MiNES
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TECHNICAL PROGRAM

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Fundamental Irradiation Damage- Session I

Tuesday AM **Room: Allegheny**
November 9, 2021 **Location: Omni William Penn Hotel**

Session Chair: M. G. Burke, Oak Ridge National Laboratory

8:00 AM Invited
Cancelled: On the Exploitation of Databases to Predict the Embrittlement of Reactor Pressure Vessels: *M. Serrano*[1]; L. Malerba[1]; D. Ferreño[2]; [1]Ciemat; [2]Universidad de Cantabria E.T.S. de Ingenieros de Caminos
The integrity assessment of the RPV is traditionally based on the estimation of the radiation damage (hardening and embrittlement) by means of generic embrittlement trend curves (ETC). In this paper, the first results of tasks 4.2 "Machine learning to model RPV LTO" of the EU-funded project ENTENTE, on the estimation of transition temperature shift the based on the use of the ASTM PLOTTER database to train and validate a number of Machine Learning regression models. These results outperform the prediction ability of existing embrittlement trend curves. In addition, the Permutation Importance algorithm was used to identify the most relevant features on the shift and the Partial Dependence Plots were used to estimate the individual influence of each of the features. This work received partial financial support in the frame of the Euratom research and training programme 2019-2020 under grant agreement No 900018 (ENTENTE project)

8:40 AM
Next Steps for Improved Defect Production and Mixing Parameters: Beyond NRT DPA, ARC-DPA and RPA: *S. Zinkle*[1]; [1]University of Tennessee
Quantitatively accurate model predictions of radiation effects processes in materials requires knowledge of several defect production and mixing parameters. The international benchmark for defect production (NRT dpa) was developed in the mid 1970s based on relatively simplistic binary collision approximation simulations, and was shown to be inaccurate for energetic displacement cascades within two years of its publication. Two improved parameters known as athermal recombination corrected (ARC-DPA) and replacements per atom (RPA) have recently been recommended to account for in-cascade recombination and mixing in energetic displacement cascades. However, these parameters are only valid for temperatures near absolute zero. Consideration of correlated recombination effects leads to additional modifications of the NRT dpa value for all irradiation sources. This presentation will summarize experimental and modeling studies that indicate the correlated recombination-corrected defect production (CORR-DPA) at elevated temperatures is ~20-30% of the NRT dpa for energetic cascades and electron irradiations, respectively.

9:00 AM
Comparison of Temperature-dependent Swelling Behavior in FCC Compositionally Complex Alloys and 316H Stainless Steel under Heavy-ion Irradiation: *C. Parkin*[1]; M. Moorehead[1]; M. Elbakhshwan[1]; K. Sridharan[1]; L. He[2]; A. Couet[1]; [1]University of Wisconsin-Madison; [2]Idaho National Laboratory
In-core structural materials for advanced reactor designs are expected to demonstrate superior resistance to environmental degradation to currently-licensed stainless steels and ferritic-martensitic steels. Compositionally complex alloys (CCAs), which have already shown reduced void swelling compared to less complex binary and ternary alloys, present the opportunity to advance fundamental understanding of matrix composition as a design parameter for irradiation resistance, opening novel alloy design pathways for advanced reactor applications. To compare their swelling behavior to conventional structural materials, two FCC CCA compositions were irradiated to 100 dpa alongside 316H stainless steel at the UW Ion Beam Laboratory using 4MeV Ni ions at multiple temperatures. TEM characterization of irradiated samples is performed to determine the swelling as function of temperature as well as void size and elemental distribution as function of depth. The swelling-temperature bell shape curves are used to assess the void swelling resistance of CCAs relative to more conventional alloys.

9:20 AM
Free Surface Impact on Radiation Damage in Pure Nickel by In-situ Self-ion Irradiation: Can It be Avoided?: K. Ma[1]; B. Décamps[2]; T. Jourdan[1]; F. Prima[3]; *M. Loyer-Prost*[1]; [1]Cea; [2]CNRS/ Université Paris-Saclay; [3]PSL Research University, Chimie ParisTech-CNRS
In-situ irradiation in a Transmission Electron Microscope (TEM) is a powerful tool to study microstructural evolution, and obtain an insight into dynamic mechanisms of fundamental radiation damage. Howerver, a major issue of these studies is the influence of free surfaces, acting as a strong sink for radiation-induced defects.In this work, in-situ irradiation experiments are combined with a calculation model to get a better understanding of the so-called surface effect and determine in which conditions it could be avoided. Nickel is chosen for the high mobility of its self-interstitials. Ultra-high purity Ni thin foils are in-situ irradiated by 2 MeV $Ni2^{+}$ ions at high temperatures (400-700°C) using the JANNuS-Orsay facility. Microstructural evolution and dislocation loop characteristics are finely analyzed in function of specimen thickness.

9:40 AM
Pushing towards the Limits in Characterization of Radiation Damage: J. Lim[1]; E. Prestat[2]; A. Sand[3]; D. Mason[1]; A. Fellman[4]; Q. Ramasse[5]; *G. Burke*[2]; [1]UKAEA/CCFE; [2]University of Manchester; [3]University of Aalto; [4]University of Helsinki; [5]University of Leeds
Being able to image and characterize the nature and characteristics of irradiation-induced defects (ID) at various damage levels in nuclear material is crucial for physics understanding, performance prediction and next-generation materials development. No characterization technique yet exists to provide detailed analysis of ID from less than 1 nm and at atomic level. According to Molecular Dynamics (MD) estimates, ID clusters that are less than 2 nm in size may contribute to ~97% of the overall defect population at low DPA, and these 'invisible' ID will have a significant contribution to the hardening effects on the irradiated material. AtomCRaD is a EUROfusion funded project to develop modern advanced Scanning Transmission Electron Microscopy (STEM) technique that couple with STEM image simulation and outputs from MD simulations to characterize small ID, < 2nm in diameter, in crystalline materials. In this talk, we will present the outcomes of AtomCRaD and limitations of this technique.

