

Focused Session 2: Computational Design, Modeling, and Simulation of Ceramics and Composites

Monday, January 23, 2012 **Simulation of Structure and Properties of Advanced Ceramics**

1:30 PM-5:40 PM

Room: Ponce de Leon

Session Chair(s): Hans Seifert, Brian Good

1:30 PM

(ICACC-FS2-001-2012) Modeling of radiation damage in nanocrystalline silicon carbide (Invited)

Izabela Szlufarska*, Dane Morgan, Narasimhan Swaminathan, Ming-Jie Zheng, University of Wisconsin, USA

2:00 PM

(ICACC-FS2-002-2012) Thermal Conductivity of Amorphous Ceramics from Ab-Initio Molecular Dynamics Simulations (Invited)

Peter Kroll*, Babak Kouchmeshky, UT Arlington, USA

2:20 PM

(ICACC-FS2-003-2012) Transferable variable charge potential for the study of energy conversion materials in Lithium ion batteries

Ying Ma*, Glenn Lockwood, Stephen Garofalini, Rutgers University, USA

2:40 PM

(ICACC-FS2-004-2012) Phase stability of Al₃BC₃: first-principles calculation and in situ Raman experiments (Invited)

Jingyang Wang*, Huimin Xiang, Institute of Metal Research, China; Yanchun Zhou, Aerospace Research Institute of Materials and Processing Technology, China

3:00 PM

Break

3:20 PM

(ICACC-FS2-005-2012) First Principles Calculations of Temperature and Pressure Dependent Physical Properties of MAX Phase Materials (Invited)

Lizhi Ouyang*, Tennessee State University, USA

3:40 PM

(ICACC-FS2-006-2012) Understanding the Behavior of Native Point Defects in ZrC by First-Principles Calculation

Yanhui Zhang*, Jingyang Wang, Institute of Metal Research, China; Yanchun Zhou, Aerospace Research Institute of Materials and Processing Technology, China

4:00 PM

(ICACC-FS2-007-2012) Mechanical properties of apatite crystals using multi-axial tensile experiment and construction of failure envelope (Invited)

Wai-Yim Ching*, Sitram Aryal, Anil Misra, University of Missouri-Kansas City, USA

4:30 PM

(ICACC-FS2-008-2012) Modeling hardness of materials and its application to the search for superhard materials from first-principles calculations (Invited)

Xingqiu Chen*, Haiyang Niu, Dianzhong Li, Yiyi Li, Institute of Metal Research, Chinese

Academy of Sciences, China

4:50 PM

(ICACC-FS2-009-2012) Multiscale modeling of ultra high temperature ceramics (UHTC) ZrB₂ and HfB₂: application to lattice thermal conductivity (Invited)

John W Lawson*, NASA Ames Research Center, USA; Murray S Daw, Clemson University, USA; Thomas H Squire, Charles W Bauschlicher, NASA Ames Research Center, USA

5:20 PM

(ICACC-FS2-010-2012) Atomistic reconstruction of pyrocarbons: from imaging to property computation (Invited)

Jean-Marc Leyssale, CNRS, France; Jean-Pierre Da Costa, University Bordeaux, France; Baptiste Farbos, CNRS, France; Christian Germain, University Bordeaux, France; Gerard L. Vignoles*, University Bordeaux 1, France

Tuesday, January 24, 2012

Characterization and Modeling of Surfaces, Interfaces and Grain Boundaries at Multiple Scales

8:00 AM-11:40 AM

Room: Ponce de Leon

Session Chair(s): Jingyang Wang, Wai-Yim Ching

8:00 AM

(ICACC-FS2-011-2012) Combining X-ray Diffraction Contrast Tomography and Mesoscale Grain Growth Simulations in STO: an integrated approach for the investigation of microstructure evolution (Invited)

Melanie Syha*, Wolfgang Rheinheimer,

Michael Baeurer, Karlsruhe Institute of Technology, Germany; Wolfgang Ludwig, European Synchrotron Radiation Facility, France; Erik M Lauridsen, Risø National Laboratory, Denmark; Daniel Weygand, Peter Gumbsch, Karlsruhe Institute of Technology, Germany

8:20 AM

(ICACC-FS2-012-2012) Growth Stress in SiO₂ during Oxidation of SiC Fibers

Randall Hay*, Air Force Research Laboratory, USA

8:40 AM

(ICACC-FS2-013-2012) A Density-Functional Theory Investigation of Oxidative Corrosion of the UO₂(111) Surface (Invited)

Anne Chaka*, Gloria Oxford, NIST, USA

9:00 AM

(ICACC-FS2-014-2012) Effect of Absorbates and Surface Defects on Work Function of ZnO Based on First Principles DFT Calculations

Jincheng Du*, Yun Li, University of North Texas, USA

9:20 AM

(ICACC-FS2-015-2012) Sintering of multi-phase Mo-Si-B and the effects of doping

Jae-Il Jung*, Jian Luo, Clemson University, USA

9:40 AM

Break

10:00 AM

(ICACC-FS2-016-2012) Modeling of Oxide Interfaces (Invited)

Craig Fisher*, Akihito Kuwabara, Hiroki Moriwake, Japan Fine Ceramics Center, Japan; Hideki Oki, Toyota Motor Corporation, Japan; Yuichi Ikuhara, University of Tokyo, Japan

10:30 AM

(ICACC-FS2-017-2012) Modeling Grain Boundary Phase Behaviors (Invited)

