SYMPOSIUM EN17

Structure–Property Processing Performance Relationships in Materials for Nuclear Technologies
December 2 - December 5, 2019

Symposium Organizers
Chaitanya Deo, Georgia Institute of Technology
Maik Lang, University of Tennessee
Simon Middleburgh, Bangor University
Maria Okuniewski, Purdue University

* Invited Paper

SESSION EN17.01: Thorium Based Nuclear Fuels
Session Chairs: David Andersson and Maria Okuniewski
Monday Morning, December 2, 2019
Sheraton, 3rd Floor, Hampton

8:30 AM *EN17.01.01
Fission Products in Thoria Robin W. Grimes 1, Navaratnarajah Kunganathan 2, Partho S. Ghosh 3 and Ashok K. Arya 4; 1Imperial College London, United Kingdom; 2Bhabha Atomic Research Centre, India; 3Los Alamos National Laboratory, United States; 4CEA, France

9:00 AM *EN17.01.02
Radiation Effects in ThO2 Tiankai Yao 1, Viny S. Chauhan 2, Maniesha Kaur Salaken Singh 1, Zilong Hua 3, Antar El-Azab 3, Matthew Mann 4, Thierry Wiss 5, Jian Gan 1, David Hurley 1 and Lingfeng He 2; 1Idaho National Laboratory, United States; 2Purdue University, United States; 3Air Force Research Laboratory, United States; 4Pacific Northwest National Laboratory, United States; 5European Commission Joint Research Centre, Germany

9:30 AM EN17.01.03
Atypical Melting Behaviour of (Th,U)O2, (Th,Pu)O2 and (Pu,U)O2 Mixed Oxides Conor O. Galvin 1,2,3, Patrick A. Burr 1, Bryant B. Jerome 1, 2,3, Matteo Vanazzi 1,2, Matteo Cabrioli 1,2, Boris Paladino 1, Daniele Iadicicco 1,2, Erkka Frankberg 1, 2, Koba Van Loo 2, Jozef Vleugels 3, Konstantina Lambrimou 4 and Fabio Di Fonzo 1, 2, 4; 1Istituto Italiano di Tecnologia, Italy; 2Politecnico di Milano, Italy; 3KU Leuven, Belgium; 4SCK-CEN, Belgium

9:45 AM EN17.01.04
Equilibrium and Irradiation-Induced Point-Defect Disorder in ThO2 and U-Doped ThO2—Modeling and Ion Irradiation Experiments Maniesha Kaur Salaken Singh 1, Tiankai Yao 1, Lingfeng He 2, Antar El-Azab 3 and Sanjoy Kumar Mazumder 4; 1Purdue University, United States; 2Idaho National Laboratory, United States; 3Los Alamos National Laboratory, United States; 4University of Manchester, United Kingdom

10:00 AM BREAK

SESSION EN17.02: Accident Tolerant and Advanced Nuclear Fuels
Session Chairs: Michael Cooper and Shenyang Hu
Monday Morning, December 2, 2019
Sheraton, 3rd Floor, Hampton

10:30 AM EN17.02.01
Atomic Level Study of Oxidation of CeSi2 as an Accident Tolerant Nuclear Fuel Surrogate Robert W. Harrison 1, Robert Worth 1, James Buckley 1 and Tim Abram 1; 1University of Manchester, United Kingdom

10:45 AM EN17.02.02
Specific Heat Measurements on USi from 2.4 K to 398 K Jason Baker 1, Joshua White 1, Aiping Chen 1, Robert Roback 1 and Hongwu Xu 1; 1Los Alamos National Laboratory, United States

11:00 AM EN17.02.03
Fission Gas and Creep Behaviour in U/Si: from DFT Calculations and Atomistic Simulations David Andersson 1, Michael W. Cooper 2, Xiang-Yang Liu 1, Benjamin Beeleer 3, Kyle Gamble 3 and Giovanni Pastore 2; 1Los Alamos National Laboratory, United States; 2Idaho National Laboratory, United States

