

SYMPOSIUM ES5

Advances in Materials, Experiments and Modeling for Nuclear
Energy
April 18 - April 21, 2017

Symposium Organizers

Dilpuneet Aidhy, University of Wyoming
Kazuto Arakawa, Shimane University
Estelle Meslin, CEA Saclay
Haixuan Xu, University of Tennessee

Proceedings Statement

All authors are invited to submit articles based on their 2017 MRS Spring Meeting presentations to the journals in the MRS portfolio (www.mrs.org/publications-news). Papers submitted and accepted for publication in MRS Advances (www.mrs.org/mrs-advances) will be available as symposium collections. Visit the MRS/Cambridge University Press Publications Booth #100 in the Exhibit Hall to learn more, including MRS Advances print options available at special rates during the meeting week only.

* Invited Paper

SESSION ES5.1: Metallic Systems I

Session Chairs: Kazuto Arakawa and Charlotte Becquart
Tuesday Morning, April 18, 2017
PCC North, 200 Level, Room 223

10:30 AM *ES5.1.01

Deferred Achievement of a Steady State Microstructure in Radiation-Resistant Alloys [Gary S. Was](#); University of Michigan, United States.

11:00 AM ES5.1.02

Microstructural and Micro-Mechanical Changes in Tungsten under High Flux Plasma Exposure [Dmitry Terentyev](#); SCKCEN, Belgium.

11:15 AM ES5.1.03

High Temperature Defect Migration Mechanism in Ni and Ni-Based Concentrated Solid-Solution Alloys [Taini Yang](#); University of Michigan, United States.

11:30 AM ES5.1.04

Defect Formation in Helium Irradiated Y₂O₃ Doped W-Ti Alloys Studied by Positron Annihilation and Nanoindentation [Asta Richter](#); Technical University of Applied Sciences Wildau, Germany.

11:45 AM ES5.1.05

Exploring the Stability of TPBAR Liner with *In Situ*, Triple-Beam, Ion Irradiation TEM [Khalid Hattar](#); Sandia National Labs, United States.

SESSION ES5.2: Metallic Systems II

Session Chairs: Cristelle Pareige and Tomoaki Suzudo
Tuesday Afternoon, April 18, 2017
PCC North, 200 Level, Room 223

1:30 PM *ES5.2.01

Point Defect Clusters and Loops in Fe—Interaction with Solute Atoms and Insights from DFT Calculations [Charlotte S. Becquart](#); Univ de Lille 1, France.

2:00 PM ES5.2.02

Experimental Measurement of the 1D Diffusivity of <100> Dislocation Loops in Iron [Kazuto Arakawa](#); Shimane University, Japan.

2:15 PM ES5.2.03

Contribution of Helium and Injected Self-Ions to Void Swelling Reduction in Ion-Irradiated High Purity α -Fe [Arunodaya Bhattacharya](#)^{1,2}; ¹University of Paris-Saclay, France; ²Centre de Sciences Nucléaires et de Sciences de la Matière (CSNSM/IN2P3/CNRS), University of Paris-Saclay, France.

2:30 PM ES5.2.04

Microstructure and Mechanical Property Evaluation of Oxide Dispersion Strengthened Ferritic Steels [Wahida R. Ilaham](#); Indian Institute of Technology, Kharagpur, India.

2:45 PM BREAK

SESSION ES5.3: Metallic Systems III

Session Chairs: Kazuto Arakawa and Gary Was
Tuesday Afternoon, April 18, 2017
PCC North, 200 Level, Room 223

3:15 PM *ES5.3.01

On the Correlation between Damage and Ion Injected Profile and Clustering in FeCr(NiSiP) Alloys [Cristelle Pareige](#); University of Rouen, France.

3:45 PM *ES5.3.02

How Rhenium and Osmium in Tungsten Crystals Suppress Radiation-Induced Defects [Tomoaki Suzudo](#); JAEA, Japan.

4:15 PM ES5.3.03

Integrated Computational and Experimental Study of Radiation Damage Effects in Alloy 709 [Haixuan Xu](#); University of Tennessee, United States.

4:30 PM ES5.3.04

Investigation of Creep-Fatigue Damage in Alloy 617 at High Temperatures [Frazz Tahir](#); Arizona State University, United States.

4:45 PM ES5.3.05

Ion Irradiation Defects in Austenitic Alloy 709 and Ferritic-Martensitic Steel Grade 92 for Nuclear Applications [Li He](#); University of Wisconsin-Madison, United States.