10:00 AM Break

Nuclear Fuel Cycles- Session I

Tuesday AM **Room: Conference Center A**
November 9, 2021 **Location: Omni William Penn Hotel**

Session Chair: C. Yablinsky, Los Alamos National Laboratory

8:00 AM Invited
Recent Advances in Pyroprocessing of Light Water Reactor Fuel: *K. Hawthorne*[1]; [1]Argonne National Laboratory
Reprocessing of used nuclear fuel is a key step in enabling the deployment of advanced nuclear reactors and minimizing the amount of radioactive material that must be disposed of as waste. Pyroprocessing safely and efficiently recycles used nuclear fuel into usable components by applying electrochemical operations in molten salt electrolytes. For light water reactor (LWR) fuel, the oxide is electrochemically reduced to metal, then electrorefined to recover a pure uranium product. The fission products are removed from the salt electrolyte and immobilized in durable waste forms for disposal. These processes are well understood at the laboratory scale, but the impacts of salt chemistry and cell geometry on process efficiencies must be determined on scaled-up systems to optimize production methods, process controls and monitoring, and product quality. Recent work at Argonne National Laboratory on understanding aspects of the process electrochemistry and engineering at multiple scales will be discussed.

8:40 AM
Instrumentation in Molten Salt Systems: Commercial Availability, Custom Solutions, and Gaps: *A. Burak*[1]; X. Sun[1]; E. Hamilton[2]; M. Simpson[2]; D. Killinger[3]; S. Phongikaroon[3]; [1]University of Michigan; [2]University of Utah; [3]Virginia Commonwealth University
Few commercial instruments can be applied to molten salt work. Others require fabrication/construction in-house and some do not exist or are in their infancy. Monitoring molten salt parameters such as temperature, composition, and redox potential is essential to infer the property evolution of materials exposed to molten salts. Commercialized technology is sparse for measuring parameters in molten salts. To measure parameters, more difficult than temperature, there is a dearth of technologies commonly requiring instruments to be built in-house. Reliable, optimized instruments, with quantified uncertainty, facilitate advanced and comparable studies. The use of uniform instrumentation reduces time spent designing and characterizing instrumentation, which can be better spent designing experiments, and ease comparison between different studies in the literature. This work discusses commercially available instruments for molten salts, prevalent in-house solutions, and where development of new instrumentation is needed. In addition, recent advances in instrumentation development for the VTR will be discussed.

9:00 AM
Deliquescence of Eutectic LiCl-KCl Diluted with NaCl for Interim Waste Salt Storage: *C. Decker*[1]; J. Howard[1]; L. Gardner[2]; A. Harward[1]; G. Fredrickson[3]; T. Yoo[3]; M. Simpson[1]; K. Carlson[1]; [1]University of Utah; [2]Argonne National Laboratory; [3]Idaho National Laboratory
Molten eutectic LiCl-KCl is a widely used electrolyte for electrorefining uranium from spent nuclear fuel. Due to the hygroscopic nature of this salt, careful handling and storage is required to avoid deliquescence and corrosion of container materials. This study investigated a potential processing path for reducing the deliquescence through dilution with NaCl. The hydration behavior of LiCl-KCl diluted with NaCl was evaluated in terms of mass gain due to water absorption, visual evidence of deliquescence, and visual evidence of corrosion to stainless-steel containers in a humid air environment. Pure LiCl-KCl exhibited a 50 mass% increase due to water absorption and exhibited deliquescence after 24 hours. 89 mass% NaCl was required in order to prevent deliquescence. Dilution with 89% NaCl was also found to protect stainless steel crucibles from corrosion. Corrosion, thus, appears to require deliquescence. While NaCl dilution decreases steady state hydration and eliminates deliquescence, storage volume is increased ~10x.

9:20 AM
Perovskite-derived Cs2SnCl6-Silica Composites as Advanced Waste Forms for Chloride Salt Wastes: Y. Kun[1]; B. Riley[2]; J. Vienna[2]; D. Zhao[1]; *J. Lian*[1]; [1]Rensselaer Polytechnic Institute; [2]Pacific Northwest National Laboratory
Advanced materials and processes are required to separate halides and fission products from complex salt waste streams associated with the chemical reprocessing of used nuclear fuels and molten salt reactor technologies and immobilize them into chemically durable waste forms. We explore an innovative concept using metal-halide perovskites (MHPs) as advanced host phases to incorporate Cs and Cl with very high waste loadings. Wet chemistry-synthesized Cs2SnCl6 powders from CsCl salts are encapsulated into a silica matrix to form a composite using spark plasma sintering with tunable Cs and Cl loadings. The MHP-silica composites display exceptional chemical durability with the long-term release rates of Cs and Cl comparable to or outperforming the state-of-the-art waste form materials despite significantly higher waste loadings. The scalable synthesis of the MHPs from wet-chemistry opens up new opportunities in designing advanced salt waste forms for the sustainable development of advanced fuel cycles and next-generation reactor technologies.

9:40 AM
A First-principles Database Approach to Predicting Trans-uranic Waste Forms: M. Christian[1]; H. Tisdale[1]; G. Morrison[1]; A. Hines[1]; H. zur Loye[1]; T. Besmann[1]; *A. Mofrad*[1]; [1]University of South Carolina
First-principles density-functional theory (DFT) provides an efficient way to screen trans-uranic (TRU) waste form candidates. To this end, the Center for Hierarchical Waste form Materials (CHWM) has created a structural database based on known parent structures to generate hypothetical TRU crystal structures. The calculated formation enthalpies for the candidate structures are then compared to formation enthalpies of competing reaction products, following the methodology of the Open Quantum Materials Database (OQMD). The results provide relative stabilities that are used to speculate on formation probability. Our calculations using this approach have led to the discovery of new structures, encouraging its expanded adoption.

