup>1</sup>; Bo WANG<sup>1</sup>; <sup>1</sup>Northeastern University

3:40 PM

**Study on Flow-Reaction Desulfurization of RH by Physical Experiment:** *Hongbo Yang*<sup>1</sup>; Jingshe Li<sup>1</sup>; Zengfu Gao<sup>1</sup>; Fangfang Song<sup>1</sup>; Wanliang Yang<sup>1</sup>; <sup>1</sup>USTB

4:00 PM Break

4:10 PM

**Modeling of Transient Fluid Flow, Solidification Processes and Bubble Transport in Continuous Casting Mold:** *Zhongqiu Liu*<sup>1</sup>; Baokuan Li<sup>1</sup>; Maofa Jiang<sup>1</sup>; <sup>1</sup>Northeastern University, China

4:30 PM

**Numerical Analysis of Coupled Fluid Flow, Heat Transfer and Solidification in Ultra-thick Slab Continuous Casting Mold:** *Xin Xie*<sup>1</sup>; Dengfu Chen<sup>1</sup>; Mujun Long<sup>1</sup>; Leilei Zhang<sup>1</sup>; Jialong Shen<sup>1</sup>; Youguang Ma<sup>1</sup>; <sup>1</sup>Chongqing University

4:50 PM

**Numerical Simulations of Inclusion Behavior in a Gas-Stirred Ladle with a CFD-PBM Coupled Model:** *Wentao Lou*<sup>1</sup>; Miaoyong Zhu<sup>1</sup>; <sup>1</sup>Northeastern University

5:10 PM

**Considering Heat Advection in Thin Wall Casting:** *Charles Monroe*<sup>1</sup>; <sup>1</sup>University of Alabama at Birmingham



5:30 PM

**Effect of Free Surface Variation on Intermixed Amount in Continuous Casting Tundish Steelmaking Tundish:** *Pradeep Jha*<sup>1</sup>; Md. Irfanul Siddiqui<sup>1</sup>; <sup>1</sup>IIT Roorkee

5:50 PM

**Measurement and Observation of the Filling Process of Steel Castings:** *Jinwu Kang*<sup>1</sup>; Haimin Long<sup>1</sup>; <sup>1</sup>Tsinghua University

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## **Materials Research Applied to National Needs (MARANN) in Honor of Professor Morris E. Fine: Materials Research Applied to National Needs (MARANN) II**

*Sponsored by:* TMS Structural Materials Division, TMS: Chemistry and Physics of Materials Committee

*Program Organizers:* Peter Liaw, University of Tennessee; Gongyao Wang, University of Tennessee; Semyon Vaynman, Northwestern University; Yip Wah Chung, Northwestern University

Monday PM  
March 4, 2013

Room: 006A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* Semyon Vaynman, Northwestern University

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2:00 PM

**Precipitation-Strengthened Ferritic Steels with Increased Strength and Ductility:** *Semyon Vaynman*<sup>1</sup>; Monica Kapoor<sup>1</sup>; Gautam Ghosh<sup>1</sup>; Dieter Isheim<sup>1</sup>; Yip-Wah Chung<sup>1</sup>; Morris Fine<sup>1</sup>; <sup>1</sup>Northwestern University

2:30 PM

**Steel Research Applied to National Needs - A Company Perspective:** *Shrikant Bhat*<sup>1</sup>; Richard Sussman<sup>1</sup>; <sup>1</sup>ArcelorMittal

3:00 PM

**Investigation on Ferritic Superalloys with Improved Creep Resistance by Computational Design and Experimental Validation:** *Peter Liaw*<sup>1</sup>; Mark Asta<sup>2</sup>; David Dunand<sup>3</sup>; Morris Fine<sup>3</sup>; Gautam Ghosh<sup>3</sup>; Chain Liu<sup>4</sup>; Hong Ding<sup>2</sup>; Shenyan Huang<sup>1</sup>; Michael Michael Rawlings<sup>3</sup>; Zhiqian Sun<sup>1</sup>; Gian Song<sup>1</sup>; Zhenke Teng<sup>1</sup>; Gongyao Wang<sup>1</sup>; Christian Liebscher<sup>2</sup>; <sup>1</sup>University of Tennessee; <sup>2</sup>University of California, Berkeley; <sup>3</sup>Northwestern University; <sup>4</sup>City University of Hong Kong

3:30 PM Break

3:50 PM

**Synchrotron Radiation Mapping of the Indented Fe-added Nickel Aluminide Alloys:** *Tian-Yu Lin*<sup>1</sup>; E-Wen Huang<sup>1</sup>; Morris Fine<sup>2</sup>; Peter Liaw<sup>3</sup>; <sup>1</sup>National Central University; <sup>2</sup>Northwestern University; <sup>3</sup>University of Tennessee

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## **Materials Science in Reduced Gravity: Facilities and Metallic Glasses**

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

*Program Organizers:* Douglas Matson, Tufts University; Robert Hyers, University of Massachusetts Amherst; Hani Henein, University of Alberta

Monday PM  
March 4, 2013

Room: Lone Star Salon E  
Location: Grand Hyatt

*Session Chair:* Hani Henein, University of Alberta - Edmonton

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2:00 PM Introductory Comments

2:10 PM Invited

**DIXI - A Radiography Facility for Materials Science Investigations Onboard ISS:** *Stefan Klein*<sup>1</sup>; Florian Kargl<sup>1</sup>; Andreas Meyer<sup>1</sup>; Christian Stenzel<sup>2</sup>; <sup>1</sup>DLR; <sup>2</sup>Astrium GmbH

2:40 PM

**MASER12-XRMON-GF: A Sounding Rocket Experiment Devoted to the X-Ray Radiographic Observation of Directional Solidification:** *Guillaume Reinhart*<sup>1</sup>; Henri Nguyen-Thi<sup>1</sup>; *Georges Salloum Abou Jaoudé*<sup>1</sup>; Ragnvald Mathiesen<sup>2</sup>; Gerhard Zimmermann<sup>3</sup>; Ylva Houltz<sup>4</sup>; Daniela Voss<sup>5</sup>; <sup>1</sup>IM2NP - Aix-Marseille Univ; <sup>2</sup>NTNU; <sup>3</sup>ACCESS e.V.; <sup>4</sup>Swedish Space Corporation; <sup>5</sup>ESA

3:00 PM

**Drop-Tube Processing of Ni-Si Alloys:** *Andrew Mullis*<sup>1</sup>; Leigang Cao<sup>1</sup>; Robert Cochran<sup>1</sup>; <sup>1</sup>University of Leeds

3:20 PM

**Electromagnetic Levitation Onboard the ISS: The EML Payload:** *Achim Seidel*<sup>1</sup>; Wolfgang Soellner<sup>1</sup>; Christian Stenzel<sup>1</sup>; <sup>1</sup>Astrium

3:40 PM

**Electrostatic Levitation Furnace for ISS:** *Keiji Murakami*<sup>1</sup>; <sup>1</sup>JAXA

4:00 PM Break

4:20 PM Invited

**Microgravity Research on Bulk Metallic Glasses and Composites:** *Douglas Hofmann*<sup>1</sup>; <sup>1</sup>NASA JPL/Caltech

4:50 PM Invited

**Electrostatic Levitation Studies of Cu-Zr Liquids:** *Ken Kelton*<sup>1</sup>; James Bendert<sup>1</sup>; Matthew Blodgett<sup>1</sup>; Anup Gangopadhyay<sup>1</sup>; Nicholas Mauro<sup>1</sup>; <sup>1</sup>Washington University

5:20 PM

**Growth Kinetics of Cu-Zr:** *Jan Gegner*<sup>1</sup>; Raphael Kobold<sup>1</sup>; Fan Yang<sup>1</sup>; Dirk Holland-Moritz<sup>1</sup>; Olga Shuleshova<sup>1</sup>; Dieter Herlach<sup>1</sup>; <sup>1</sup>DLR

5:40 PM

**Fabrication and Optical Properties of Glass and Crystalline Rare-Earth Aluminates by Containerless Levitation Process:** *Malahalli Vijaya Kumar*<sup>1</sup>; Takehiko Ishikawa<sup>1</sup>; Junpei Okada<sup>1</sup>; Yuki Watanabe<sup>2</sup>; Kazuhiko Kuribayashi<sup>3</sup>; <sup>1</sup>Japan Aerospace Exploration Agency; <sup>2</sup>Advanced Engineering Service; <sup>3</sup>Shibaura Institute of Technology

## Mesoscale Computational Materials Science of Energy Materials: Phase Field Modeling and Microstructural Evolutions

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

*Program Organizers:* Pascal Bellon, University of Illinois; Alfredo Caro, LANL; Long Qing Chen, Penn State University; Anter El-Azab, Florida State University; Ming Tang, Lawrence Livermore National Laboratory

Monday PM  
March 4, 2013

Room: 218  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Pascal Bellon, University of Illinois at Urbana-Champaign; Ken Elder, Oakland University

### 2:00 PM Invited

**Multiscale Modeling of Multiferroics Using Phase Field Crystal Modeling and Complex Amplitude Expansions:** *Ken Elder*<sup>1</sup>; <sup>1</sup>Oakland University

### 2:30 PM Invited

**Simulation in 3D of Microstructure-Resolved Thermal Stress Leading to Whisker Formation:** Benjamin Anglin<sup>1</sup>; John Blendell<sup>2</sup>; W.H. (Aska) Chen<sup>2</sup>; Pylon Sarobol<sup>2</sup>; Carol Handwerker<sup>2</sup>; *Anthony Rollett*<sup>1</sup>; <sup>1</sup>Carnegie Mellon University; <sup>2</sup>Purdue University

### 3:00 PM

**Adaptive Atomistic-Phase-Field Dislocation Dynamics Model:** *Lei Cao*<sup>1</sup>; Hojin Kim<sup>1</sup>; Alejandro Strachan<sup>1</sup>; Marisol Koslowski<sup>1</sup>; <sup>1</sup>Purdue University

### 3:20 PM

**Discrete Dislocation Simulations of Taper Effects in Micropillar Compression:** *Babak Kondori*<sup>1</sup>; Amine Benzerga<sup>1</sup>; <sup>1</sup>Texas A&M University

### 3:40 PM Break

### 3:50 PM

**A Nucleation Algorithm in the Coupled Conserved/Non-conserved Phase Field Model:** *Andrea Jokisaari*<sup>1</sup>; Katsuyo Thornton<sup>1</sup>; <sup>1</sup>University of Michigan

### 4:10 PM Invited

**Phase-Field-Crystal Modeling of Nanocrystalline Pattern Evolution:** *Alain Karma*<sup>1</sup>; Ari Adland<sup>1</sup>; <sup>1</sup>Northeastern University

### 4:40 PM

**Modeling and Characterization of 3D Photovoltaics:** *Jon Guyer*<sup>1</sup>; Daniel Josell<sup>1</sup>; <sup>1</sup>NIST

### 5:00 PM

**Diffuse Interface Field Approach (DIFA) to Modeling and Simulation of Capillarity-Related Self-Organization Phenomena in Colloidal Systems:** *Tian-Le Cheng*<sup>1</sup>; Yu Wang<sup>1</sup>; <sup>1</sup>Michigan Technological University