SESSION ES5.4: Complex Behaviors in Ceramics I

Session Chairs: Haixuan Xu and Yongfeng Zhang
Wednesday Morning, April 19, 2017
PCC North, 200 Level, Room 223

8:00 AM *ES5.4.01

Experimental and Modelling Studies of Nuclear Materials for Fission and Fusion Energy [Gregory R. Lumpkin](#); ANSTO, Australia.

8:30 AM *ES5.4.02

On the Relationship between Chemical Disorder and Mass Transport in Complex Oxides [Blas P. Uberuaga](#); Los Alamos National Laboratory, United States.

9:00 AM ES5.4.03

Radiation Damage in Borosilicate and Iron Phosphate Glass [Roger Smith](#); Loughborough University, United Kingdom.

9:15 AM ES5.4.04

Effects of Ionization in Ion-Irradiation Studies of Damage Evolution in Nuclear Ceramics [William J. Weber](#)^{1,2}; ¹University of Tennessee, United States; ²Oak Ridge National Laboratory, United States.

9:30 AM ES5.4.05

Atomic Resolution STEM Imaging of Epsilon Phase Formation in Doped Ceria by Irradiation and Thermal Annealing [Michele A. Conroy](#); Pacific Northwest National Lab, United States.

9:45 AM ES5.4.06

Defect Kinetics and Long-Term Evolution of Grain Boundaries in Irradiated Silicon Carbide [Hao Jiang](#); University of Wisconsin Madison, United States.

10:00 AM BREAK

SESSION ES5.5: Microstructure and Irradiation
Session Chairs: Estelle Meslin and Dane Morgan
Wednesday Morning, April 19, 2017
PCC North, 200 Level, Room 223

10:30 AM *ES5.5.01

Solving the Puzzle of Nonequilibrium Precipitation in Irradiated Tungsten Using Parameter-Free Modeling Jaime Marian; University of California, Los Angeles, United States.

11:00 AM ES5.5.02

Plastic Straining in Presence of Radiation-Induced Defects—A 3D Dislocation Dynamics Investigation Christian Robertson; CEA Saclay, France.

11:15 AM ES5.5.03

Concurrent Atomistic-Continuum Simulations of Sequential Dislocation/Obstacle Interactions in Face-Centered Cubic Metals Shuozhi Xu; Georgia Tech, United States.

11:30 AM ES5.5.04

Epsilon Phase Fission Products in Spent Nuclear Fuel Cladding—A Complimentary Atomic Resolution Electron Microscopy and Atom Probe Tomography Study Michele A. Conroy; Pacific Northwest National Lab, United States.

11:45 AM ES5.5.05

Multiscale Approach on the Understanding of the Growth Mechanisms of Zirconium Alloys under Irradiation Benjamin Christiaen^{1,2,3}; ¹EDF R&D, France; ²UMET (Unité matériaux Et Transformation), France; ³EM2VM (Etude et Modélisation des Microstructures pour le Vieillessement des Matériaux), France.

SESSION ES5.6: Thermodynamics and Modeling
Session Chairs: Jaime Marian and Blas Uberuaga
Wednesday Afternoon, April 19, 2017
PCC North, 200 Level, Room 223

1:30 PM *ES5.6.01

Modeling Cu-Mn-Ni-Si Precipitate Evolution and Hardening in Reactor Pressure Vessel Steels Dane Morgan; University of Wisconsin-Madison, United States.

2:00 PM ES5.6.02

A Comprehensive Thermodynamic Study of the U-Am-O Ternary System—Multiple Experimental Investigations and Calphad Modelling Enrica Epifano; CEA Marcoule, France.

2:15 PM ES5.6.03

Molecular Dynamics Analysis of Thermodynamic and Kinetic Properties of Bulk PdH_x Xiaowang Zhou; Sandia National Labs, United States.

2:30 PM BREAK

SESSION ES5.7: Chemical Effects
Session Chairs: Gregory Lumpkin and William Weber
Wednesday Afternoon, April 19, 2017
PCC North, 200 Level, Room 223

3:30 PM *ES5.7.01

Atomistic to Mesoscale Understanding of Hydride Formation in Alpha-Zr Yongfeng Zhang; Idaho National Lab, United States.

4:00 PM ES5.7.02

Fast and Ultrahigh-Capacity Uranium Extraction from Sea Water by Electrochemical Method Chong Liu; Stanford University, United States.