10:00 AM Break

Versatile Test Reactor

Tuesday AM **Room: Urban**
November 9, 2021 **Location: Omni William Penn Hotel**

Session Chair: A. Couet, University of Wisconsin-Madison

8:00 AM Invited
Overview of in Reactor Mechanical Testing in the Versatile Test Reactor: *T. Saleh*[1]; J. Tucker[2]; S. Briggs[2]; M. Okuniewski[3]; C. Topbasi[4]; [1]Los Alamos National Laboratory; [2]Oregon State University; [3]Purdue University; [4]Electric Power Research Institute (EPRI)
The Versatile Test Reactor (VTR) is a fast spectrum test reactor proposed by the U.S. Department of Energy to provide a relevant experimental environment to test materials in conditions expected for advanced reactors. Instrumented in-reactor fast neutron spectrum mechanical testing is currently very difficult globally due to loss of experimental capability and limited numbers of fast test reactors. The VTR will provide a robust experimental environment for both materials irradiations and in-reactor mechanical and environmental testing. Among a large design team consisting of national laboratories, universities and industrial partners, the materials team, led by Los Alamos National Laboratory, Oregon State University, Purdue University and EPRI, has been working to design in-reactor mechanical testing rigs, associated diagnostics, as well as an open test assembly to house the experiments. This talk will review the status of these mechanical testing designs, environmental considerations, and plans for integrating them in the reactor.

8:40 AM
In Situ Mechanical Testing Method for Materials in Gaseous Environments: *P. Beck*[1]; J. Quincey[1]; D. Mangus[1]; A. Koziol[1]; G. Young[1]; G. Mignot[1]; S. Briggs[1]; J. Tucker[1]; [1]Oregon State University
Advanced heat transfer fluids (such as He, supercritical CO_2) for Gen IV reactor designs are being considered for their increased efficiency and power density at high temperatures. In situ mechanical testing of structural materials is needed to qualify materials for safe use in reactor designs. Simulated operating conditions make such work challenging due to high temperature, pressure, and geometric constraints impeding traditional crack growth testing. This work presents a novel, low-profile mechanism for crack growth testing in reactor environments, featuring a metal bellows and using a modified electric potential drop method. This compact device can be deployed in-core and will enable environmentally assisted crack growth testing. Low-cycle fatigue tests are performed on 316/316L stainless steel in a variety of elevated temperature (550°C) gaseous environments, including air, He, and supercritical CO_2. Analogous tests are conducted in a traditional load frame to compare and validate the new testing method.

9:00 AM
Cancelled: Emissivity Measurements of Silicon Carbide Cladding Samples for Use in Gas Cooled Fast Reactor: *N. Sutton*[1]; R. Vaghetto[1]; Y. Hassan[1]; P. Sabharwall[2]; [1]TA&M Thermal Hydraulics Lab; [2]Idaho National Laboratory
There is a strong need for further characterization and measurements of thermal properties of the materials to be tested in the Gas Cooled Fast Reactor (GFR) cartridge during irradiation test campaigns that will be conducted at the Versatile Test Reactor (VTR). Due to high operating temperature, radiation heat transfer is expected to play an important role in the GFR core heat transfer, and must be properly characterized. Emissivity measurements of cylindrical silicon carbide cladding samples have been conducted to study the dependency on the operating temperature and surface roughness. The measurement system is based on infrared technology and utilizes a reference with known properties of emissivity. High-temperature paint, with known emissivity as a function of temperature, was selected as the reference to conduct the measurements and estimate the uncertainty. Emissivity of the samples was measured for samples of two different surface roughness and at temperatures up to approximately 500 °C.

9:20 AM
Design and Operation of an Out-of-pile Liquid Sodium Experimental Facility for Mechanical Testing: *D. Mangus*[1]; P. Beck[1]; G. Mignot[1]; W. Marcum[1]; J. Tucker[1]; S. Briggs[1]; [1]Oregon State University
The U.S. Department of Energy initiated the Versatile Test Reactor (VTR) program to address the capability gap pertaining to in-pile testing of engineering materials in prototypical environments proposed for the Generation IV fission reactors. Oregon State University (OSU) is performing work to develop a mechanical and environmentally assisted crack growth testing apparatus that can be housed within a fully instrumented VTR cartridge loop. OSU's newly developed Glovebox for Experimental Liquid Sodium (GELS) facility is an out-of-pile thermal-hydraulic system that can provide purified liquid sodium to experimental loops and vessels within an inert glovebox. Integrated into GELS is the Corrosion Experimental Loop (CEL) which will house a compact loading mechanism to assess the viability of the loading systems' ability to facilitate crack growth in structural alloys tested in liquid sodium media. This presentation will highlight the capabilities of OSU's GELS facility for materials degradation testing in support of SFR-related research.

9:40 AM
Fracture Mechanics-based Testing and DCPD in FLiNaK: *X. Quintana*[1]; J. Quincey[1]; P. Beck[1]; G. Young[1]; S. Briggs[1]; J. Tucker[1]; [1]Oregon State University
Advanced reactor coolants such as molten salts pose unique challenges for test systems designed to study environmentally assisted cracking (EAC). Challenges with in-situ testing include immersing the sample in molten salt while preventing air exposure and providing sample access for real-time load control and monitoring of crack initiation and growth. An in-situ mechanical test system has been developed that addresses these challenges and is capable of state-of-the-art, fracture mechanics-based EAC testing in molten salt. Slow strain rate and K-controlled fatigue crack growth tests were performed utilizing DCPD for in-situ data collection. Initial tests have been conducted using 316 stainless steel in molten FLiNaK at temperatures up to 700°C. Samples were characterized post-test via scanning electron microscopy to elucidate the salt's influence on stress corrosion cracking. Inductively coupled plasma-based salt impurity measurements are also used to correlate specimen performance in the salt environment.