### 5:20 PM

**Prediction of Contact Mechanics for Microsystems by a Multiscale Model with Uncertainties Quantification:** *Hojin Kim*<sup>1</sup>; Alejandro Strachan<sup>1</sup>; <sup>1</sup>Purdue University

### 5:40 PM

**Phase-Field Simulations of Orientation-Dependent GaN Growth By Selective Area Epitaxy:** *Larry Aagesen*<sup>1</sup>; Michael Coltrin<sup>2</sup>; Jung Han<sup>3</sup>; Katsuyo Thornton<sup>1</sup>; <sup>1</sup>University of Michigan; <sup>2</sup>Sandia National Laboratories; <sup>3</sup>Yale University

## Microstructural Processes in Irradiated Materials: Ferritic/Martensitic Steels II

*Sponsored by:* TMS Structural Materials Division, TMS/ASM: Nuclear Materials Committee

*Program Organizers:* Thak Sang Byun, Oak Ridge National Laboratory; Dane Morgan, University of Wisconsin-Madison; Yasuyoshi Nagai, Tohoku University; Zhijie Jiao, University of Michigan-Ann Arbor; Christine Guéneau, CEA-Saclay

Monday PM  
March 4, 2013

Room: 203A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Arthur Motta, Penn State University; Brian Wirth, University of Tennessee

### 2:00 PM Invited

**Multiscale Modeling of Defect Cluster Evolution in Irradiated Structural Materials:** *Brian Wirth*<sup>1</sup>; Donghua Xu<sup>1</sup>; Aaron Kohnert<sup>2</sup>; <sup>1</sup>University of Tennessee; <sup>2</sup>University of California, Berkeley

### 2:30 PM

**Modelling Helium Bubble Nucleation in Alpha-Iron for Thermal Desorption Experiments: A Cluster Dynamics Approach:** Thomas Jourdan<sup>1</sup>; Jean-Paul Crocombette<sup>1</sup>; Sandra Moll<sup>1</sup>; Hélène Lefaix<sup>1</sup>; <sup>1</sup>CEA

### 2:50 PM

**Multi-Scale Modeling of Hydrogen and Helium Bubbles in BCC Iron:** *Erin Hayward*<sup>1</sup>; Chaitanya Deo<sup>2</sup>; Chu Chun Fu<sup>1</sup>; <sup>1</sup>CEA-Saclay; <sup>2</sup>Georgia Institute of Technology

### 3:10 PM

**Influence of Hydrogen and Point Defects in BCC Iron: An Ab Initio Study:** M. Bhatia<sup>1</sup>; *Kiran Solanki*<sup>1</sup>; M. Tschopp<sup>2</sup>; <sup>1</sup>Arizona State University; <sup>2</sup>Mississippi State University

### 3:30 PM Break

### 3:40 PM Invited

**Radiation Damage Using In Situ Charged Particle Irradiation:** *Arthur Motta*<sup>1</sup>; <sup>1</sup>Penn State University

### 4:10 PM

**On the Effects of Helium-DPA Interactions on Microstructural Evolution in Tempered Martensitic Steels: A Summary of In-Situ He Injection Results and a Model Based Analysis:** *Takuya Yamamoto*<sup>1</sup>; Yuan Wu<sup>1</sup>; G. Robert Odette<sup>1</sup>; Richard Kurtz<sup>2</sup>; Danny Edwards<sup>2</sup>; Bo Yao<sup>2</sup>; <sup>1</sup>University of California Santa Barbara; <sup>2</sup>Pacific Northwest National Laboratory

### 4:30 PM

**Role of Helium and Beam Rastering on Swelling Behavior in Ion Irradiated HT9 Steel:** *Elizabeth Beckett*<sup>1</sup>; Gary Was<sup>1</sup>; Zhijie Jiao<sup>1</sup>; Kai Sun<sup>1</sup>; <sup>1</sup>University of Michigan

### 4:50 PM

**Atomistic Modeling of He Embrittlement at Various Grain Boundaries of  $\alpha$ -Fe:** *Tomoaki Suzudo*<sup>1</sup>; Masatake Yamaguchi<sup>1</sup>; Tomohito Tsuru<sup>1</sup>; <sup>1</sup>Japan Atomic Energy Agency

### 5:10 PM

**Atomic Scale Understanding of Defect Sink Property of Grain Boundaries in Fe:** *Di Chen*<sup>1</sup>; Jing Wang<sup>1</sup>; Tianyi Chen<sup>1</sup>; Lin Shao<sup>1</sup>; <sup>1</sup>Texas A&M University

## Modeling and Experimental Validation of Multiscale Mechanical Behavior from Atomic Scale to Macro Scale: Multiscale Deformation Mechanisms

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS Structural Materials Division, TMS: Integrated Computational Materials Engineering Committee, TMS/ASM: Mechanical Behavior of Materials Committee, TMS: Nanomechanical Materials Behavior Committee, TMS: Process Technology and Modeling Committee, TMS: Shaping and Forming Committee

*Program Organizers:* Nathan Mara, Los Alamos National Laboratory; Jian Wang, Los Alamos National Laboratory; Brad Boyce, Sandia National Laboratories; Jennifer Carter, Case Western Reserve University; Anthony Rollett, Carnegie Mellon University; Jonathan Zimmerman, Sandia National Laboratories

Monday PM  
March 4, 2013

Room: 211  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Julia Greer, California Institute of Technology; Scott Mao, University of Pittsburgh

### 2:00 PM Invited

**Fabrication and Deformation in Nanocrystalline and Bi-Crystalline Nano Structures:** *Julia Greer*<sup>1</sup>; X Gu<sup>1</sup>; Peri Landau<sup>1</sup>; Qiang Guo<sup>1</sup>; <sup>1</sup>California Institute of Technology

### 2:30 PM

**EBS and TEM Studies to Inform and Guide the Mechanistic Modelling of Deformation in P22 Steel:** *Dhriti Bhattacharyya*<sup>1</sup>; Pranesh Dayal<sup>1</sup>; Michael Drew<sup>1</sup>; Warwick Payten<sup>1</sup>; Ken Snowden<sup>1</sup>; Robert Harrison<sup>1</sup>; Lyndon Edwards<sup>1</sup>; <sup>1</sup>Australian Nuclear Science and Technology Organization

### 2:50 PM

**Deformation Behavior in Nano-Polycrystalline Zirconium:** Margarita Ruda<sup>1</sup>; *Carlos Ruestes*<sup>2</sup>; Graciela Bertolino<sup>3</sup>; Diana Farkas<sup>4</sup>; Eduardo Bringa<sup>1</sup>; <sup>1</sup>CAB-CNEA; <sup>2</sup>Universidad Nacional de Cuyo; <sup>3</sup>CONICET; <sup>4</sup>Virginia Tech

### 3:10 PM Invited

**Multiscale Modeling of Nanostructured Shape Memory Alloys by Molecular Dynamics, Monte Carlo and Phase Field Methods:** *Ting Zhu*<sup>1</sup>; Yuan Zhong<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

### 3:40 PM

**Analysis of Pole Mechanisms for (10-12) Twin Nucleation in Mg:** *Maryam Ghazisaeidi*<sup>1</sup>; W. A. Curtin<sup>1</sup>; <sup>1</sup>Brown University

### 4:00 PM Break

### 4:10 PM Invited

**Plasticity in Small Volume: Stochastic Not Deterministic:** *Hussien Zbib*<sup>1</sup>; Shuai Shao<sup>1</sup>; Samantha Lawrence<sup>1</sup>; David Bahr<sup>1</sup>; <sup>1</sup>Washington State University

### 4:40 PM

**Size-Related Dislocation Plasticity and Deformation Twinning Behavior in Mg:** *Qian Yu*<sup>1</sup>; Liang Qi<sup>2</sup>; Ju Li<sup>2</sup>; Raj Mishra<sup>3</sup>; Andrew Minor<sup>1</sup>; <sup>1</sup>UC Berkeley; <sup>2</sup>MIT; <sup>3</sup>GM

### 5:00 PM Invited

**Partial Dislocation Controlled Plasticity in Nanometer-Sized Au Single Crystal:** *Scott Mao*<sup>1</sup>; He Zheng<sup>1</sup>; Christopher Weinberger<sup>2</sup>; Jianyu Huang<sup>2</sup>; Li Zhong<sup>1</sup>; <sup>1</sup>Department of Mechanical Engineering and Materials Science, University of Pittsburgh; <sup>2</sup>Sandia National Laboratories

### 5:30 PM

**Strengthening Mechanisms, Nanoscale Precipitation, and Twin Morphology in a High-Strength Bulk Nanostructured Cu-Zn-Al Alloy:** *Haiming Wen*<sup>1</sup>; Troy Topping<sup>1</sup>; Dieter Isheim<sup>2</sup>; David Seidman<sup>2</sup>; Enrique Lavernia<sup>1</sup>; <sup>1</sup>University of California, Davis; <sup>2</sup>Northwestern University

## Modeling of Multi-Scale Phenomena in Materials Processing - III: Microstructure Evolution II

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS/ASM: Computational Materials Science and Engineering Committee, TMS: Process Technology and Modeling Committee, TMS: Integrated Computational Materials Engineering Committee

*Program Organizers:* Adrian Sabau, Oak Ridge National Laboratory; Anthony Rollett, Carnegie Mellon University; Laurentiu Nastac, The University of Alabama; Jonathan Madison, Sandia National Laboratories; Mei Li, Ford Motor Company

Monday PM  
March 4, 2013

Room: 216  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Mei Li, Ford Motor Company; Sergio Felicelli, Mississippi State University

### 2:00 PM Introductory Comments

### 2:05 PM Invited

**Computational Multi-Phase Modeling of Cast Energetic Materials:** *Ruslan Mudryy*<sup>1</sup>; Laurentiu Nastac<sup>2</sup>; <sup>1</sup>US ARMY; <sup>2</sup>The University of Alabama

### 2:50 PM

**Flow Characteristics in Molten Metal Processing Using Ultrasonic Stirring Technology:** *Laurentiu Nastac*<sup>1</sup>; Shian Jia<sup>1</sup>; Xiaoda Liu<sup>1</sup>; <sup>1</sup>The University of Alabama

### 3:15 PM

**Large Scale Parallel Lattice Boltzmann Model of Dendritic Growth:** *Bohumir Jelinek*<sup>1</sup>; Mohsen Eshraghi<sup>1</sup>; Sergio Felicelli<sup>1</sup>; <sup>1</sup>Mississippi State University

### 3:40 PM Break

### 4:10 PM

**Thin Wall Ductile Iron Castings Modeling by Cellular Automaton:** Daniel Gurgul<sup>1</sup>; *Andriy Burchenko*<sup>1</sup>; Marcin Górny<sup>1</sup>; Wojciech Kapturkiewicz<sup>1</sup>; <sup>1</sup>AGH University of Science and Technology