11:15 AM EN17.02.04
Ceramic Oxide Coatings for Accident Tolerant Fuel Concept in Light Water Reactors Mattia Cabrioli 1, 2, Matteo Vanazzi 1, Erika Frankberg 1, Koba Van Loo 2, Jozef Vleugels 3, Konstantina Lambrimou 4 and Fabio Di Fonzo 1, 2, 4; 1Istituto Italiano di Tecnologia, Italy; 2Politecnico di Milano, Italy; 3KU Leuven, Belgium; 4SCK-CEN, Belgium

11:30 AM EN17.02.05
DFT+U Point Defect Calculations of Uranium Mononitride Ground State and Metastable States Bryant B. Jerome 1 and Dilipunet S. Aidhy 1; University of Wyoming, United States

11:45 AM EN17.02.06
Multifunctional Nano-Ceramic Coatings—The Enabling Technology for Next Generation Nuclear Reactors (Including Fusion) Matteo Vanazzi 1, Mattia Cabrioli 1, Boris Paladino 1, Daniele Iadicicco 1, Erika Frankberg 1 and Fabio Di Fonzo 1, 2, 4; Istituto Italiano di Tecnologia, Italy

12:30 PM EN17.02.07
Specific Heat Measurements on USi from 2.4 K to 398 K Jason Baker 1, Joshua White 1, Aiping Chen 1, Robert Roback 1 and Hongwu Xu 1; 1Los Alamos National Laboratory, United States

1:00 PM EN17.02.08
Fission Gas and Creep Behaviour in U/Si: from DFT Calculations and Atomistic Simulations David Andersson 1, Michael W. Cooper 2, Xiang-Yang Liu 1, Benjamin Beeleer 3, Kyle Gamble 3 and Giovanni Pastore 2; 1Los Alamos National Laboratory, United States; 2Idaho National Laboratory, United States

1:15 PM EN17.02.09
Ceramic Oxide Coatings for Accident Tolerant Fuel Concept in Light Water Reactors Mattia Cabrioli 1, 2, Matteo Vanazzi 1, Erika Frankberg 1, Koba Van Loo 2, Jozef Vleugels 3, Konstantina Lambrimou 4 and Fabio Di Fonzo 1, 2, 4; 1Istituto Italiano di Tecnologia, Italy; 2Politecnico di Milano, Italy; 3KU Leuven, Belgium; 4SCK-CEN, Belgium

SESSION EN17.03: Metallic Nuclear Fuels
Session Chairs: Gianguido Baldinozzi and Maik Lang
Monday Afternoon, December 2, 2019
Sheraton, 3rd Floor, Hampton

1:30 PM *EN17.03.01
Microstructure-Based Model of Gas Bubble Swelling in Polycrystalline U-Mo Fuels by Integrating Cluster Dynamics and Phase-Field Approaches Shenyang Hu 1, Benjamin Beeleer 2 and Douglas Burkes 1; 1Pacific Northwest National Laboratory, United States; 2Idaho National Laboratory, United States

2:00 PM EN17.03.02
Modeling Irradiation Induced Grain Refinement Utilizing Cahn’s Time Cone Method Alejandro L. Figueroa 1, Joshua Pribel 1, Walter J. Williams 1, 2, Rayaprolu Goutham Sreekar Annadanam 1, Edwin Garcia 1 and Maria Okuniewski 1; 1Purdue University, United States; 2Idaho National Laboratory, United States

2:15 PM EN17.03.03
The Effects of Fabrication Parameters on the Microstructure of Monolithic U-Mo Nuclear Fuels Jan-Fong Hwu 1, Dennis Keiser 1, Adam Robinson 1, Brandon Miller 1, Jian Gan 1 and Glenn Moore 1; Idaho National Laboratory, United States

2:30 PM EN17.03.04
Density Functional Theory Study of Uranium-Based Compounds Edmanuel Torres 1, Thaneswvar Kaloni 1 and Jeremy Pencer 1; Canadian Nuclear Laboratories, Canada