10:00 AM Break

Fuels and Actinide Materials- Fabrication Methodology

Tuesday AM **November 9, 2021**

Room: Urban **Location: Omni William Penn Hotel**

Session Chair: D. Andersson, Los Alamos National Laboratory

10:30 AM Invited
Advanced Technology Fuel Accelerated Development at Bangor University: *S. Middleburgh*[1]; P. Makrurunje[1]; F. Martini[1]; M. Bolukbasi[1]; M. Rushton[1]; W. Lee[2]; [1]Bangor University; [2]Bangor University; Imperial College London
Bangor University's Nuclear Futures Institute was initiated in 2017 to grow expertise and train new scientists and engineers in the North Wales region of the UK. Developing new technologies for the nuclear fuel cycle has played a central role in the group, linking to our strong international collaborators within universities, national laboratories, and industry. Advanced technology fuels (ATFs) are being developed simultaneously using experimental efforts and through modelling methods, accelerating our understanding towards a commercially viable concept. The focus of this presentation will be to highlight the advances made in several kernel fuel and composite fuel concepts that incorporate higher uranium densities (e.g. with the inclusion of UN), burnable absorbers (for example ZrB2), high thermal conductivity or a combination thereof. The experimental techniques applied have an eye to industrial scalability, and the modelling techniques consider not only the materials aspects but also the fuel cycle economics.

11:10 AM
Synthesis of UN-U3Si2 Composite Fuels by Spark Plasma Sintering and Properties Characterization: *B. Gong*[1]; E. Kardoulaki[2]; A. Broussard[1]; D. Zhao[1]; J. White[2]; K. Metzger[3]; M. Sivack[3]; K. Mcclellan[2]; E. Lahoda[3]; J. Lian[1]; [1]Rensselaer Polytechnic Institute; [2]Los Alamos National Laboratory; [3]Westinghouse Electric Company
UN-U3Si2 composites are considered as a potential candidate of accident tolerant fuels because of their high uranium density and thermal conductivity. However, the UN-U3Si2 composite experiences thermal mismatch-induced micro-cracking in the fuel pellets sintered by conventional approaches. Here, we explore the feasibility of using spark plasma sintering (SPS) to synthesize UN-U3Si2 composites with different fractions of silicides (25 ~ 75 wt%). The phase and microstructure of the UN-U3Si2 composites are characterized, and micro-cracking can be mitigated by controlling sintering conditions. Thermal-mechanical properties and oxidation resistance of the composite fuels are characterized by laser flash, indentation and dynamic oxidation tests. An UN-50 wt% U3Si2 composite displays simultaneously-high strength and fracture toughness and excellent thermal conductivity. The onset temperatures of the composites are close to 530 °C, suggesting an improved oxidation resistance than monolithic UN. These results highlight the potential of synergizing UN and U3Si2 in composites with enhanced properties.

11:30 AM
Fabrication of Potentially High Burnup Annular U-10Zr Fuel by SPS: *D. Zhao*[1]; M. Benson[2]; F. Lemma[2]; J. Lian[1]; [1]Rensselaer Polytechnic Institute; [2]Idaho National Laboratory
Contrasting with a solid fuel design, the annular metallic fuel (U-10Zr, wt%) shows ultra-high burnup potential, better fuel-cladding chemical interaction performance, and no need for sodium bonding. During irradiation of U-10Zr, an interconnected porosity allows fission gas to escape to the plenum. Here, annular U-10Zr fuel pellets with controlled porosity and pore structure was fabricated by spark-plasma-sintering (SPS) with a special graphite die design. To mimic the irradiated structure for metallic fuel, pressure-less die design and sacrificed pore formers were used to fabricate the bi-model pore structure fuel, which has interconnected large-sized (20~30 μm) pores embedded with micron-sized fine pores. The homogenous microstructure is achieved by controlling the current flow during the sintering process. The results not only show the capabilities of SPS for advanced fuel fabrication, but can also be used to investigate the properties of irradiated metallic fuel structure with a thermal gradient, simulating the nuclear reactor environment.

Fundamental Irradiation Damage- Session II

Tuesday AM **November 9, 2021**

Room: Allegheny **Location: Omni William Penn Hotel**

Session Chair: Y. Zhang, University of Wisconsin

10:30 AM Invited
Physical Understanding of Radiation Hardening of Neutron Irradiated FeCr Alloys: *C. Pareige*[1]; A. Etienne[1]; P. Gueye[1]; M. Hernandez-Mayoral[2]; A. Ulbricht[3]; F. Bergner[3]; C. Heintze[3]; L. Malerba[2]; N. Castin[4]; G. Bonni[4]; M. Konstantinovic[4]; [1]Normandie Univ, UNIROUEN, INSA Rouen, CNRS, Groupe de Physique des Matériaux; [2]Materials of Energy Interest Division, Technology Department, CIEMAT, Avda. Complutense 40; [3]Institute of Resource Ecology, Helmholtz-Zentrum Dresden - Rossendorf; [4]SCKCEN, NMS institute
High-chromium ferritic-martensitic steels are promising candidates for structural components in Gen-IV and fusion reactors because of their excellent swelling resistance and good thermal properties. At low temperature, the operating window is limited by irradiation hardening and the correlated embrittlement. These are influenced by Cr content but also by impurity content (Ni, Si, P and C) and initial microstructure (ferritic vs martensitic). We investigated these factors in neutron irradiated Fe9Cr alloys and steels with advanced experimental techniques, including PAS, SANS, TEM, APT and mechanical testing. These experimental results are simulated and interpreted from the point of view of the physical mechanisms that drive the microstructure evolution using a physical model that also provides a quantitative prediction of the ensuing radiation hardening and embrittlement, bridging the formation of nano-sized solute clusters with hardening or embrittlement. This work is part of the H2020/M4F project and of the EERA/JPNM.