### 4:55 PM

**Coupled Flow-Thermal-Microstructural Modeling of the Scanning Laser Epitaxy Process:** *Ranadip Acharya*<sup>1</sup>; Justin Gambone<sup>1</sup>; Rohan Bansal<sup>1</sup>; Paul Cilino<sup>1</sup>; Suman Das<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

### 5:20 PM

**Modeling of Effective Thermal Conductivities of Cu-Ni Alloy Series as a Function of Temperature in the Liquid Region:** *Shahid Mehmood*<sup>1</sup>; <sup>1</sup>Quaid-e-Azam University Islamabad



## Nanostructured Materials for Lithium Ion Batteries and for Supercapacitors: Nanostructured Materials for Lithium Ion Batteries and for Supercapacitors Session II

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Energy Conversion and Storage Committee  
*Program Organizer:* David Mitlin, University of Alberta and NINT NRC

Monday PM  
March 4, 2013

Room: 007B  
Location: Henry B. Gonzalez Convention Center

*Session Chairs:* Reza Shahbazian-Yassar, Michigan Technological University; David Mitlin, University of Alberta and NINT NRC; Zhi Li, University of Alberta and NINT NRC; Peter Kalisvaart, University of Alberta and NINT NRC

### 2:00 PM Invited

**Graphene-Based and Graphene-Derived Materials for Supercapacitors and Li Ion Batteries:** Rodney Ruoff<sup>1</sup>; *TaeYoung Kim*<sup>1</sup>; <sup>1</sup>The University of Texas at Austin

### 2:20 PM Invited

**Graphene Based Anodes for Li-ion Batteries:** *Nikhil Koratkar*<sup>1</sup>; <sup>1</sup>Rensselaer Polytechnic Institute

### 2:40 PM Invited

**Graphene Oxide Supercapacitors: Computer Simulation Study:** *Hyung Kim*<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

### 3:00 PM Invited

**Asymmetrical Supercapacitor Based on Graphene-Nickel Cobaltite Nanocomposite and Activated Carbon Electrodes with Commercial Level Mass Loading:** *Huanlei Wang*<sup>1</sup>; Chris Holt<sup>1</sup>; Zhi Li<sup>1</sup>; Xuehai Tan<sup>1</sup>; Babak Shalchi Amirkhiz<sup>1</sup>; Zhanwei Xu<sup>1</sup>; Brian C. Olsen<sup>1</sup>; Tyler Stephenson<sup>1</sup>; David Mitlin<sup>1</sup>; <sup>1</sup>University of Alberta and NINT NRC

### 3:20 PM Invited

**Graphene-Based Nano-Composites for Electrochemical Energy Storage:** *Jie Lian*<sup>1</sup>; Xiang Sun<sup>1</sup>; Ming Xie<sup>2</sup>; Steven George<sup>2</sup>; <sup>1</sup>Rensselaer Polytechnic Institute; <sup>2</sup>University of Colorado at Boulder

### 3:40 PM Break

### 4:00 PM Invited

**Controlled Synthesis and Functionalization of Carbon Nanomaterials for Energy Storage:** *Liming Dai*<sup>1</sup>; <sup>1</sup>Case Western Reserve University

### 4:20 PM Invited

**Electrolytes and Electrodes for High-energy Secondary Batteries:** *Lynden Archer*<sup>1</sup>; <sup>1</sup>Cornell University

### 4:40 PM Invited

**Composite Electrodes for Electrochemical Supercapacitors:** *Igor Zhitomirsky*<sup>1</sup>; <sup>1</sup>McMaster University

### 5:00 PM Invited

**Effect of Concentration-Dependent Ductility on Fracture Behavior in Li-alloy Electrode Materials:** Yifan Gao<sup>1</sup>; *Min Zhou*<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology

### 5:20 PM Invited

**Designing Nanostructured Hybrid Materials for Energy Storage Technologies:** *Guihua Yu*<sup>1</sup>; <sup>1</sup>The University of Texas at Austin

### 5:40 PM Invited

**Synthesis of High Voltage Spinel LiNi<sub>0.5</sub>Mn<sub>1.5</sub>O<sub>4</sub> Nano-Powders by the Polyol Process for Lithium Ion Batteries:** *Kyler Carroll*<sup>1</sup>; Hyungman Cho<sup>1</sup>; Hyojung Yoon<sup>1</sup>; Shirley Meng<sup>1</sup>; <sup>1</sup>University of California, San Diego

### 6:00 PM Invited

**Charge Storage in New Electrode and Electrolyte Materials: Surprises and Opportunities:** *Rui Qiao*<sup>1</sup>; Jingsong Huang<sup>2</sup>; Vincent Meunier<sup>3</sup>; Bobby Sumpter<sup>2</sup>; <sup>1</sup>Clemson University; <sup>2</sup>Oak Ridge National Laboratory; <sup>3</sup>Rensselaer Polytechnic Institute

### 6:20 PM Invited

**Enabling High Energy Density Redox Chemistries and 3D Electrode Architectures for Lithium Batteries:** *Jagjit Nanda*<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

### 6:40 PM Invited

**Core-Shell Type Nanowires for Electrodes of Flexible Electrochemical Cells:** *Jung-Kun Lee*<sup>1</sup>; Bo Ding<sup>1</sup>; Junhong Noh<sup>2</sup>; <sup>1</sup>University of Pittsburgh; <sup>2</sup>Korea Research Institute of Chemical Technology

## Neutron and X-ray Studies of Advanced Materials VI: Centennial and Beyond: In Honor of Prof. T.R. Welberry: "What Can We Learn from Diffuse Scattering?"

*Sponsored by:* TMS Structural Materials Division, TMS/ASM: Mechanical Behavior of Materials Committee  
*Program Organizers:* Rozaliya Barabash, Oak Ridge National Laboratory; Xun-Li Wang, City University of Hong Kong; Jaimie Tile, US Air Force Research Laboratory; Gernot Kostorz, ETH Zurich; Brent Fultz, California Institute of Technology; Peter Liaw, University of Tennessee

Monday PM  
March 4, 2013

Room: 209  
Location: Henry B. Gonzalez Convention Center

*Session Chairs:* Thomas Proffen, SNS, Oak Ridge National Laboratory; Darren Goossens, Australian National University

### 2:00 PM Introductory Comments

### 2:05 PM Invited

**Unlocking the 'True' Structure of Complex Materials Using Total Scattering:** *Thomas Proffen*<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory

### 2:25 PM Invited

**Diffuse Scattering Studies Supported by Ab-Initio Calculations:** *Matthias Gutmann*<sup>1</sup>; <sup>1</sup>Rutherford Appleton Laboratory

### 2:45 PM Invited

**Investigating Disorder as a Matter of Routine?:** *Thomas Weber*<sup>1</sup>; <sup>1</sup>ETH Zurich

### 3:05 PM Invited

**Local Structure and Dynamics of Quantum Paraelectric Perovskites:** *Marek Paszciak*<sup>1</sup>; Richard Welberry<sup>2</sup>; Jiri Hlinka<sup>1</sup>; <sup>1</sup>Academy of Sciences of the Czech Republic; <sup>2</sup>Australian National University

### 3:25 PM Invited

**Modulated Structures, Functional Materials and the TEM: from Relaxor Ferroelectrics to Nano Chessboards:** *Ray Withers*<sup>1</sup>; <sup>1</sup>The Australian National University

### 3:45 PM Break

### 3:55 PM Invited

**Combined Diffraction and Computational Modelling Studies of Structural Disorder in Energy Storage Materials:** *Bill David*<sup>1</sup>; <sup>1</sup>ISIS Neutron Source

**4:15 PM Invited**

**Distinguishing Types of Disorder in Diffuse Scattering: A Numerical Study:** *Darren Goossens*<sup>1</sup>; T Welberry<sup>1</sup>; <sup>1</sup>Australian National University

**4:35 PM Invited**

**Inter-Slab Interactions and Disorder in Gd<sub>5</sub>Si<sub>4</sub>-xBi:** *Branton Campbell*<sup>1</sup>; Volodymyr Svitlyk<sup>2</sup>; Yuriy Mozharivskyj<sup>2</sup>; <sup>1</sup>Brigham Young University; <sup>2</sup>McMaster University

**4:55 PM Invited**

**Structural Analysis of Complex Materials:** *Takeshi Egami*<sup>1</sup>; <sup>1</sup>University of Tennessee

**5:15 PM Invited**

**X-Ray Scattering from Amorphous Solids:** *Zbigniew Stachurski*<sup>1</sup>; <sup>1</sup>Australian National University

**5:35 PM Invited**

**Beyond the Structure: Investigating Properties in Molecular Materials:** *Lynne Thomas*<sup>1</sup>; <sup>1</sup>University of Bath

**5:55 PM Invited**

**Pair Distribution Function Measurements of Functional Materials:** *Peter Chupas*<sup>1</sup>; <sup>1</sup>Argonne National Laboratory

**Ni-Co 2013: Ni Laterite Hydrometallurgy**

*Sponsored by:* The Minerals, Metals and Materials Society, Metallurgical Society of the Canadian Institute of Mining Metallurgy and Petroleum, Chinese Society for Metals, GDMB Society for Mining, Metallurgy, Resource and Environmental Technology, Society for Mining Metallurgy and Exploration, Mining and Materials Processing Institute of Japan, Associacao Brasileira de Metalurgia, Materiais e Mineracao, Southern African Institute of Mining and Metallurgy (SAIMM), Minerals Engineering International Online, Cobalt Development Institute, Societe Francaise de Metallurgie et de Materiaux, TMS Extraction and Processing Division, TMS: Hydrometallurgy and Electrometallurgy Committee, TMS: Pyrometallurgy Committee  
*Program Organizer:* Thomas Battle, Midrex Technologies

Monday PM  
March 4, 2013

Room: 007D  
Location: Henry B. Gonzalez Convention Center

*Session Chairs:* Shafiq Alam, Memorial University of Newfoundland; Corby Anderson, Colorado School of Mines

**2:00 PM**

**Acid Leaching of Nickel Laterites with Jarosite Precipitation:** *David White*<sup>1</sup>; James Gillaspie<sup>2</sup>; <sup>1</sup>Snowden Mining Industry Consultants; <sup>2</sup>Freeport-McMoRan Copper & Gold Inc.

**2:25 PM**

**Extraction of Nickel, Cobalt and Iron from Laterite Ores by Mixed Chloride Leach Process:** *V.I. Lakshmanan*<sup>1</sup>; Ram Sridhar<sup>1</sup>; Jonathan Chen<sup>1</sup>; Robert DeLaat<sup>1</sup>; M.A. Halim<sup>1</sup>; Raja Roy<sup>1</sup>; <sup>1</sup>Process Research Ortech Inc.