4:15 PM ES5.7.03

Reaction Model for Fluorination of Uranium Dioxide Using Improved Unreacted Shrinking Core Model for Expanding Spherical Particles Artur Braun; EMPA, Switzerland.

4:30 PM ES5.7.04

In Situ X-Ray Diffraction Study of the Steam Oxidation of Zirconium and Zirconium Alloys Mohamed Elbakhshwan; Brookhaven National Laboratory, United States.

4:45 PM ES5.7.05

Joint Experimental and Theoretical Investigation of Cement Paste under Electron Irradiation Lucile Dezerald^{1,3}; ¹Institut Jean Lamour, France; ³Massachusetts Institute of Technology, United States.

SESSION ES5.8: Poster Session
Wednesday Afternoon, April 19, 2017
8:00 PM - 10:00 PM
Sheraton, Third Level, Phoenix Ballroom

ES5.8.01

Transport of Hydrogen Isotopes in CuCrZr and the Isotope Effect for Nuclear Applications Woo Jun Byeon; Dankook University, Korea (the Republic of).

ES5.8.02

Examination of High Burnup Behavior of Nuclear Fuels Using a Modified Potts Model Richard T. Hoffman; Georgia Institute of Technology, United States.

ES5.8.03

Multi-Scale Simulation of the Experimental Response of Ion-Irradiated Zirconium Carbide Jean-Paul Crocombette; CEA Saclay, France.

ES5.8.04

Irradiation Effects of Helium Ions on the Deuterium Retention and Desorption in the Reduced Activation Martensitic Steel ARAA Hae Won Shin; Dankook University, Korea (the Republic of).

ES5.8.05

Structure of La-U-O Compounds Luis Casillas; University of Tennessee, United States.

ES5.8.06

A Complete Study on the Evolution of W and W-Re Alloy under Irradiation Using Monte Carlo Simulation Methods Chen-Hsi Huang; University of California, Los Angeles, United States.

ES5.8.07

Cladding Fretting Wear Comparison of APMT Steel and Zircaloy-4 Thomas Winter; Georgia Institute of Technology, United States.

ES5.8.08

Microstructural Evolution in Hot Rolled Monotectoid Zr-Nb Jacob Startt; Georgia Institute of Technology, United States.

ES5.8.09

Hydrogen Solidification on Template Materials for Nuclear Fusion Applications Swanee J. Shin; Lawrence Livermore National Laboratory, United States.

ES5.8.10

Modeling Diffusion of Fission Products in SiC High-Energy Grain Boundaries Hyunseok Ko; University of Wisconsin-Madison, United States.

ES5.8.11

Efficient Ab Initio Modeling of Nuclear Materials George Beridze; Forschungszentrum Juelich GmbH, Germany.

ES5.8.12

OKMC Simulation of Absorption Kinetics of Point Defects by Dislocations and Defect Clusters Denise Carpentier; CEA Saclay, France.

ES5.8.13

Multiscale Modelling of Delayed Hydride Cracking Mitesh Patel; Imperial College London, United Kingdom.

SESSION ES5.9: Metallic Systems IV

Session Chairs: Chaitanya Deo and Estelle Meslin
Thursday Morning, April 20, 2017
PCC North, 200 Level, Room 223

8:00 AM *ES5.9.01

Toward a Mechanistic Understanding of Interfacial Damage Tolerance Mitra L. Taheri; Drexel University, United States.

8:30 AM *ES5.9.02

Influence of Chemical Disorder on Defect Dynamics in Concentrated Solid-Solution Alloys Yanwen Zhang^{1,2}; ¹Oak Ridge National Lab, United States; ²University of Tennessee, United States.

9:00 AM ES5.9.03

Defect Properties in Concentrated Solid-Solution Alloys Shijun Zhao; Oak Ridge National Lab, United States.

9:15 AM ES5.9.04

Cr-Induced Fast Vacancy Cluster Formation in Ni Alloys Dilpuneet S. Aidhy; University of Wyoming, United States.

9:30 AM ES5.9.05

Evaluating Irradiation Effects and Defect Kinetics in a Co-Free High Entropy Alloy Congyi Li; University of Tennessee, United States.

9:45 AM ES5.9.06

Effect of Sinks on the Kinetics of Cr Precipitation in FeCr Alloys under Irradiation—APT versus AKMC Modeling Estelle Meslin; CEA Saclay, France.