11:10 AM
The Kinetics and Stability of Alpha Prime (a') Precipitates in FeCr Binary Alloy under Ion Irradiations: Y. Zhao[1]; *A. Bhattacharya*[2]; C. Pareige[3]; C. Massey[2]; J. Poplawsky[2]; P. Zhu[1]; J. Henry[4]; *S. Zinkle*[1]; [1]University of Tennessee Knoxville; [2]Oak Ridge National Laboratory; [3]Université et INSA de Rouen; [4]CEA, DEN, Service de Recherches Métallurgiques Appliquées, Laboratoire d'Analyse Microstructurale des Matériaux, Université Paris-Saclay F-91191 Gif-sur-Yvette, France
Cr-enriched a' precipitates severally degrade the mechanical property of FeCr based Ferritic-Martensitic steels. However, the kinetics and stability of a' precipitation under higher dose rate ion irradiation conditions are not well understood. In this study, High purity Fe-(10-18%)Cr specimens in either solid solution state or pre-aged to form a' precipitates were irradiated with 8 MeV Fe ions at 300-450 °C and 10-5-10-3 dpa/s to final doses of 0.37 or 3.7 dpa. The quantification of a' precipitates after irradiations was performed with atom probe tomography (APT) located at ORNL's CNMS. The critical irradiation condition (temperature and dose rate) for a' to form was found to be 300 °C and 10-3 dpa/s in Fe18Cr. At conditions where a' were observed, the evolution of size and number density of precipitates follows an Ostwald ripening mechanism, the kinetics of which is modified by the irradiation dose rate and temperature.

11:30 AM

Effect of Cr and Temperature on Dislocation Loops in Heavy Ion Irradiated Ultra-high Purity FeCr Alloys: *Y. Li*[1]; A. Bhattacharya[2]; L. Wang[1]; Y. Zhao[1]; S. Zinkle[1]; J. Henry[3]; [1]University of Tennessee Knoxville; [2]Oak Ridge National Laboratory; [3]The French Alternative Energies and Atomic Energy Commission

In Fe and Fe-Cr alloys, a/2<111> and a<100> type loops are observed after irradiations. In this study, we performed multi-temperature (300-450°C) irradiation using 8 MeV Fe ions (ion range of 2 µm) to midrange doses of ~0.35 and 3.5 dpa at dose rates of 10-5 and 10-4 dpa/s on Fe and Fe-xCr model alloys (x = 3- 18wt.%). Loop identification used a combination of conventional diffraction contrast TEM imaging techniques and the g·b method. Nearly all loops were interstitial-type. We observed petal-shaped loop clusters in samples at 450 °C and 0.35 dpa. At 350°C and 0.35 dpa, dislocations decorated by loops were the major phenomenon. At 350°C and 3.5 dpa midrange dose, ½ <111> loop fraction increased with increasing irradiation depth, from16% in the near-surface region (0-300nm) to 81% in the beyond-damage region (2350-2600nm) in Fe. Mean loop diameter decreased from 20 nm to 7nm with Cr addition.

Nuclear Fuel Cycles- Session II

Tuesday AM **Room: Conference Center A**
November 9, 2021 **Location: Omni William Penn Hotel**

Session Chair: J. Lian, Rensselaer Polytechnic Institute

10:30 AM Invited

How Does PUREX Actually Work and What Do Chemists Do?: *J. Shafer*[1]; [1]Colorado School of Mines

The Plutonium, Uranium, Reduction, Extraction Process (PUREX) is the de facto approach for post-irradiation separations of plutonium and uranium. While this process has been in place for 70 years, the underpinning chemistry that controls PUREX is diabolically complicated and only recently have approaches been developed that can provide the near-molecular resolution necessary to understand process dynamics. This presentation will focus on recent developments in understanding the PUREX process, how this new understanding can explain undesirable phenomena like interfacial precipitates (CRUDs) and liquid third phase formation, and the benefits of new technologies that are not centered on PUREX chemistry. These new technologies include online monitoring, monoamide extractants and mixed actinide recovery approaches which could efficiently support a fast reactor fuel cycle. The presentation will be presented in a way to hopefully answer the question, "PUREX has been in use for roughly 70 years, why are chemists still working on this process?".

11:10 AM

Development and Application of an Interatomic Potential for the Investigation of Mixed Oxide Compounds Containing Americium: *M. Bertolus*[1]; S. Orlat[1]; B. Labonne[1]; [1]CEA

Americium is a chemical element produced in nuclear reactors, whose strong radiotoxicity is a major issue for the management of nuclear waste. One solution envisaged to reduce the amount of americium in waste is to separate it and to transmute it in reactor into a less radiotoxic element. This requires, among other things, a very good knowledge of the thermodynamic properties of Am bearing oxides to control the manufacturing process and predict the phases formed under irradiation. Atomic scale modelling, e.g. classical Molecular Dynamics, is a suitable tool for the calculation of thermodynamic properties to complement experimental characterizations. It requires, however, precise interatomic potentials.We parameterized a potential for Americium with oxidation state + III in the formalism developed by Cooper, Rushton and Grimes and validated it against available experimental data. The potential was then applied to determine thermodynamic properties of (U,Am)O2 as a function of Am content and/or temperature. This project has received funding from the Euratom research and training programme 2019-2020 under grant agreement No 945077.