2:45 PM EN17.03.05
Defect Clustering in Irradiated Alpha Uranium—Cluster Dynamics Modeling and Ion Irradiation Experiments Fabia Farlin Athena 1, Tiankai Yao 1, Lingfeng He 2, Antar El-Azab 3 and Sanjoy Kumar Mazumder 1; 1Purdue University, United States; 2Idaho National Laboratory, United States

3:00 PM BREAK
2:00 PM EN17.07.02
First Principles Investigation of Cr Segregation Behaviors in Ni-Cr Alloy in Molten Salt Systems Jacob Statt1, Stephen S. Raman2 and Chaitanya Deo3; 1Georgia Institute of Technology, United States; 2Oak Ridge National Laboratory, United States

2:15 PM EN17.07.03
Corrosion Mechanism of Molten Salts on Haynes 230 Alloy Studied Using In Situ Neutron Reflectometry Joohyun Seo, Mathieu Doucet, Gabriel M. Veith, Sheng Dai and James F. Browning; Oak Ridge National Laboratory, United States

2:30 PM EN17.07.04
Trinitium Mobility and Local Chemistry in Fluoride Molten Salts Stephen Lam, Ronald Ballinger, Ju Li and Charles Forsberg; Massachusetts Institute of Technology, United States

2:45 PM EN17.07.05
High Temperature Cell for In Situ Reflectometry of Molten Salts Mathieu Doucet, James F. Browning, Joohyun Seo and Gabriel M. Veith; Oak Ridge National Laboratory, United States

3:00 PM BREAK

3:30 PM EN17.08.02
Free-Energy Functional of the Zirconium-Hydride System from First Principle Calculations Michele Fallarino1, Simon R. Phillpot1, Yongfeng Zhang2 and Larry K. Aagesen3; 1University of Florida, United States; 2University of Colorado, Boulder, United States; 3University of Wisconsin-Madison, United States

3:45 PM EN17.08.03
Oxygen Stoichiometry Deviation in Amorphous ZrO2 and Yttria-Stabilized Zirconia Simon C. Middleburgh1, Michael Rushton2, Ilia Ipatova1, Lee Evitts1 and William E. Lee2; 1Bangor University, United Kingdom; 2Imperial College London, United Kingdom

4:00 PM EN17.08.04
Deformation and fracture of Zirconium Hydrides During Plastic Straining of Zr-4 Luca Real1, Said El Chemaa, Daniel S Balint, Mark R. Wennman and Adrian P. Sutton; Imperial College London, United Kingdom

4:15 PM EN17.08.05
Hydrogen Pickup and Oxidation Kinetics of Zirconium Alloy—Dopant Effects from the Chemo-Mechanical Perspective Jing Yang, Mostafa Yousef and Bilge Yildiz; Massachusetts Institute of Technology, United States

4:30 PM EN17.08.06
Influence of Boron Isotope Ratio on the Thermal Conductivity of Uranium Diboride (UB2) and Zirconium Diboride (ZrB2) Lee Evitts1, Simon C. Middleburgh1, Erofili Kardoulaki2, Michael Rushton1, Ilia Ipatova1 and William E. Lee1,2; 1Bangor University, United Kingdom; 2Imperial College London, United Kingdom

SESSION EN17.09: Poster Session
Session Chairs: Chaitanya Deo, Maik Lang, Simon Middleburgh and Maria Okuniewski
Tuesday Afternoon, December 3, 2019
8:00 PM - 10:00 PM
Hynes, Level 1, Hall B

EN17.09.03
Detection of Low Dose Gamma-Ray Using Color Change of the Organic Conjugated Molecules Seung-Hwan Oh, Jin-Moon Yun and Hyun Bin Kim; Korea Atomic Energy Research Institute, Korea (the Republic of)

EN17.09.04
Anode Material Development for Scale-Up Oxide Reducer in Pyroprocessing Sung-Wook Kim, Min Ku Jeon, Sang-Kwon Lee and Eun-Young Choi; Korea Atomic Energy Research Institute, Korea (the Republic of)