**2:50 PM**

**Pilot Plant Study on the Nitric Acid Pressure Leaching Technology for Limonitic Laterite Ores:** Baozhong Ma<sup>1</sup>; *Chengyan Wang*<sup>1</sup>; Weijiao Yang<sup>1</sup>; Bo Yang<sup>1</sup>; Fei Yin<sup>1</sup>; Yongqiang Chen<sup>1</sup>; Yongqiang Yang<sup>1</sup>; <sup>1</sup>Beijing General Research Institute of Mining and Metallurgy

**3:15 PM**

**Reductive Leaching of Limonitic Laterites Using Ferrous Sulphate:** *Mariela Zuniga*<sup>1</sup>; Edouard Asselin<sup>1</sup>; <sup>1</sup>University of British Columbia

**3:40 PM Break**

**4:00 PM**

**Sulfuric Acid Leaching Characteristics of Ni-Doped Goethite:** *Guanghui Li*<sup>1</sup>; Wen Cai<sup>1</sup>; Mingjun Rao<sup>1</sup>; Qian Zhi<sup>1</sup>; Tao Jiang<sup>1</sup>; <sup>1</sup>School of Minerals Processing and Bioengineering, Central South University

**4:20 PM**

**Characteristics of Nickel Laterite Crushed Ore Agglomerates:** Adirek Janwong<sup>1</sup>; Nikhil Dhawan<sup>1</sup>; Thien Vethsodsakda<sup>1</sup>; *Michael Moats*<sup>2</sup>; <sup>1</sup>University of Utah; <sup>2</sup>Missouri University of Science and Technology

**4:40 PM**

**Update and Outlook of Hydrometallurgical Process for Nickel Laterite Ore:** *Yoshitomo Ozaki*<sup>1</sup>; Sumitomo Metal Mining Co., Ltd.

**5:00 PM**

**Recovery of High Purity Metals Using Molecular Recognition Technology:** Neil Izatt<sup>1</sup>; Ronald Bruening<sup>1</sup>; *Steven Izatt*; <sup>1</sup>IBC Advanced Technologies, Inc.

**Novel Synthesis and Consolidation of Powder Materials : Thermal Spray and Cold Spray Processing**

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS: Powder Materials Committee  
*Program Organizers:* Ma Qian, The University of Queensland; Iver Anderson, The Ames Laboratory

Monday PM  
March 4, 2013

Room: Lone Star Salon C  
Location: Grand Hyatt

*Session Chairs:* Iver Anderson, The Ames Laboratory; Mingxing Zhang, The University of Queensland

**2:00 PM Keynote**

**Thermal Spray as a Consolidation Process to Form Advanced Materials: Future Horizons:** *Christopher Berndt*<sup>1</sup>; Mitchell Sesso<sup>2</sup>; Andrew Ming<sup>2</sup>; <sup>1</sup>Swinburne University of Technology ; <sup>2</sup>Swinburne University of Technology

**2:40 PM**

**Cold Spray Processing of Bulk Nanocrystalline Aluminum AA5083:** Enrique Barrera<sup>1</sup>; *Andres Rodela*<sup>1</sup>; David Chan<sup>1</sup>; George Kim<sup>2</sup>; Enrique Laverna<sup>3</sup>; Victor Champagne<sup>4</sup>; <sup>1</sup>Rice University; <sup>2</sup>Perpetual Technologies; <sup>3</sup>University of California, Davis; <sup>4</sup>Army Research Laboratory

**3:00 PM**

**Cold Spray Synthesis Of Nanodiamond-Reinforced Aluminum Composites:** *Luke Brewer*<sup>1</sup>; Brian Sneed<sup>1</sup>; Filipe Peerally<sup>1</sup>; Dong Jin Woo<sup>1</sup>; Joseph Hooper<sup>1</sup>; Sebastian Osswald<sup>1</sup>; <sup>1</sup>Naval Postgraduate School

**3:20 PM Break**

**3:40 PM Invited**

**Development of a Novel Direct Manufacturing Technology Via Cold Spray Route:** *Stefan Gulizia*<sup>1</sup>; Mahnaz Jahedi<sup>2</sup>; Saden Zahiri<sup>2</sup>; Andrew Urban<sup>2</sup>; Darren Fraser<sup>2</sup>; Tang Caixian<sup>2</sup>; <sup>1</sup>CSIRO Materials Science & Engineering/Future Manufacturing Flagship; <sup>2</sup>CSIRO Materials Science & Engineering

**4:10 PM**

**Synthesis of Nickel-Encapsulated Particles for High-Strain-Rate Deposition in Cold-Spray:** Maryam Neshastehriz; *Ivi Smid*<sup>1</sup>; Al Segall<sup>1</sup>; Lisa Stark<sup>1</sup>; Tim Eden<sup>1</sup>; <sup>1</sup>Penn State

4:30 PM

**Hot Deformation Behavior of Spray Formed FGH4095 Superalloy during Compression at Elevated Temperature:** *Xu Yi*<sup>1</sup>; <sup>1</sup>Southwest Jiaotong University

4:50 PM Invited

**Development of Novel Packed Powder Diffusion Coating Techniques for Light Alloys:** *Mingxing Zhang*<sup>1</sup>; Shoumou Miao<sup>1</sup>; <sup>1</sup>The University of Queensland

## Pb-free Solders and Emerging Interconnect and Packaging Technologies: 3D Interconnect and Novel Packaging Approaches

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Electronic Packaging and Interconnection Materials Committee

*Program Organizers:* Nikhilesh Chawla, Arizona State University; Srinivas Chada, Whirlpool; Darrel Frear, Freescale Semiconductor; John Elmer, LLNL; Tae-Kyu Lee, Cisco Systems; Yan Li, Intel; Laura Turbini, Research In Motion; Kwang-Lung Lin, National Cheng Kung University; Sohoon Yoo, Korea Institute of Industrial Technology

Monday PM  
March 4, 2013

Room: 217B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chair:* To Be Announced

2:00 PM

**Au and Pd Embrittlement in Space-Confining Soldering Reactions for 3D IC Applications:** *Yu-Jen Chen*<sup>1</sup>; C. Robert Kao<sup>1</sup>; <sup>1</sup>National Taiwan University

2:20 PM

**Comparison and Optimization of Mechanical Stresses in Cu Through-Silicon Via (TSV) as Revealed by Synchrotron X-ray Microdiffraction for 3-D Integration:** *Arief Budiman*<sup>1</sup>; H. Shin<sup>2</sup>; K. Byun<sup>3</sup>; K. Hummler<sup>4</sup>; Tian Tian<sup>5</sup>; Y. Joo<sup>2</sup>; Larry Smith<sup>4</sup>; N. Tamura<sup>6</sup>; <sup>1</sup>Los Alamos National Laboratory (LANL); <sup>2</sup>Seoul National University (SNU); <sup>3</sup>SK Hynix Inc.; <sup>4</sup>SEMATECH; <sup>5</sup>UCLA; <sup>6</sup>Advanced Light Source (ALS)

2:40 PM

**Cu-Sn Intermetallics and Voids Formation: Is Cu-Sn an Option for 3D Interconnect?:** *George Vakanas*<sup>1</sup>; Wenqi Zhang<sup>2</sup>; Kenneth Rebibis<sup>2</sup>; Eric Beyne<sup>2</sup>; Fay Hua<sup>3</sup>; Kabirkumar Mirpuri<sup>3</sup>; Paul Zimmerman<sup>3</sup>; <sup>1</sup>IMEC/INTEL; <sup>2</sup>IMEC; <sup>3</sup>Intel Corp

3:00 PM

**Fabrication of nEarly Void-Free Cu<sub>3</sub>Sn Microbumps for 3D IC Packaging:** *Wei-Lan Chiu*<sup>1</sup>; Chih Chen<sup>1</sup>; <sup>1</sup>NCTU

3:20 PM Break

3:40 PM Invited

**Fluxless Bonding of Silicon to Aluminum Using Tin and Silver-Indium System:** *Chin Lee*<sup>1</sup>; Shou-Jen Hsu<sup>1</sup>; Yuanyun Wu<sup>1</sup>; <sup>1</sup>University of California, Irvine

4:00 PM

**Low-Temperature Bonding Technique Using Cu Nanoparticles:** *Toshitaka Ishizaki*<sup>1</sup>; Ryota Watanabe<sup>1</sup>; Toshikazu Satoh<sup>1</sup>; Kunio Akedo<sup>1</sup>; <sup>1</sup>Toyota Central R&D Laboratories Inc.

4:20 PM

**Interfacial Reaction of TSV Filled Sn Alloy and Cu Pillar Bump:** *Young-Ki Ko*<sup>1</sup>; Myong-Suk Kang<sup>2</sup>; Hiroyuki Kokawa<sup>3</sup>; Yutaka Sato<sup>3</sup>; Chang-Woo Lee<sup>1</sup>; Sehoon Yoo<sup>1</sup>; <sup>1</sup>KITECH/Micro-Joining Center; <sup>2</sup>University of Science and Technology; <sup>3</sup>Tohoku University

4:40 PM

**Undercooling of Pb-Free Alloys: Solder Size and Configuration System Effect:** *Fiqiri Hodaj*<sup>1</sup>; <sup>1</sup>Grenoble Institute of Technology

## Phase Stability, Phase Transformations, and Reactive Phase Formation in Electronic Materials XII: Phase Equilibria and Transformations of the Pb-free Solders and Energy Materials

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Alloy Phases Committee

*Program Organizers:* Chao-hong Wang, National Chung Cheng University; Chih-Ming Chen, National Chung Hsing University; Jae-Ho Lee, Hongik University; Ikuro Ohnuma, Tohoku University; Clemens Schmetterer, TU Bergakademie Freiberg; Yee-Wen Yen, National Taiwan University of Science and Technology; Shien-Ping Feng, The University of Hong Kong; Shih-Kang Lin, National Cheng Kung University

Monday PM  
March 4, 2013

Room: 203B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Clemens Schmetterer, Forschungszentrum Juelich GmbH; Ikuro Ohnuma, Tohoku University

2:00 PM Invited

**Characteristics of Beta/Alpha Transformations in High Purity Tin:** *Kazuhiro Nogita*<sup>1</sup>; Christopher Gourlay<sup>2</sup>; Stuart McDonald<sup>1</sup>; Shoichi Suenaga<sup>3</sup>; Jonathan Read<sup>1</sup>; Guang Zeng<sup>1</sup>; Qinfen Gu<sup>4</sup>; <sup>1</sup>The University of Queensland; <sup>2</sup>Imperial College, London; <sup>3</sup>Nihon Superior Co, Ltd.; <sup>4</sup>Australian Synchrotron

2:20 PM Invited

**Experimental Thermodynamics of Ni-Sn-Zn as a New HT LF-Solder System:** *Hans Flandorfer*<sup>1</sup>; Divakar Rajamohan<sup>1</sup>; Siegfried Fürtauer<sup>1</sup>; Herbert Ipser<sup>1</sup>; <sup>1</sup>University of Vienna

2:40 PM

**Effect of Zn, Au and In on the Phase Stability and Thermal Expansion of Cu<sub>6</sub>Sn<sub>5</sub> Intermetallics:** *Guang Zeng*<sup>1</sup>; Stuart McDonald<sup>1</sup>; Qinfen Gu<sup>2</sup>; Kazuhiro Nogita<sup>1</sup>; <sup>1</sup>The University of Queensland; <sup>2</sup>The Australian Synchrotron

2:55 PM

**Metastable Intermetallics in Sn-Ni Couples:** *Sergey Belyakov*<sup>1</sup>; C. Gourlay<sup>1</sup>; <sup>1</sup>Imperial College London