11:30 AM

Radiation Damages Bohr's Metrics: The Elemental Landscape: *J. Sublet*[1]; M. Gilbert[2]; [1]IAEA; [2]United Kingdom Atomic Energy Authority

Nuclear interactions can be the source of atomic displacement; post-short-term cascade annealing defects; atomic, lattice interstitial gas dislocation; atomic activation, transmutation and heating in irradiated structural materials. Such quantities are derived from, or can be correlated to, nuclear kinematic simulations of the energy spectra of primary atomic recoil distributions, and the quantification of the numbers of secondary defects produced per primary as a function of the available recoils, residual or transmutant and emitted particles. Novel data forms for 83 naturally occurring element that include total and partial neutron defect-energy production, gas production cross section and kinetic energy release in material KERMA factors, have been systematically derived from ENDF/B-VIII.0, JENDL-4.0, JEFF-3.3, TENDL-2019 and CENDL-3.2 libraries. Numerical instance of integral damage quantities for legacy and novel nuclear components material alloys in NNPs, piles, fusion and accelerator devices typical irradiation conditions are been simulated in order to applicably founds material damage metrics landscape.

Fuels and Actinide Materials- HTGR Fuels

Tuesday PM **Room: Urban**
November 9, 2021 **Location: Omni William Penn Hotel**

Session Chair: E. Sooby, University of Texas at San Antonio

1:30 PM

Cluster Dynamics Simulations of Fission Gas and Product (Xe, Ag) Diffusivities in TRISO UCO Fuel Kernels: X. Liu[1]; C. Matthews[1]; W. Jiang[2]; M. Cooper[1]; J. Hales[2]; *D. Andersson*[1]; [1]Los Alamos National Laboratory; [2]Idaho National Laboratory

The UCO fuel kernels used in TRISO particles consist of a uranium dioxide (UO_2) and uranium carbide (UC_2) mixture. UC_2 is added to suppress the formation of carbon monoxide gas, however it also alters the chemistry (non-stoichiometry) of the UO_2 matrix by imposing reducing conditions, which is known to influence diffusion parameters governing gas and fission product release. In the present study, density functional theory (DFT) and empirical potential calculations are used to determine the diffusion mechanisms of Xe (fission gas) and Ag (fission product) in UO_2 under the reducing conditions generated by the presence of UC_2. The calculated diffusion parameters are first used in thermodynamic and kinetic models to predict diffusion for intrinsic conditions, after which the same information is utilized in cluster dynamics simulations to estimate the impact of irradiation on defect transport. The application of the resulting diffusion model in Bison fuel performance simulations is demonstrated.

1:50 PM
Microstructural Analysis of Oxidized Tristructural Isotropic Particles (TRISO) in Mixed Gas Atmospheres: *K. Montoya*[1]; B. Brigham[1]; T. Gerczak[2]; E. Sooby[1]; [1]University of Texas at San Antonio; [2]Oak Ridge National Laboratory
Certain, proposed off-normal scenarios lead to the exposure of HTGR fuel elements to steam. Subsequently, graphite matrix degradation and OPyC evolution will produce volatile gaseous oxidation products and potentially expose the TRISO particle's SiC layer to a mixed gas atmosphere. The SiC layer acts as the structural component and primary fission product barrier; oxidation induced damage to the SiC can lead to particle failure. This study investigates the impact of steam ingress to the SiC layer by characterizing microstructure evolution of the oxidized surface. Surrogate, SiC exposed, TRISO particle oxidation testing atmospheres in the thermogravimetric analyzer included low partial pressures of steam (<0.2 atm H2O) and carbon monoxide (<1000 ppm) at high temperatures (1300°C < T <1600 °C). Microstructural analysis of the oxidized SiO2-SiC interface was performed utilizing focused ion beam milling, scanning electron microscopy and limited transmission electron microscopy in addition to surface chemistry analysis via x-ray photoelectron spectroscopy.

2:10 PM
Oxidation Performance of High Uranium Density Fuels for Light Water Reactors: *J. White*[1]; J. Stull[1]; S. Paisner[1]; T. Coons[1]; E. Kardoulaki[1]; K. McClellan[1]; [1]Los Alamos National Laboratory
High uranium density fuels are currently being considered for drop in replacement in the nuclear reactor fleet. This class of fuels, such as UN, provides higher thermal conductivity and improved plant economics relative to native UO2, while also overcoming the neutronic penalties of accident tolerant based alloys. Many of the fundamental mechanisms underlying the oxidation behavior of UN has not been properly investigated in the literature to date. To this end, this work investigates the fundamental corrosion mechanisms in high temperature steam and hydrogen environments to elucidate the governing corrosion mechanisms. Application of inert coatings on UN using electroless deposition will be discussed as a potential method to mitigate washout in these fuels with steam oxidation and microstructural evaluations. Discussion will assess the practical application of coatings in a commercial setting as well as evaluating this as a method to minimizing or preventing oxidation in this class of nuclear fuels.

2:30 PM
Fabrication and Properties of Uranium Dioxide-uranium Boride Composites: *E. Kardoulaki*[1]; [1]Los Alamos National Laboratory
UO_2 composites with UB_2 and UB_4 have been proposed as advanced fuel candidates due to their high thermal conductivity, high melting point, high fissile density and their ability to incorporate a built-in burnable poison by tailoring the targeted $^{10}B/^{11}B$ ratio. In this work, UO_2-UB_2 and UO_2-UB_4 composites were fabricated via spark plasma sintering. The thermal diffusivities of the samples were measured (299 to 1273 K) and were found to increase as a function of boride weight fraction. Our results confirm that UO_2 composites with either UB_2 or UB_4 have increased thermal diffusivity compared to UO_2 across the studied temperature range. Assessment of these results also indicated that in-situ reactions between the UO_2 and boride phases occur that suppress the diffusivity above 800 K. Oxidation of the boride phase was proposed as the underlying reaction and was confirmed through microstructural and crystallographic characterization performed on these samples.