EN17.09.05
Interaction Behavior between U-Zr Alloy Containing Lanthanides and Reusable Crucible Materials Seoungwoo Kuk, KyungChai Jeong, SeokJin Oh, KiHwan Kim and Jeong-Yong Park; KAERI, Korea (the Republic of)

EN17.09.06
Reaction Characterization between Graphite Crucible and U-Zr Melt Seung-Jun H1,2, Jeong-Yong Park3, Seoungwoo Kuk3, KyungChai Jeong4, Sang Gyu Park2, Young-Mo Ko5, Yoon-Myung Woo5 and Young-Kook Lee1; 1Yonsei University, Korea (the Republic of); 2Korea Atomic Energy Research Institute, Korea (the Republic of)

EN17.09.07
Combined Ab Initio and Empirical Model for Irradiated Metal Alloys with Focus on Uranium Alloy Fuel Thermal Conductivity Shuxiang Zhou1,2, Ryan Jacobs1 and Dane Morgan; 1University of Wisconsin-Madison, United States; 2Idaho National Laboratory, United States

EN17.09.08
Effects of Initial Microstructure on the Hot Extrusion Properties of Annular Fuel after Extrusion Sang Gyu Park, Seoungwoo Kuk and Jeong-Yong Park; KAERI, Korea (the Republic of)

EN17.09.10
Determination of Dose Effects on Defect Accumulation under Irradiation in Nanoporous Gold and Niobium via Atomistic Simulations Daniel E. Vizoso1,2; Chattany Deo1 and Remi Dingreville1; 1Georgia Institute of Technology, United States; 2Sandia National Laboratories, United States

EN17.09.11
Reusable Multifunctional 3D Graphene Electrode for Highly Efficient In Situ Extraction of Uranium from Mining and Contaminated Solution Ahmed Elwakeil, Chao Wang and Ju Li; Massachusetts Institute of Technology, United States

EN17.09.13
Glass Degradation and pH Changes in Narrow Openings of Cracks Rama Krishna Chinnam1,2 and William E. Lee2,3; 1University of Limerick, Ireland; 2Imperial College London, United Kingdom; 3Bangor University, United Kingdom

EN17.09.14
Investigations in the UB2-UO2 Advanced Fuel System Fabio Martini1, Iuliia Ipatova1, Lee Evitts1, William E. Lee1, Michael J. Rushton1, Antoine Claisse2 and Simon C. Middleburgh1; 1Bangor University, United Kingdom; 2Westinghouse Electric Sweden AB, Sweden

EN17.09.15
Multifunctional Nanoceramic Barrier for DEMO Breeding Blanket Concepts Boris Paladino1,2, Daniele Iadicicco1, Matteo Vanazzi1,2, Patrizia Munoz1, Teresa Hernandez1, Serena Bassini1, Marco Ulti1 and Fabio Di Fonzo1; 1Istituto Italiano di Tecnologia, Italy; 2Politecnico di Milano, Italy; 3CIEMAT, Spain; 4ENEA, Italy
EN17.09.16 Experimental and Computational Study of Lattice Anharmonicity Effects in Oxide Nuclear Fuels Zilong Hu1, Amey Khanolkar1, Marat Khafizov2, Yuzhou Wang3, Chris Marianetti3, Lyuwen Fu4 and David Hurley1; 1Idaho National Laboratory, United States; 2The Ohio State University, United States; 3Columbia University, United States

EN17.09.17 Combined Molecular Dynamics and Sol-Gel Synthesis to Investigate the Properties of the Pellet-Clad Bonding Layer Dillon Frost1,2, Jessica Carolan-Velisek1, Conor O. Galvin1, Edward Obbard1, Michael W. Cooper2 and Patrick A. Burr2; 1UNSW, Australia; 2Australian Nuclear Science and Technology Organisation, Australia; 3Los Alamos National Laboratory, United States