3:10 PM

**Experimental Study and Thermodynamic Assessment of Ternary Cu-Pd-Sn Phase Relations Focused on the Sn-Rich Region:** *Md. Arifur Rahman*<sup>1</sup>; Cheng-En Ho<sup>1</sup>; Wojciech Gierlotka<sup>1</sup>; <sup>1</sup>Yuan Ze University

3:25 PM

**Thermodynamic Modeling of the Ternary Ag-Sb-Te System:** *Wojciech Gierlotka*<sup>1</sup>; Md. Arifur Rahman<sup>1</sup>; <sup>1</sup>YuanZe University

3:40 PM Break

3:55 PM Invited

**Experimental and Theoretical Study of the In-Ni-Sn System:** *Clemens Schmetterer*<sup>1</sup>; Divakar Rajamohan<sup>2</sup>; Ales Kroupa<sup>3</sup>; Adela Zemanova<sup>3</sup>; Herbert Ipser<sup>2</sup>; Hans Flandorfer<sup>2</sup>; <sup>1</sup>Forschungszentrum Juelich; <sup>2</sup>University of Vienna; <sup>3</sup>Academy of Sciences of the Czech Republic

4:15 PM Invited

**Calorimetric Investigation of the Lithium-Manganese-Oxygen Cathode Material System for Lithium Ion Batteries:** *Damian Cupid*<sup>1</sup>; Alexandra Reif<sup>1</sup>; Hans Seifert<sup>1</sup>; <sup>1</sup>Karlsruhe Institute of Technology



4:35 PM

**New Phase in Stoichiometric Cu<sub>6</sub>Sn<sub>5</sub> and Effect of Ni Addition on Phase Stabilization in Wide Temperature Range:** *Yueqin Wu*<sup>1</sup>; John Barry<sup>2</sup>; Tomokazu Yamamoto<sup>3</sup>; Qinfen Gu<sup>4</sup>; Han Huang<sup>1</sup>; Syo Matsumura<sup>3</sup>; Kazuhiro Nogita<sup>1</sup>; <sup>1</sup>The University of Queensland; <sup>2</sup>Queensland University of Technology; <sup>3</sup>Kyushu University; <sup>4</sup>The Australian Synchrotron

4:50 PM

**Superhydrophobic Coating of Chemical Functionalized Nickel Hydroxide Nanostructures on Transparent Conductive Substrates:** *Shien Ping Feng*<sup>1</sup>; Ya-Huei Chang<sup>1</sup>; <sup>1</sup>The University of Hong Kong

5:05 PM

**Phase Relations and Thermodynamic Data in the System Cu-Li-Sn and the Binary Constituent Systems:** *Siegfried Fürtauer*<sup>1</sup>; Andriy Yakymovych<sup>1</sup>; Erdenebat Tserenjav<sup>2</sup>; Hans Flandorfer<sup>1</sup>; <sup>1</sup>University of Vienna; <sup>2</sup>University of Mongolia

5:20 PM

**Thermoelectric Performance of Spark-Plasma-Sintering Bi<sub>2</sub>Te<sub>3</sub> System:** *Ting-Chun Chen*<sup>1</sup>; Albert Wu<sup>1</sup>; <sup>1</sup>National Central University

## Phase Transformation and Microstructural Evolution: General Phase Transformations - Non-Ferrous: Part I

*Sponsored by:* TMS Materials Processing and Manufacturing Division, TMS: Chemistry and Physics of Materials Committee, TMS/ASM: Computational Materials Science and Engineering Committee, TMS: Integrated Computational Materials Engineering Committee, TMS/ASM: Phase Transformations Committee, TMS: Process Technology and Modeling Committee, ASM: Alloy Phase Diagrams Committee

*Program Organizers:* Amy Clarke, Los Alamos National Laboratory; Sudarsanam Suresh Babu, Ohio State Univ; Rajarshi Banerjee, Univ of North Texas; John Morral, Ohio State University; Brian Gleeson, University of Pittsburgh; Carelyn Campbell, National Institute of Standards & Tech; Yongho Sohn, University of Central Florida; Yunzhi Wang, Ohio State University

Monday PM  
March 4, 2013

Room: 204B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Srinivasan Srivilliputhur, University of North Texas; Peter Collins, University of North Texas

2:00 PM Invited

**Phase Transformations and Microstructure Evolution in Two-Phase Titanium Alloys:** Taewook Heo<sup>1</sup>; Yanzhou Ji<sup>1</sup>; Donald Shih<sup>2</sup>; *Long Qing Chen*<sup>1</sup>; <sup>1</sup>Pennsylvania State University; <sup>2</sup>Boeing Company

2:30 PM Invited

**The Formation Mechanism of Precipitate Plates and the Role of Micro-Alloying Elements in Magnesium and Aluminum Alloys:** *Jian-Feng Nie*<sup>1</sup>; <sup>1</sup>Monash University

3:00 PM

**Alpha Nucleation Mediated by Boride Precipitates in Titanium Alloys:** *Peeyush Nandwana*<sup>1</sup>; Niraj Gupta<sup>1</sup>; Priya Gopal<sup>1</sup>; Soumya Nag<sup>1</sup>; Jaimie Tiley<sup>2</sup>; Srivilliputhur Srinivasan<sup>1</sup>; Rajarshi Banerjee<sup>1</sup>; <sup>1</sup>UNT; <sup>2</sup>Air Force Research Laboratory

3:20 PM

**Compositionally Dependent Displacive Transformation from Beta to Omega Phase in Titanium Alloys:** *Soumya Nag*<sup>1</sup>; Robert Williams<sup>2</sup>; Arun Devaraj<sup>3</sup>; Niraj Gupta<sup>1</sup>; Jaimie Tiley<sup>4</sup>; Srinivasan Srivilliputhur<sup>1</sup>; Hamish Fraser<sup>2</sup>; Rajarshi Banerjee<sup>1</sup>; <sup>1</sup>University of North Texas; <sup>2</sup>Ohio State University; <sup>3</sup>Pacific Northwest National Laboratory; <sup>4</sup>Air Force Research Laboratory

3:40 PM Break

4:00 PM

**Crystallographic and Energetic Prediction for Variant Selection of Grain Boundary Alpha in Titanium Alloys:** *Rongpei Shi*<sup>1</sup>; Vikas Dixit<sup>1</sup>; Ning Zhou<sup>2</sup>; Hamish Fraser<sup>1</sup>; Yunzhi Wang<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>GE Global Research Center

4:20 PM

**Grain-Boundary Parameters Controlled Evolution of Allotriomorphic Alpha in Beta-Processed Titanium Alloys:** *Vikas Dixit*<sup>1</sup>; Rongpei Shi<sup>1</sup>; G.B. Viswanathan<sup>2</sup>; Yunzhi Wang<sup>1</sup>; W.A.T. Clark<sup>1</sup>; Hamish Fraser<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>Air Force Research Laboratory

4:40 PM

**Influence of Heat Treatment on Microstructure and Tensile Properties of Massively Transformed High-Ta TiAl Alloys:** *Zhijin Cai*<sup>1</sup>; Huimin Lu<sup>1</sup>; Chenguang Tian<sup>1</sup>; <sup>1</sup>Beihang University

5:00 PM

**Microstructural Evolutions of the Earliest and Intermediate Stages of the Equiaxed Alpha Particles in  $\alpha + \beta$  Processed Titanium Alloys:** *Iman Ghamarian*<sup>1</sup>; Brian Welk<sup>2</sup>; P. Collins<sup>1</sup>; <sup>1</sup>University of North Texas; <sup>2</sup>The Ohio State University

5:20 PM

**Formation of Transformation Texture in Supertransus Heat Treated Ti-6Al-2Sn-4Zr-6Mo:** *Gordon Sargent*<sup>1</sup>; Adam Pilchak<sup>2</sup>; Christopher Szczepanski<sup>2</sup>; Kacey Kinsel<sup>3</sup>; Lee Semiatin<sup>2</sup>; <sup>1</sup>Consultant; <sup>2</sup>Air Force Research Laboratory; <sup>3</sup>Wright State University

## Physical and Mechanical Metallurgy of Shape Memory Alloys: Novel and NiTi-based Shape Memory Alloys

*Sponsored by:* TMS/ASM: Phase Transformations Committee  
*Program Organizers:* Haluk Karaca, University of Kentucky; Ibrahim Karaman, Texas A&M University; Othmane Benafan, NASA Glenn Research Center; Ryosuke Kainuma, Tohoku University; Hans Jurgen Maier, University of Paderborn

Monday PM  
March 4, 2013

Room: Lone Star Salon B  
Location: Grand Hyatt

*Session Chairs:* Haluk Karaca, University of Kentucky; Hideki Hosoda, Tokyo Institute of Technology

2:00 PM

**Phase Constitution, Mechanical and Shape Memory Properties of (Pt,Co)Ti Alloys:** *Hideki Hosoda*<sup>1</sup>; Satoshi Tsutsumi<sup>1</sup>; Masaki Tahara<sup>1</sup>; Tomonari Inamura<sup>1</sup>; Yoko Yamabe-Mitarai<sup>2</sup>; <sup>1</sup>Tokyo Institute of Technology; <sup>2</sup>National Institute of Materials Science

2:20 PM

**Mechanical and Material Characterization of Ternary Nitinol Alloys:** *Chandan Pulletikurthi*<sup>1</sup>; Puneet Gill<sup>1</sup>; Norman Munroe<sup>1</sup>; Amit Datye<sup>2</sup>; <sup>1</sup>Florida International University; <sup>2</sup>The University of Tennessee

2:40 PM

**Effect of Heat Treatment on Deformation Behavior of Ti-Au-Cr-Zr Shape Memory Alloys:** *Yuri Shinohara*<sup>1</sup>; Masaki Tahara<sup>1</sup>; Tomonari Inamura<sup>1</sup>; Hideki Hosoda<sup>1</sup>; Shuichi Miyazaki<sup>2</sup>; <sup>1</sup>Tokyo Institute of Technology; <sup>2</sup>University of Tsukuba

3:00 PM

**Martensitic Transformation in Co-Cr-Al-Si System:** *Kenji Hirata*<sup>1</sup>; Xiao Xu<sup>1</sup>; Makoto Nagasako<sup>1</sup>; Toshihiro Omori<sup>1</sup>; Ryosuke Kainuma<sup>1</sup>; <sup>1</sup>Tohoku University

3:20 PM

**Effect of Oxygen Addition on Microstructure and Shape Memory Behavior of Ti-Nb Alloy:** *Masaki Tahara*<sup>1</sup>; Tomonari Inamura<sup>1</sup>; Hee Young Kim<sup>2</sup>; Hideki Hosoda<sup>1</sup>; Shuichi Miyazaki<sup>2</sup>; <sup>1</sup>Tokyo Institute of Technology; <sup>2</sup>University of Tsukuba

3:40 PM

**Elastic Deformation in Fe-31.2Pd (at.%) Alloy Exhibiting Lattice Softening:** *Fei Xiao*<sup>1</sup>; Takashi Fukuda<sup>1</sup>; Tomoyuki Kakeshita<sup>1</sup>; <sup>1</sup>Osaka University