2:50 PM
A Review of Current Understanding of Fluff Formation in Metallic Fuel via EBR-II Data and Modelling and Simulations: *J. Fay*[1]; F. Di Lemma[2]; L. Capriotti[2]; P. Medvedev[2]; J. Lian[1]; A. Gribok[2]; D. Porter[2]; [1]Rensselaer Polytechnic Institute; [2]Idaho National Laboratory
As metallic fuel rods undergo axial swelling in a reactor setting the tops of the fuel rods begin to form a porous structure currently labeled "fluff", which impacts source term release and core reactivity. The mechanisms and environmental factors that control fluff formation are currently unknown and need to understood and modeled for the advancement of reactor designs that utilize metallic fuels. This project is a first step in this process and primarily involves examining past experimental data from the experimental breeder reactor II experiment (EBR II) in order to build correlations between fluff formation and key factors such as operating temperature, fuel composition, and burnup. The end goal of this project will be to create accurate fluff models and to incorporate them into the BISON fuel code in order to improve simulation of metallic fuels.

3:10 PM Break

Fundamental Irradiation Damage- Session III

Tuesday PM — **Room: Allegheny**
November 9, 2021 — **Location: Omni William Penn Hotel**

Session Chair: B. Uberuaga, Los Alamos National Laboratory

1:30 PM Invited
Point Defect Evolution under Irradiation: Finite Size Effects and Spatio-temporal Correlations: *E. Martinez Saez*[1]; F. Soisson[2]; M. Nastar[2]; [1]Clemson University; [2]DEN-Service de Recherches de Metallurgie Physique, CEA, Universite Paris-Saclay
We show a large discrepancy in the defect concentrations between standard rate theory (SRT) and the atomistic kinetic Monte Carlo (AKMC) when the average number of defects in the AKMC simulation box is close or lower than one. The reason is that AKMC naturally captures strong space and time correlations between vacancies and interstitials generated by the finite size of the periodic simulation box. These correlations strongly affect the recombination rate and the point defect concentrations but SRT fails to predict them. We introduce a Correlated Pair Theory (CPT) which fully takes into account the correlations between vacancy and interstitial pairs and predicts point defect concentrations in good agreement with AKMC simulations. Inversely, we show here that the CPT can be used to modify the elimination rates in the AKMC simulations, so as to yield point defect concentrations in agreement with SRT.

2:10 PM
Cavity Formation in Ion Irradiated Fe and Fe-Cr Ferritic Alloys: *Y. Lin*[1]; A. Bhattacharya[2]; J. Henry[3]; S. Zinkle[1]; [1]University of Tennessee; [2]Oak Ridge National Laboratory; [3]CEA
To provide a better understanding of the formation of cavities in ferritic steels, we have performed multi-temperature (400-550˚C) simultaneous dual-beam ex-situ and in-situ irradiations on a series of ultra-high purity Fe, Fe-Cr alloys (3-14 wt% Cr), and several advanced ferritic steels. Helium production rates of 0.1 and 10 appm He/dpa were selected to examine the helium synergistic effects. Transmission electron microscopy was used to characterize the microstructures in more than 50 different irradiated samples. Cavities were observed in all the irradiated samples between 400-550˚C. This indicates that the narrow temperature range of observable cavities reported in prior ion irradiation studies is likely an artifact associated with the use of low ion energies. Cavity swelling as a function of the Cr content is non-monotonic and could be controlled by solute trapping of defects or formation of alpha-prime precipitates leading to increased recombination. Higher He/dpa content resulted in a higher peak swelling temperature.

2:30 PM
Explorations in Automated Cavity Detection Using an Expanded Machine Learning Training Data Domain: *M. Lynch*[1]; R. Jacobs[2]; S. Chen[1]; R. Graham[1]; D. Morgan[2]; K. Field[1]; [1]University of Michigan - Ann Arbor; [2]University of Wisconsin - Madison
The quantification of cavities in post irradiated microscopy is key to understanding materials performance. However, manual detection is a time-consuming process. Recently, machine learning (ML) models have successfully detected and analyzed defects. These models perform at near human levels, but with increased speed and repeatability. A downfall of current models are they are mostly built around a single material/irradiation, meaning their use domain is narrow. Here, we explore the influence of expanding dataset sizes and domain for cavity features. This is accomplished via two expansions of the training data. Firstly, a 30,000+ instances experimental database has been developed to provide an expanded domain space. Secondly, using simplified physics and unirradiated micrographs, artificial data were automatically created and labeled at essentially no cost. Incremental and expanding model training using this combination revealed the correlation between training domain and test instances with model generality increasing with increased training domains.

2:50 PM
Impact of Grain Boundary and Surface Diffusion on Fission Gas Release in UO_2 Nuclear Fuel Using a Phase Field Model: *M. Muntaha*[1]; M. Tonks[1]; D. Kim[1]; [1]University of Floirda
This study aims to quantify the importance of grain boundary and surface diffusion on the fission gas release mechanism in UO_2 nuclear fuel. Most computational studies of fission gas bubble behavior found in the available literature do not consider faster diffusion along grain boundaries, triple junctions, and gas-bubble surfaces. Our study has investigated the importance of grain boundary and surface diffusion on fission gas release in UO_2 nuclear fuel. To do that, we have added a free surface on a specific boundary on the domain to observe the gas release amount through the free surface. We have incorporated diffusion heterogeneity for providing a faster diffusion path along the grain boundary and interface. We have developed and applied a phase-field model using an open-source finite element tool MOOSE for mesoscale modeling. Our model predicts that incorporating diffusion heterogeneity changes the way microstructure evolves and changes the fission gas release rate.