EN17.09.19 Measuring Retention and Erosion Properties of SiC and W-SiC Coatings Exposed to High-Flux Ion Irradiation in an RF Plasma Source Gregory Sinclair1, Tyler Abrams2, Stefan Bringuier3, Dan Thomas4, Leo Holland3,4, Sean Goedermans5, Gokul Vasudevanmuthy6, Jonathan Yu7 and Russell Doerner7; 1Oak Ridge Associated Universities, United States; 2General Atomics, United States; 3University of California, San Diego, United States

EN17.09.20 The Effect of Flux on the Irradiation-Induced Precipitation in AlSi-316L—An In Situ TEM Study, Italo M. Oyarzabal1,2, Mathew A. Tunes2, Osmane Camara2, Emily Arad2, Inamul Haq Mtr3, Gaetano Greaves2, Jonathan A. Hinks4, Paulo F. Fichtner1 and Stephen Donnelly5; 1IFRGS, Brazil; 2University of Huddersfield, United Kingdom

SESSION EN17.10: Nuclear Materials—Ceramics and Composites

Wednesday Morning, December 4, 2019
Sheraton, 3rd Floor, Hampton

8:15 AM *EN17.10.01 Radiation Damage in Ceramics—The View From Microscopy Karl R. Whittle; University of Liverpool, United Kingdom

8:45 AM EN17.10.02 Modelling of Crack Nucleation and Propagation in SiC/SiC Accident-Tolerant Fuel During Routine Operational Transients Using Peridynamics Thomas Haynes and Mark R. Wenman; Imperial College London, United Kingdom

9:00 AM EN17.10.03 Irradiation of Carbide Composites for Next Generation Nuclear Reactors Daniel Runtil; University of Liverpool, United Kingdom

9:15 AM EN17.10.04 Radiation Tolerance of Stabilized Alumina Coatings—An In Situ Irradiation Study Matteo Vanazzi1, Davide Lotiacono1,2, Wei Chen1, Meimei Li1, Marco G. Beghi2 and Fabio Di Fonzo1; 1Istituto Italiano di Tecnologia, Italy; 2Politecnico di Milano, Italy; 3Argonne National Laboratory, United States

9:30 AM EN17.10.05 Metal/Carbon Nanotube Composites Enhance Strength and Ductility, Even During Radiation Damage Kang Pyo So1, Penghui Cao1,2, Young Hee Lee1, Michael P. Short1 and Ju Li2; 1Institute of Technology, United States; 2University of California, Irvine, United States; 3Sungkyunkwan University, Korea (the Republic of)

9:45 AM EN17.10.06 Investigation of Helium Precipitates in Ta(Ti)/Zr(Ti) Nanocomposites Sisi Xiang, Kelvin Y. Xie, Jan Metcalf and Michael J. Demkowicz; Texas A&M University, United States

SESSION EN17.11: Irradiation Simulations and Performance

Wednesday Afternoon, December 4, 2019
Sheraton, 3rd Floor, Hampton

1:30 PM *EN17.11.01 We Need More Realistic Corrosion Tests to Provide Confidence in Safety Cases for Radwaste Disposal William E. Lee; Bangor University, United Kingdom

2:00 PM EN17.11.02 Structure-Property Relationships of Copper Coating Materials for Canada’s Used Nuclear Fuel Containers Jason Tam1, Bosco Yu1,2, Weiwei Li1, Jason Giallonardo1, Jane Howe1 and Uwe Frost1,2; 1University of Toronto, Canada; 2McMaster University, Canada; 3Nuclear Waste Management Organization, Canada

2:15 PM EN17.11.03 Complexation/Speciation—New Insight Studies of the Secondary Phase Formation under Repository Conditions Nieves Rodríguez-Villagra, L.J. Bonales and J. Cobos; CIEMAT, Spain

2:30 PM BREAK
Radiation Tolerant Ceramics for Nuclear Waste Immobilization—Structure and Stability of Zinc Substituted Hollandites with High Cesium Loading
Kyle S. Brinkman, Clemson University, United States