4:00 PM Break

4:20 PM

**Effects of Heat Treatments and Applied Stress on the Shape Memory Behavior of Highly Ni-Rich NiTi Alloys:** *Irfan Kaya*<sup>1</sup>; Hirobumi Tobel<sup>1</sup>; Haluk Karaca<sup>1</sup>; Makoto Nagasako<sup>2</sup>; Ryosuke Kainuma<sup>2</sup>; <sup>1</sup>University of Kentucky; <sup>2</sup>Tohoku University

4:40 PM

**Effect of Precipitates on Cyclic Actuation Response of Ni<sub>50.7</sub>Ti<sub>49.3</sub> Shape Memory Alloys:** *Ceylan Hayrettin*<sup>1</sup>; Ibrahim Karaman<sup>1</sup>; Ebubekir Dogan<sup>1</sup>; James Mabe<sup>2</sup>; David Rodin<sup>1</sup>; <sup>1</sup>Texas A&M University; <sup>2</sup>Boeing Phantom Works

5:00 PM

**Fatigue Analysis of Laser-Treated Nitinol Wires:** *Janet Gbur*<sup>1</sup>; Hossein Lavvafi<sup>1</sup>; Melissa Young<sup>2</sup>; John J Lewandowski<sup>1</sup>; <sup>1</sup>Case Western Reserve University; <sup>2</sup>Cleveland Clinic

5:20 PM

**Effect of Cold Working Rate on Shape Memory Characteristics of Ti-50.4 at.% Ni Alloy with Time Gradient Annealing:** *Won Ki Ko*<sup>1</sup>; Chang Suk Bae<sup>1</sup>; Jae Il Kim<sup>1</sup>; <sup>1</sup>Donga-A University

5:40 PM

**Mechanical Properties of NiTi42.5Cu7.5 (wt.%) Shape Memory Alloy during Aging Heat Treatment:** *Emad Omrani*<sup>1</sup>; Ali Shokuhfar<sup>2</sup>; <sup>1</sup>University of Wisconsin - Milwaukee; <sup>2</sup>K.N. Toosi University of Technology

## Production, Refining and Recycling of Rare Earth Metals: Production, Refining and Recycling of Rare Earth Metals

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS Extraction and Processing Division, TMS Materials Processing and Manufacturing Division, TMS: Magnetic Materials Committee, TMS: Process Technology and Modeling Committee  
*Program Organizers:* Lifeng Zhang, University of Science and Technology Beijing; Oliver Gutfleisch, IFW Dresden; Jeffrey S. Spangenberg, Argonne National Laboratory

Monday PM  
March 4, 2013

Room: 006B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Lifeng Zhang, University of Science and Technology Beijing; Jeffrey S. Spangenberg, Argonne National Laboratory

2:00 PM

**Enrichment of Rare Earth Elements from Neodymium Magnet by Liquid Phase Separation in Nd<sub>2</sub>O<sub>3</sub>-B<sub>2</sub>O<sub>3</sub> System:** *Hidehiro Sekimoto*<sup>1</sup>; Takahiro Kubo<sup>1</sup>; Katsunori Yamaguchi<sup>1</sup>; <sup>1</sup>Iwate University

2:20 PM

**Intrinsic Magnetic Properties of Alloys Synthesized from Recycled Rare Earth Metals:** *Ryan Ott*<sup>1</sup>; Larry Jones<sup>2</sup>; Kevin Dennis<sup>2</sup>; R. McCallum<sup>2</sup>; <sup>1</sup>Ames Laboratory (USDOE); <sup>2</sup>Ames Laboratory (USDOE)

2:40 PM

**Rare Earth Extraction by Molten Oxide Electrolysis:** *Guillaume Lambotte*<sup>1</sup>; Tessa Green<sup>1</sup>; Rachel DeLucas<sup>1</sup>; Yen Yeh<sup>1</sup>; Donald Sadoway<sup>1</sup>; Antoine Allanore<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology

3:00 PM

**Recycling of Different Sintered Magnet Grades by Hydrogen Processing Yielding Anisotropic Resin Bonded Magnets:** *Konrad G  th*<sup>1</sup>; Thomas George Woodcock<sup>1</sup>; Oliver Gutfleisch<sup>2</sup>; <sup>1</sup>IFW Dresden; <sup>2</sup>Technical University of Darmstadt

3:20 PM

**Thermodynamic Modeling of Nd Extraction from FeNdB Magnet:** *Marie-Aline Van Ende*<sup>1</sup>; *In-Ho Jung*<sup>1</sup>; <sup>1</sup>McGill University

3:40 PM

**The Ternary System Thermodynamics of Phase Diagram Analysis of Cerium Rare Earth Oxides in Supercritical Water:** *Hongxu Li*<sup>1</sup>; chao Li<sup>1</sup>; Chuanqi Jiao<sup>1</sup>; Yu Chen<sup>1</sup>; <sup>1</sup>University of Science and Technology

4:00 PM

**Removing Aluminum from Chlorinated Rare Earth Solution by Hydrolysis:** *Shufang Ding*<sup>1</sup>; Wei Chen<sup>2</sup>; Cuicui Ji<sup>2</sup>; Zhiqiang Shan<sup>3</sup>; Fukun Yan<sup>3</sup>; <sup>1</sup>Heilongjiang Institute of Science and Technology; <sup>2</sup>Heilongjiang Institute of Science and Technology; <sup>3</sup>Heilongjiang Institute of Science and Technology

4:20 PM

**Synthesis of a New Asymmetric Dialkylphosphinic Acid and Its Extraction and Separation Performance for Rare Earth Metals in HNO<sub>3</sub> Solutions:** *Shengming Xu*<sup>1</sup>; Junlian Wang; Linyan Li; Gang Xu; <sup>1</sup>Tsinghua University

## Recent Developments in Biological, Electronic, and Functional Thin Films and Coatings: Biological, Electronic, and Functional Thin Films and Coatings II

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Thin Films and Interfaces Committee  
*Program Organizers:* R. Narayan, UNC/NCSU Joint Department of Biomedical Engineering; Choong-Un Kim, University of Texas at Arlington; Jian Luo, Clemson University; Nancy Michael, University of Texas at Arlington; Nuggehalli Ravindra, New Jersey Institute of Technology; Adele Carrado, IPCMS

Monday PM  
 March 4, 2013  
 Room: 214D  
 Location: Henry B. Gonzalez Convention Center

*Session Chair:* Choong-un Kim, UT Arlington

### 2:00 PM

**Advanced Plasma-Based Nanocoatings for the Innovation in Cardiovascular Devices:** *Diego Mantovani*<sup>1</sup>; <sup>1</sup>Laval University

### 2:40 PM Invited

**Using Nanoscale Building Blocks to Make Electronic and Photonic Devices:** *Federico Rosei*<sup>1</sup>; <sup>1</sup>INRS

### 3:20 PM

**Improved Mobility and Transmittance of Room Temperature Deposited a-IGZO Films with Low Temperature Post-Fabrication Anneals:** *Terry Alford*<sup>1</sup>; Mandar Gadre<sup>2</sup>; Rajitha Vemuri<sup>1</sup>; <sup>1</sup>Arizona State University; <sup>2</sup>Solidigm Inc.

### 3:40 PM Break

### 4:00 PM

**Growth and Characterization of Lu<sub>2</sub>O<sub>3</sub>:Eu<sup>3+</sup> Thin Film on Single Crystal Yttria-Doped Zirconia Substrates:** *Sudesna Roy*<sup>1</sup>; Stephen Topping<sup>1</sup>; Vinod Sarin<sup>1</sup>; <sup>1</sup>Boston University

### 4:20 PM

**Optical Emission of Doped Sol-Gel Films Deposited on Silicon:** *Sufian Abedrabbo*<sup>1</sup>; Bashar Lahlouh; Hassan Juwhari; Oktay Gokce; Anthony Fiory; Nuggehalli Ravindra; <sup>1</sup>University of Jordan

### 4:40 PM

**Production and Characterization of Cerium-Based Conversion Coatings on Galvanized Steel and Aluminum Alloys:** *Carlos Castano*<sup>1</sup>; Surender Maddela<sup>1</sup>; Matthew O'Keefe<sup>1</sup>; <sup>1</sup>Missouri University of Science and Technology

### 5:00 PM

**Solution-Based Method to Fabricate Diamond-Like Carbon Nanocomposite Coatings:** *Vasiliki Poenitzsch*<sup>1</sup>; Carol Ellis-Terrell<sup>1</sup>; Ronghua Wei<sup>1</sup>; Kent Coulter<sup>1</sup>; <sup>1</sup>Southwest Research Institute

### 5:20 PM

**Impacts of Accelerated Aging on the Mechanical Properties of Cu-Nb Nanolaminates:** *Marian Kennedy*<sup>1</sup>; Bradley Schultz<sup>1</sup>; David Economy<sup>1</sup>; <sup>1</sup>Clemson University

## Recent Developments in the Processing, Characterization, Properties, Performance and Applications of Metal Matrix Composites: Processing, Microstructure and Mechanical Properties I

*Sponsored by:* TMS Structural Materials Division, TMS/ASM: Composite Materials Committee  
*Program Organizers:* Martin Pech-Canul, Centro de Investigacion y de Estudios Avanzados del Instituto Politecnico Nacional; Zariff Chaudhury, Materion Coporation; Golam Newaz, Wayne State University

Monday PM  
 March 4, 2013  
 Room: Bowie A  
 Location: Grand Hyatt

*Session Chairs:* Zariff Chaudhury, Materion Corporation; Martin Pech-Canul, CINVESTAV IPN SALTILLO

### 2:00 PM

**Mechanical Property and Abrasive Wear Characteristics of In-Situ Synthesized Al-12Si/10TiC Composites:** *Manas Mahapatra*<sup>1</sup>; Belete Yigezu<sup>1</sup>; P. K. Jha<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Roorkee

### 2:20 PM

**Columnar-to-Equiaxed Transition in Metal Matrix Composites:** *Alicia Ares*<sup>1</sup>; *Carlos Schvezov*<sup>1</sup>; <sup>1</sup>CONICET/FCEQyN-UNaM

### 2:40 PM

**Creep Resistant Submicron-Structured Composite with Fe-Al Matrix and Al<sub>2</sub>O<sub>3</sub> Particles:** *Jiri Svoboda*<sup>1</sup>; *Bohuslav Masek*<sup>2</sup>; Hana Jirkova<sup>2</sup>; Andrea Ronesova<sup>2</sup>; Stepan Jenicek<sup>2</sup>; <sup>1</sup>Academy of Sciences of the Czech Republic, v. v. i.; <sup>2</sup>University of West Bohemia in Pilsen, Research Centre of Forming Technology

### 3:00 PM

**Deformation and Structure-Property Correlation of ECAP AA2024 Aluminium Alloy and Influence of Fly-Ash Composites:** *Ajit Bhandakkar*<sup>1</sup>; Akshaya Behera<sup>1</sup>; R C Prasad<sup>1</sup>; *Shankar Sastry*<sup>2</sup>; <sup>1</sup>IIT, Bombay; <sup>2</sup>Washington University at St. Louis