Jian Luo*, Clemson Univ, USA

11:00 AM

(ICACC-FS2-018-2012) Atomistic simulations and TEM measurements of Si₃N₄-amorphous SiO₂ interface with La and Lu

Iskander G Batyrev*, Jennifer Synowczynski, Neil S Weingarten, Betsy M Rice, Jan Andzelm, Jeff J Swab, US Army Research Laboratory, USA; Juan C Idrobo, ORNL, USA

11:20 AM

(ICACC-FS2-019-2012) Molecular Dynamics Simulations of La Doped Intergranular Films in Silicon Nitride: Effect of Structure on Properties

Yun Jiang*, Stephen H Garofalini, Rutgers University, USA

Novel Simulation Method and Virtual Material Design

1:30 PM-5:10 PM

Room: Ponce de Leon

Session Chair(s): Jian Luo, John Lawson

1:30 PM

(ICACC-FS2-020-2012) Kinetic Monte Carlo Simulation of Oxygen Diffusion in Doped Zirconia-Based Materials. (Invited)

Brian S Good*, NASA Glenn Research Center, USA

2:00 PM

(ICACC-FS2-021-2012) Materials Thermodynamics and Phase Modeling in the Li-Mn-O System (Invited)

Hans Juergen Seifert*, Damian M Cupid, Karlsruhe Institute of Technology, Germany

2:30 PM

(ICACC-FS2-022-2012) Electronic Structure, Bonding, and Optical Properties of Mo Based Alloys in the Mo-Si-B Phase Diagram (Invited)

Paul Rulis*, Wai-Yim Ching, University of Missouri - Kansas City, USA

3:00 PM

Break

3:20 PM

(ICACC-FS2-023-2012) Micromechanical Finite Element Simulations and Determination of Effective Properties in Silicon Nitride (Invited)

Thomas Böhlke*, Johannes Wippler, Karlsruhe Institute of Technology, Germany

3:50 PM

(ICACC-FS2-024-2012) A new anisotropic constitutive model for ceramic materials failure

Simone Falco*, Claire Dancer, Richard Todd, Nik Petrinic, University of Oxford, United Kingdom

4:10 PM

(ICACC-FS2-025-2012) Inelastic Microstructure Modeling and Design of MMCs with Lamellar Microstructure

Romana Piat*, Yuriy Sinchuk, Karlsruhe Inst of Technology, Germany

4:30 PM

(ICACC-FS2-026-2012) An integrated virtual material approach for ceramic matrix composites

Guillaume Couegnat*, William Ros, Thomas Haurat, Christian Germain, Eric Martin, Gérard L Vignoles, University of Bordeaux, France

4:50 PM

(ICACC-FS2-027-2012) Microstructure-sensitive extreme value damage response in fully dense ceramic matrix composites with

unidirectional plys

Michael Braginsky*, UES, Inc., USA; Craig Paul Przybyla, Air Force Research Laboratory, USA

Focused Session 2: Poster Session

5:00 PM-7:30 PM

Room: Exhibition Hall, Ocean Center

(ICACC-FS2-P140-2012) Numerical Simulation of Temperature and Stress Field Evolution Applied to Spark Plasma Sintering

Jeffrey Allen*, Charles Welch, John Peters, US Army Corps of Engineers, Engineer Research & Development Center, USA

(ICACC-FS2-P141-2012) Electronic Structure and Interband Optical Properties of 20 MAX Phase Compounds

Yuxiang Mo, Paul Rulis, Wai-Yim Ching*, University of Missouri-Kansas City, USA

(ICACC-FS2-P142-2012) Crystalline Approximants of SiCO: Implications on Structure and Thermochemistry of Ternary Silicon Oxycarbide

Peter Kroll*, Nelli Bodiford, UT Arlington, USA

(ICACC-FS2-P143-2012) Oxidation mechanism for SiCO: theoretical study on diffusion and reaction of oxygen

Peter Kroll*, Bin Xu, Babak Kouchmeshky, UT Arlington, USA

(ICACC-FS2-P144-2012) Design of ZrO₂/SiC Composite Materials with very low-thermal conductivity

Babak Kouchmeshky, Peter Kroll*, UT Arlington, USA

(ICACC-FS2-P145-2012) Molecular dynamics simulations of hypersonic velocity impact protection properties of CNT/a-SiC**composites**

Ali Goodarzi*, Amirkabir University of Tech., Iran, Islamic Republic of; Hailey Taylor, Imperial College London, United Kingdom

(ICACC-FS2-P146-2012) Studies of gas-phase reactivity during chemical vapor deposition of boron carbide

Guillaume Reinisch, University Bordeaux 1, France; Jean-Marc Leyssale, CNRS, France; Stéphanie Patel, University Bordeaux 1, France; Georges Chollon, CNRS, France; Gerard L. Vignoles*, University Bordeaux 1, France

(ICACC-FS2-P147-2012) Image-based 2D Numerical Modeling of Oxide Formation in Self-Healing CMCs

Virginie Dréan, INRIA, France; Grégory Perrot, University Bordeaux 1, France; Guillaume Couegnat, CNRS, France; Mario Ricchiuto, INRIA, France; Gerard L. Vignoles*, University Bordeaux 1, France

(ICACC-FS2-P148-2012) First Principles Calculations of Boron Carbide

Jennifer Synowczynski Dunn*, Jerry C LaSalvia, U.S. Army Research Laboratory, USA