10:00 AM BREAK

SESSION ES5.10: Fuels

Session Chairs: Dilpuneet Aidhy and Chaitanya Deo
Thursday Morning, April 20, 2017
PCC North, 200 Level, Room 223

10:30 AM *ES5.10.01

Technical Accomplishments in Westinghouse Accident Tolerant Fuel Program Peng Xu; Westinghouse Electric Company, United States.

11:00 AM ES5.10.02

Irradiation Behavior of the Zirconium Diffusion Barrier in Monolithic U-Mo Fuels Jan-Fong Jue; Idaho National Lab, United States.

11:15 AM ES5.10.03

A Modified Embedded-Atom Method Interatomic Potential for U-Si Benjamin Beeler; Idaho National Laboratory, United States.

11:30 AM ES5.10.04

Radiation Stability of Spent Nuclear Fuel—*In Situ* Experimental Simulation Aurelie Gentils; CSNSM, Univ Paris-Sud, CNRS/IN2P3, Université Paris-Saclay, France.

11:45 AM ES5.10.05

Quantitative Image Analysis of Surrogate Fuel Blocks Imaged with X-Rays for the Transient Reactor Test Facility—A Preliminary Study Jeffery A. Aguiar; Idaho National Laboratory, United States.

SESSION ES5.11: Metals and Theory
Session Chairs: Meimei Li and Mitra Taheri
Thursday Afternoon, April 20, 2017
PCC North, 200 Level, Room 223

1:30 PM *ES5.11.01

Molecular Dynamics Simulations of Cascades with Realistic Energies—First Applications of the Cell Molecular Dynamics for Cascade (CMD-C) Code Jean-Paul Crocombette; CEA Saclay, France.

2:00 PM *ES5.11.02

Uncertainty Quantification and Sensitivity Analysis of Atomistic and Mesoscale Models of Nuclear Materials Behavior Chaitanya Deo; Georgia Institute of Technology, United States.

2:30 PM ES5.11.03

Development of Molecular Dynamics Potential for Xe-U-Si Ternary System Jianguo Yu; Idaho National Lab, United States.

2:45 PM ES5.11.04

Defect Energetics of Ni-Based Concentrated Solid-Solution Alloys Using DFT Dilpuneet S. Aidhy; University of Wyoming, United States.

3:00 PM BREAK

SESSION ES5.12: Metallic Systems V

Session Chairs: Dilpuneet Aidhy and Jean-Paul Crocombette
Thursday Afternoon, April 20, 2017
PCC North, 200 Level, Room 223

3:30 PM *ES5.12.01

Towards a Multiscale Experiment of Irradiated Material with High-Energy Synchrotron X-Rays Meimei Li; Argonne National Lab, United States.

4:00 PM ES5.12.02

Stability and Evolution of Cavities in Aluminum—Experiments and Modeling Camille Jacquelin; CEA Saclay, France.

4:15 PM ES5.12.03

Scaling Laws of Cascade and Sub-Cascade Formation in High Energy Ion and Neutron Impacts Andree De Backer; CCFE, Culham Science Center, United Kingdom.

4:30 PM ES5.12.04

Proton Irradiation Effect on Nanostructured Half-Heusler Thermoelectric Materials Nicholas Kempf; Boise State University, United States.

4:45 PM ES5.12.05

Effect of Precipitation and Precipitate Distribution on the Strength of Immiscible Cu-W Alloys during Ion Irradiation Gowtham Sriram Jawaharram; University of Illinois at Urbana-Champaign, United States.

SESSION ES5.13: Complex Behaviors in Ceramics II

Session Chairs: Dilpuneet Aidhy and Maik Lang
Friday Morning, April 21, 2017
PCC North, 200 Level, Room 223

8:15 AM *ES5.13.01

Investigating the Nature of Defect Behavior and Disorder in Nuclear Materials Maik K. Lang; University of Tennessee, United States.

8:45 AM ES5.13.02

Ultrafast Laser-Induced Irreversible Phase Transformations in Ln₂O₃ Dylan Rittman; Stanford University, United States.

9:00 AM ES5.13.03

Charge Distribution and Chemical Bonds in UO₃ Polymorphs Luis Casillas; University of Tennessee, United States.

9:15 AM ES5.13.04

Nanoscale Mechanical Behavior of Nuclear Materials Ursula Carvajal; Los Alamos National Laboratory, United States.

9:30 AM ES5.13.05

Radiation Defect Dynamics Studied by Pulsed Ion Beams Leonardus Bimo Bayu Aji; Lawrence Livermore National Laboratory, United States.

9:45 AM BREAK