### 3:20 PM

**Low Cycle Fatigue Behaviour of Hot Pressed Austenitic Steel/MG-PSZ Composite Materials:** *Horst Biermann*<sup>1</sup>; Alexander Glage<sup>1</sup>; Christian Weigelt<sup>1</sup>; Jan Räthel<sup>2</sup>; Anja Weidner<sup>1</sup>; <sup>1</sup>TU Bergakademie Freiberg; <sup>2</sup>Fraunhofer Institute for Ceramic Technologies

### 3:40 PM

**Microstructure and Wear Resistance Investigation of Ti/TiC Composite Coated on CP-Ti by TIG Cladding and Using Cored-Wire Electrode:** *Bahram Vaghefinazari*<sup>1</sup>; Amirhossein Kokabi<sup>1</sup>; <sup>1</sup>Sharif University of Technology

### 4:00 PM

**Smart, Multifunctional Metal-Matrix Composites For Repair and Damage Mitigation:** *Charles Fisher*<sup>1</sup>; Michele Manuel<sup>1</sup>; <sup>1</sup>University of Florida

### 4:20 PM

**Spark Plasma Sintering of Nickel-CNT Composites:** *Tushar Borkar*<sup>1</sup>; Junyeon Hwang<sup>2</sup>; Jaimie Tiley<sup>3</sup>; Soon-Hyung Hong<sup>4</sup>; Rajarshi Banerjee<sup>1</sup>; <sup>1</sup>University of North Texas; <sup>2</sup>Korea Institute of Science and Technology; <sup>3</sup>Air Force Research Laboratory; <sup>4</sup>Korea Advanced Institute of Science and Technology

### 4:40 PM

**Ultrasonic Fatigue of AMC225xe and AMC xfine225:** *Matthias Wolf*<sup>1</sup>; *Guntram Wagner*<sup>1</sup>; Dietmar Eifler<sup>1</sup>; <sup>1</sup>University of Kaiserslautern



5:00 PM

**Synthesis of Ti/TiC Composites by Mechanical Milling Followed by Spark Plasma Sintering of Ti-CNT Mixtures:** Vasanthakumar K<sup>1</sup>; Karthiselva S<sup>1</sup>; Niraj Chawake<sup>1</sup>; Prathap Chandran<sup>1</sup>; *Srinivasa Bakshi<sup>1</sup>*; <sup>1</sup>Indian Institute of Technology Madras

## Refractory Metals 2013: Refractory Metal-based Materials II

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

*Program Organizers:* David Honecker, Climax Molybdenum; Omer Dogan, DOE National Energy Technology Laboratory

Monday PM

March 4, 2013

Room: Mission A

Location: Grand Hyatt

*Session Chairs:* Omer Dogan, National Energy Technology Laboratory; S Varma, University of Texas at El Paso

2:00 PM

**Are Mo, Ta and W Alloying Additions Beneficial for Nb Silicide Based Alloys?:** *Panayiotis Tsakiroopoulos<sup>1</sup>*; <sup>1</sup>University of Sheffield

2:20 PM Question and Answer Period

2:25 PM

**Effect of Re on the Oxidation Behavior of Nb Alloys:** *Ruth Dasary<sup>1</sup>*; Shailendra Varma<sup>1</sup>; <sup>1</sup>The University of Texas at El Paso

2:45 PM Question and Answer Period

2:50 PM

**Interfacial Strength and Bonding between High Temperature Mo-Si-B Alloys and Silica-Based Oxidation Resistant Coatings:** *Oleg Kontsevoi<sup>1</sup>*; Arthur Freeman<sup>1</sup>; <sup>1</sup>Northwestern University

3:10 PM Question and Answer Period

3:15 PM Break

3:35 PM

**Effects of Si Doping on the Mechanical Behavior of Iridium Alloys:** D. Catoor<sup>1</sup>; C. A. Carmichael<sup>1</sup>; S. Lawson<sup>2</sup>; E. K. Ohriner<sup>1</sup>; *E. P. George<sup>1</sup>*; <sup>1</sup>Oak Ridge National Laboratory; <sup>2</sup>University of Tennessee

3:55 PM Question and Answer Period

4:00 PM

**Development of Nb-1%Zr-0.1%C Alloy as Structural Components for High Temperature Reactor Application:** Raghvendra Tewari<sup>1</sup>; Vishwanadh Bithula<sup>1</sup>; Gautam Dey<sup>1</sup>; N. Saibaba<sup>2</sup>; *Sanjay Jha<sup>2</sup>*; <sup>1</sup>Bhabha Atomic Research Centre; <sup>2</sup>Nuclear Fuel Complex

4:20 PM Question and Answer Period

4:30 PM

**Characterizing Slip System Behavior in High Purity Nb for Accelerator Cavities:** *Di Kang<sup>1</sup>*; Derek Baars<sup>1</sup>; Thomas Bieler<sup>1</sup>; Chris Compton<sup>1</sup>; <sup>1</sup>Michigan State University

4:50 PM Concluding Comments

## REWAS 2013: Enabling Materials Resource Sustainability: Plenary Session: Realizing Sustainability

*Sponsored by:* Chinese Society for Metals, The Mining and Materials Processing Institute of Japan (MMIJ), TMS Extraction and Processing Division, TMS: Recycling and Environmental Technologies Committee

*Program Organizers:* Christina Meskers, Umicore Precious Metals Refining; Anne Kvithyld, SINTEF; Markus Reuter, Outotec Oyj; Randolph Kirchain, Massachusetts Institute of Technology; Mark Schlesinger, Missouri University of Science and Technology; Gregory Krumbick, Argonne National Laboratory; Cong Wang, Saint-Gobain High Performance Materials; Gabrielle Gaustad, Rochester Institute of Technology; Diana A. Lados, Worcester Polytechnic Institute; Brajendra Mishra, Colorado School of Mines; Jeffrey S. Spangenberg, Argonne National Laboratory

Monday PM

March 4, 2013

Room: Lila Cockrell Theatre

Location: Henry B. Gonzalez Convention Center

*Funding support provided by:* Xstrata; SINTEF; Outotec; Umicore, and CR3, the Center for Resource Recovery and Recycling

*Session Chair:* Christina Meskers, Umicore Precious Metals Refining; Anne Kvithyld, SINTEF

2:00 PM Introductory Comments

2:10 PM Invited

**Sustainable Transportation Challenges and Opportunities:** *Lewis Fulton<sup>1</sup>*; <sup>1</sup>University of California, Davis

2:40 PM Invited

**Saint-Gobain's Approach Towards Materials Development for Sustainability in Habitat:** *Todd DiNoia<sup>1</sup>*; <sup>1</sup>Saint-Gobain High Performance Materials Research and Development Center

3:10 PM Invited

**iNEMI Environmental Thrust; History, Challenges, & Opportunities:** *Bill Bader<sup>1</sup>*; <sup>1</sup>iNEMI

3:40 PM Break

4:00 PM Invited

**Advanced Technology and the Scope of Large-scale Sustainability:** *Julio Friedmann<sup>1</sup>*; <sup>1</sup>Lawrence Livermore National Laboratory

4:30 PM Invited

**Global Trends in Water Treatment Technology & Sustainability:** *William Bonkoski<sup>1</sup>*; <sup>1</sup>GE Water & Process Technologies

5:00 PM Invited

**Value-in-Use and Beyond—Creating More Value from Scrap:** *Helga Vanthournout<sup>1</sup>*; <sup>1</sup>McKinsey and Ellen McArthur Foundation

## Synergies of Computational and Experimental Materials Science II: Integrated Computational Materials Engineering

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

*Program Organizers:* Katsuyo Thornton, University of Michigan; Thomas Buchheit, Sandia National Laboratories; Anthony Rollett, Carnegie Mellon University; David Rowenhorst, Naval Research Lab

Monday PM  
March 4, 2013

Room: 217A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Peter Collins, University of North Texas; Peter Lee, The University of Manchester

### 2:00 PM Introductory Comments

#### 2:05 PM Invited

**Developing a Materials Innovation Infrastructure: How Do We Bridge Simulation, Characterization, Experiment and Design?:** *Stephen Niezgoda*<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory

#### 2:35 PM Invited

**MIDAS-A Tool to Connect Experiments and Models:** *Meijie Tang*<sup>1</sup>; Jeff Florando<sup>1</sup>; Nathan Barton<sup>1</sup>; Kevin Durrenberger<sup>1</sup>; Peter Norquist<sup>1</sup>; <sup>1</sup>LLNL

#### 3:05 PM Invited

**In Situ Fast Synchrotron Tomography to Inform and Validate Microstructural Models:** *Peter D. Lee*<sup>1</sup>; Lang Yuan<sup>1</sup>; Chedtha Puncreobutr<sup>2</sup>; <sup>1</sup>The University of Manchester; <sup>2</sup>Imperial College London

#### 3:35 PM Break

#### 3:50 PM Invited

**Model-Based Regularized Inverse Methods for Developing Microstructure Models from Large Image Datasets:** *Jeff Simmons*<sup>1</sup>; Charles Bouman<sup>2</sup>; Singanallur Venkatakrishnan<sup>2</sup>; Lawrence Drummy<sup>3</sup>; Craig Przybyla<sup>1</sup>; Marc De Graef<sup>4</sup>; <sup>1</sup>AFRL; <sup>2</sup>Purdue University; <sup>3</sup>UES, Inc.; <sup>4</sup>Carnegie Mellon

#### 4:20 PM

**Using Forward Modeling to Close the Gap between 3D Experiments and Microstructure Models:** *Patrick Callahan*<sup>1</sup>; Marc De Graef<sup>1</sup>; <sup>1</sup>Carnegie Mellon University

#### 4:40 PM

**Role of Microstructure on Residual Stress Relaxation of a Shot-Peened Nickel-Base Superalloy:** *Micheal Burba*<sup>1</sup>; Michael Caton<sup>2</sup>; Dennis Buchanan<sup>1</sup>; Reji John<sup>2</sup>; <sup>1</sup>University of Dayton; <sup>2</sup>Air Force Research Laboratory (AFRL/RXC)

#### 5:00 PM

**Experimental Validation of Models Used in Automotive Sheet Metal Deformation:** *Adam Creuziger*<sup>1</sup>; Mark Iadicola<sup>1</sup>; Thomas Gnaeupel-Herold<sup>1</sup>; Andrew Reid<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

#### 5:20 PM

**Thermodynamic and Kinetic Model-Based Processing of Low Density Al Alloys:** *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>Army Research Laboratory

## Three-Dimensional Materials Science VII: Novel Material Systems in Three-Dimensional Materials Science

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

*Program Organizers:* Jonathan Madison, Sandia National Laboratories; Nikhilesh Chawla, Arizona State University; Michael Groeber, Air Force Research Laboratory

Monday PM  
March 4, 2013

Room: 212A  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Nik Chawla, Arizona State University; Francesco De Carlo, Argonne National Laboratory