Ion Irradiation-Induced Volume Swelling and Microcrackling in Multilayer Glass Ceramic and Crystalline Ceramic Nuclear Waste Forms
Ming Tang, 1 Los Alamos National Laboratory, United States; 2 Clemson University, United States

Physics-Based Mesoscale Models of Ion Exchange in Hierarchical Materials
Yulan Li, Shenyang Hu, Chuck Henager, Theodore M. Besmann, Agnes Grandjean, and Hans-Conrad Zur Loye; Pacific Northwest National Lab, United States; University of South Carolina, United States; Univ Montpellier, France; CEA, France

Progress in Flash Sintering of UO2
Erofili Kardoulaki, Darrin Byler, and Ken McClellan, Los Alamos National Laboratory, United States

Crystal Growth and Scintillation Properties of Ternary Halides for Gamma Spectroscopy
Mariya Zhuravleva and Matthew Loyd, The University of Tennessee, Knoxville, United States

Robust Perovskite Single Crystal Devices for Efficient Gamma-Ray Detection
Jeremy Tisdale, Michael Yoho, Shreuth Shreshtha, Kasun Fernando, Sergio Tretiak, Darrin Byler, and Ken McClellan; Los Alamos National Laboratory, United States

Passive Radiofrequency Dosimeter Tag Based on Flexible Radiation-Sensitive Oxide Field-Effect Transistor
Tobias Cramer, Ilaria Fratelli, Pedro Barquinha, Rodrigo Martins, Elvira Fortunato, and Beatrice Fraboni; University of Bologna, Italy; Universidade Nova de Lisboa, Portugal

Thermal Diffusivity Degradation and Defect Density Prediction in Self-Ion Implanted Tungsten Using Transient Grating Spectroscopy
Mohamed Abdallah Reza, Hongbing Yu, Kenichiro Mizohata, and Felix Hofmann; University of Oxford, United Kingdom; University of Helsinki, Finland

Processing-Structure Related Performance of Irradiated Relaxor-Ferroelectric Thin Films
Evelyn Chin, Cory D. Cress, and Nazanin Bassiri-Gharb; Georgia Institute of Technology, United States; U.S. Naval Research Laboratory, United States

Non-Destructively Uncovering Aging and Irradiation Relationships for Nuclear Material Health Assessment and Forensics
Michael P. Short, Cody Dennett, Saleem Aldajani, Benjamin Dacus, Caitlin Huotlaimen, Ulla Ehrnsten, M. Grace Burke, Kudzanai Mukihawa, Ihor Radchenko, Kai Chen, Ziv Ungarish, Michael Aizenshtein, Eyal Yahel, Phil Eftsing, Thak Sang Byun, and Joe Wall; Massachusetts Institute of Technology, United States; VT Technical Research Centre, Finland; University of Manchester, United Kingdom; Xi'an Jiaotong University, China; Nuclear Research Center Negev (NRCN), Israel; Ben-Gurion University of the Negev, Israel; Vattenfall AB, Sweden; Pacific Northwest National Laboratory, United States; Electric Power Research Institute (EPRI), United States

Thermodynamics and Electronic Structure of Actinide Based Metal-Organic Frameworks from Density Functional Theory Calculations
Shubham Pandey, Zhilin Jia, Brian Demaske, Otega Ejegbavwo, Natalia Shustova, Wahyu Setyawan, Chuck Henager, and Simon R. Phillpot; University of Florida, United States; Sandia National Laboratories, United States; University of South Carolina, United States; Pacific Northwest National Laboratory, United States

Nanoscale Cross-Plane Thermal Transport and Structural Characterization of Swift Heavy Ion Irradiated LiF Crystals
Ainur Koshkinbayeva, Azat Abdullaev, Zhanatay Nurekeyev, Vladimir Skuratov, and Zhandos Utegulov; Nazarbayev University, Kazakhstan; Flerov Laboratory of Nuclear Reactions, Joint Institute for Nuclear Research, Russian Federation; National Research Nuclear University MEPhI, Russian Federation; Dubna State University, Russian Federation