### 2:00 PM Invited

**Three-Dimensional Tomographic Characterization of Advanced Ceramic Textile Composites under In Situ Loading at Ultrahigh Temperatures:** Hrishikesh Bale<sup>1</sup>; A. Haboub<sup>2</sup>; Alastair MacDowell<sup>2</sup>; J. Nasiatka<sup>2</sup>; Brian Cox<sup>3</sup>; David Marshall<sup>3</sup>; *Robert Ritchie*<sup>1</sup>; <sup>1</sup>University of California Berkeley; <sup>2</sup>Lawrence Berkeley National Laboratory; <sup>3</sup>Teledyne Science Center

### 2:30 PM

**Grain Boundary Misorientation and Solute Segregation in Radiation-Tolerant Nanostructured Ferritic Alloys:** *Lan Yao*<sup>1</sup>; Michael Miller<sup>1</sup>; Kathy Powers<sup>1</sup>; <sup>1</sup>ORNL

### 2:50 PM

**Neutron and X-Ray Tomography of Aluminum Alloys Subjected to Fire Damage:** Stephen Pupilamp<sup>1</sup>; *Dayakar Penumadu*<sup>1</sup>; Felix Kim<sup>1</sup>; Justin Baba<sup>2</sup>; <sup>1</sup>University of Tennessee; <sup>2</sup>Oak Ridge National Laboratory

### 3:10 PM Invited

**The Use of 3D Microstructural Volumes in the Integrated Experimental Approach to the Prediction of Fatigue Behavior in an  $\alpha + \beta$  Titanium Alloy:** *Christopher Szczepanski*<sup>1</sup>; Sushant Jha<sup>2</sup>; Paul Shade<sup>1</sup>; Megna Shah<sup>3</sup>; Michael Uchic<sup>1</sup>; Michael Groeber<sup>1</sup>; James Larsen<sup>1</sup>; <sup>1</sup>US Air Force Research Laboratory; <sup>2</sup>UTC/AFRL; <sup>3</sup>UES

### 3:40 PM Break

### 3:55 PM

**Determining the Variance and Distribution of Quantified Microstructure in  $\alpha + \beta$  Processed Ti-6Al-4V by Meso-Scale 3D Serial Sectioning:** *Meg Noble*<sup>1</sup>; Daniel Huber<sup>1</sup>; John Sosa<sup>1</sup>; Vikas Dixit<sup>1</sup>; Hamish Fraser<sup>1</sup>; <sup>1</sup>The Ohio State University

### 4:15 PM

**3D Microstructural Characterization of In-Situ TiC Reinforced Ni Composites:** *Junyeon Hwang*<sup>1</sup>; Sundeep Gopagoni<sup>2</sup>; Darius Simmons<sup>3</sup>; Kristopher Mahdak<sup>3</sup>; Soumya Nag<sup>3</sup>; Jaimie Tiley<sup>4</sup>; Rajarshi Banerjee<sup>3</sup>; <sup>1</sup>Korea Institute of Science and Technology; <sup>2</sup>Johns Manville; <sup>3</sup>University of North Texas; <sup>4</sup>Air Force Research Laboratory

### 4:35 PM Break

### 4:50 PM Invited

**On Quantification of Fibrous Material:** *Ming Lei*<sup>1</sup>; Shawn Zhang<sup>1</sup>; Laurent Bernard<sup>1</sup>; Patrick Barthelémy<sup>1</sup>; <sup>1</sup>Visualization Sciences Group

### 5:20 PM

**X-Ray Microtomographic Characterisation of Deformation and Failure in Cellular Materials under Quasi-static and Dynamic Compression:** *Peifeng Li*<sup>1</sup>; <sup>1</sup>Nanyang Technological University

5:40 PM

**X-Ray Fluorescence Analysis of a Dirty Discrete White Spot in a Nickel 718 Alloy:** *Trevor Watt*<sup>1</sup>; Eric Taleff<sup>1</sup>; <sup>1</sup>The University of Texas at Austin

## 2013 Functional Nanomaterials: Synthesis, Properties and Applications: Nanomaterials General I: Electronic, Photonic, and Bio-Nano Interfaces

*Sponsored by:* TMS Electronic, Magnetic, and Photonic Materials Division, TMS: Nanomaterials Committee

*Program Organizers:* Seong Jin Koh, University of Texas at Arlington; Nitin Chopra, University of Alabama; Jiyoung Kim, University of Texas at Dallas; Yuanbing Mao, University of Texas-Pan American; Ashwin Ramasubramaniam, University of Massachusetts; Gregory Thompson, University of Alabama

Tuesday AM  
March 5, 2013

Room: 201  
Location: Henry B. Gonzalez  
Convention Center

*Funding support provided by:* Qualcomm, Inc.

*Session Chairs:* Gregory Thompson, University of Alabama; Ashwin Ramasubramaniam, University of Massachusetts Amherst

8:30 AM Invited

**Transfer Printed Semiconductor Nanomembrane Photonics:** *Weidong Zhou*<sup>1</sup>; Zhenqiang Ma<sup>2</sup>; Hongun Yang<sup>3</sup>; <sup>1</sup>University of Texas at Arlington; <sup>2</sup>University of Wisconsin-Madison; <sup>3</sup>Semerane, Inc.

9:05 AM Invited

**Tunable Nanostructures and Printed Electronics:** *Horst Hahn*<sup>1</sup>; <sup>1</sup>Karlsruhe Institute of Technology

9:40 AM

**Fabrication of Surface Channel Waveguides on a Thin Film of Rare Earth Doped Silicon:** *Matthew Murray*<sup>1</sup>; Gin Jose<sup>1</sup>; Billy Richards<sup>1</sup>; Animesh Jha<sup>1</sup>; <sup>1</sup>The University of Leeds

10:00 AM Break

10:15 AM

**Characteristic Study for Nano-Scaled 2DEG Properties of AlGaIn/GaN:** *JaeWoo Suh*<sup>1</sup>; Feyza Berber<sup>1</sup>; Harlan Harris<sup>1</sup>; <sup>1</sup>Texas A&M University

10:35 AM Invited

**Chemical Functionalization of Hydrogen-terminated Silicon Surfaces for Energy and Sensing Applications:** Oliver Seitz; Weina Peng; Peter Thissen; Louise Caillard; William De Benedetti; Hue Nguyen; Yuri Gartstein; Anton Malko; *Yves Chabal*<sup>1</sup>; <sup>1</sup>Univ of Texas at Dallas

11:10 AM Invited

**Biological Properties of Zinc Oxide-Coated Anodized Aluminum Oxide:** S. Skoog<sup>1</sup>; M. Bayati<sup>2</sup>; P. Petrochenko<sup>1</sup>; S. Stafslie<sup>3</sup>; J. Daniels<sup>3</sup>; N. Cilz<sup>3</sup>; D. Comstock<sup>4</sup>; J. Elam<sup>4</sup>; *R. Narayan*<sup>1</sup>; <sup>1</sup>UNC/NCSU Joint Department of Biomedical Engineering; <sup>2</sup>North Carolina State University Department of Materials Science and Engineering; <sup>3</sup>North Dakota State University; <sup>4</sup>Argonne National Laboratory

11:45 AM

**Quantitation of Circulating Tumor Cells Using Nanowire Substrate-Based Laser Scanning Cytometry:** *Sang-Kwon Lee*<sup>1</sup>; Rong Fan<sup>2</sup>; <sup>1</sup>Chonbuk National University; <sup>2</sup>Yale University

12:05 PM

**Synthesis and Characterization of Magnetic Silica Nanoparticles for His-tagged Proteins Capture and Separation:** Mahdi Kamali<sup>1</sup>; Mehdi Ghaffari Sharaf<sup>2</sup>; *Seyed Mostafa Amoozadeh*<sup>3</sup>; Hamidreza Javadi<sup>4</sup>; Hamid Kooshki<sup>1</sup>; Jamal Rashidani<sup>1</sup>; Amir Homayoun Keihan<sup>2</sup>; Manizheh Ramezani<sup>5</sup>; <sup>1</sup>BMSU Nano Biotechnology Research Center; <sup>2</sup>Ibb Institute, University of Tehran; <sup>3</sup>Sharif University of Technology; <sup>4</sup>National Institute of Genetic Engineering and Biotechnology (NIGEB); <sup>5</sup>University of Tehran

## 4th International Symposium on High-Temperature Metallurgical Processing: Alloy and Materials Preparation I

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

*Program Organizers:* Tao Jiang, Central South University; Jiann-Yang Hwang, Michigan Technological University; Phillip Mackey, Consultant; Onuralp Yücel, ITU; Guifeng Zhou, Wuhan Iron and Steel

Tuesday AM  
March 5, 2013

Room: 008B  
Location: Henry B. Gonzalez  
Convention Center

*Session Chairs:* Onuralp YÜCEL, Istanbul Technical University; Jilai Xue, University of Science and Technology Beijing

8:30 AM

**The Effect of Aluminum Addition to the ESR Process Slag on IN718 Superalloy Characteristics:** *Adel Sheikhhosseini*<sup>1</sup>; <sup>1</sup>IUT

8:50 AM

**Effects of Crystallization of Mould Fluxes on Property of Liquid Slag Film and Its Impact on Peritectic Steel Slab Continuous Casting:** *Xiao Long*<sup>1</sup>; Shengping He<sup>1</sup>; Lilong Zhu<sup>1</sup>; Ting Wu<sup>1</sup>; Qian Wang<sup>1</sup>; <sup>1</sup>Chongqing University

9:05 AM

**A Study on Production of Fe-Co-V Alloys by Self Propagating High Temperature Synthesis:** *Murat Alkan*<sup>1</sup>; Ozlem Altinordu<sup>1</sup>; Seref Sönmez<sup>1</sup>; Bora Derin<sup>1</sup>; Onuralp Yücel<sup>1</sup>; Vladimir Sanin<sup>2</sup>; Vladimir Yuhvid<sup>2</sup>; <sup>1</sup>Istanbul Technical University; <sup>2</sup>Institute of Structural Macrokinetics and Materials Science

9:20 AM

**Hot Ductility of Nb-V-Containing Microalloyed Steel during Solidification:** Yanhui Sun<sup>1</sup>; *Yanan Zeng*<sup>1</sup>; Kaike Cai<sup>1</sup>; <sup>1</sup>University of Science and Technology, Beijing

9:40 AM

**Co-Cr-Mo Alloys Production by Self Propagating High Temperature Synthesis:** *Ozlem Okur*<sup>1</sup>; Murat Alkan<sup>1</sup>; Onuralp Yücel<sup>1</sup>; <sup>1</sup>Istanbul Technical University

10:00 AM Break

10:20 AM

**High-Temperature Oxidation and Corrosion Behaviors of NiFe Alloy for Inert Anode Materials in Aluminum Electrolysis:** *Jilai Xue*<sup>1</sup>; Luxing Feng<sup>1</sup>; MengDong Gu<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing

10:30 AM

**Production of Molybdenum Containing Iron Based Alloys via Metallurgical Processes:** *Dilek Kirgöz*<sup>1</sup>; Murat Alkan<sup>1</sup>; Onuralp Yücel<sup>1</sup>; <sup>1</sup>Istanbul Technical University