3:10 PM Break

Nuclear Fuel Cycles- Session III

Tuesday PM	**Room: Conference Center A**
November 9, 2021	**Location: Omni William Penn Hotel**

Session Chair: J. Shafer, Colorado School of Mines

1:30 PM Invited
Beta Transmutations in Apatite with Ferric Iron as an Electron Acceptor – Implication for Nuclear Waste form Development: *J. Wang*[1]; [1]Louisiana State University
Apatite-structured materials are considered for immobilization of fission products from reprocessing nuclear fuel because of their chemical durability and compositional and structural flexibility. It was hypothesized that the effect of beta decay on stability can be mitigated by introducing an appropriate electron acceptor at the neighboring sites in the structure. Decay series ^{137}Cs ^{137}Ba and ^{90}Sr ^{90}Y ^{90}Zr were investigated using a spin-polarized DFT approach to test the hypothesis. Apatites with compositions of $Ca_{10}(PO_4)_6F_2$ and $Ca_4Y_6(SiO_4)_6F_2$ were selected for radionuclides Cs and Sr incorporation respectively. Ferric iron was introduced in the structure as an electron acceptor. Electron density of states, crystal and defect structure, and energies confirm the structural and compositional adaptability of apatites upon beta transmutations. The study suggests that apatite-structured materials could be promising nuclear waste forms to mitigate the beta decay-induced instability, by incorporating variable valence cations such as ferric iron in the structure.

2:10 PM
The Effect of Phase Structure on the Aqueous Corrosion of Yttrium Disilicate: *K. Bryce*[1]; K. Yang[1]; J. Lian[1]; [1]Rensselaer Polytechnic Institute
In deep geological repositories, rare earth elements may react with silicates found in the surrounding engineered barrier systems to form rare earth disilicates ($RE_2Si_2O_7$). This study investigates the chemical durability of $Y_2Si_2O_7$ polymorphs with different phases (amorphous, alpha, beta, and gamma) in dense sintered pellets by semi-dynamic leaching tests. The gamma phase showed the lowest leaching rates for both Y and Si, followed by beta, alpha and the amorphous pellet, suggesting a strong impact of phases on chemical durability of disilicates. Incongruent leaching was observed for all phases with a preferential release of Y from the matrix. Microstructural analysis of the post leaching sample revealed variations in the level of corrosion of the surface grains for the beta and gamma pellets.

2:30 PM
Predicting Phase Stability of Potential Actinide-bearing Hollandite Waste Forms Using First Principles Calculations: *A. Mofrad*[1]; M. Christian[1]; J. Shcorne-Pinto[1]; T. Besmann[1]; [1]University of South Carolina
Fission product, cesium-137 with a half-life of approximately 30 years, has been well known as problematic for waste forms. Titanate-based hollandites have long been considered effective phases for sequestering cesium, having the formula $A_{1.33}(Ti^{4+},B)_8O_{16}$, where A is an alkali/alkaline earth element and B is a metal. Due to the beta decay of ^{137}Cs, hollandites must be energetically stable not only to immobilize cesium, but also to remain stable when it is replaced by its decay product, barium. In this study, we have investigated the structural stability of actinide (U, Np, and Pu)-bearing hollandites, that is, when actinides co-exist at B-sites with titanium, to allow their consideration as both a cesium/barium and actinide waste form. The predicted formation enthalpies from density functional theory have provided insight into the stability of these hollandites as a function of composition which are being used to target synthesis efforts.

2:50 PM Break

Plenary

Tuesday PM	**Room: Grand Ballroom**
November 9, 2021	**Location: Omni William Penn Hotel**

Session Chair: C. Yablinsky, Los Alamos National Laboratory

4:00 PM Introductory Comments

4:30 PM Plenary
The Xe-100 Advanced Reactor Concept: *E. Mulder*[1]; [1]X-energy
X-energy's ARDP concept is a pebbled bed reactor based on HTGR technology. The Xe-100 has a continuously fueled, multi-pass fuel cycle based on the UCO TRISO-coated fuel particles developed as part of the DOE's NGNP program. This presentation highlights some of the safety characteristics due to the choice of materials in the reactor design. Aspects of the multi-physics simulation of the reactor, its materials and associated fuel cycle will be addressed.

Fuels and Actinide Materials- Metallic Fuels I

Wednesday AM **Room: Grand Ballroom**
November 10, 2021 **Location: Omni William Penn Hotel**

Session Chair: B. Beeler, North Carolina State University

8:00 AM Invited
3D-reconstruction via Genetic Algorithms: Application to Metallic Fuel: R. Genoni[1]; D. Pizzocri[1]; F. Antonello[1]; T. Barani[1]; L. Luzzi[1]; *F. Cappia*[2]; [1]Politecnico di Milano; [2]Idaho National Laboratory
Advanced microscopy for nuclear fuels has increased over the last years supporting the understanding of nuclear material irradiation effects. Focused ion beam/scanning electron microscopy (FIB-SEM) serial reconstruction or X-ray tomography are used to determine three-dimensional (3D) microstructure features. These techniques provide fundamental 3D information, but they present some limitations in applications to nuclear fuels, as both techniques can investigate only small amount of material. A cost-effective approach is the reconstruction of the 3D multi-phase material from two-dimensional images. Such approach, despite intrinsically ill-posed, is of great value and applied in many fields. Here we study the fission gas bubbles of irradiated metallic fuels with a combination of image analysis and an optimization technique based on genetic algorithm (GA). The aim is to provide quantitative information regarding the porosity in 3D in U-Pu-Zr fuel with minor actinides and to obtain a correlation between the 3D properties and the measurable 2D quantities.

8:40 AM
Identifying Crystalline Phases in Irradiated U-Pu-Zr Fuels Using TEM: *A. Aitkaliyeva*[1]; T. Rahn[1]; L. Capriotti[2]; [1]University of Florida; [2]Idaho National Laboratory
The structure of metal fuel used in fast reactors is a complex function of composition, porosity, sodium content, texture, defect concentration, and crystalline phases. Of these, crystalline phases are arguably the most important in determining thermal, mechanical, and chemical behaviors of the fuel, and thus dominate the response of the fuel to a given set of operational conditions. This contribution will report on the crystalline phases observed in irradiated U-Pu-Zr fuels, which have been identified using selective area electron diffraction (SAED). In the past, phase identification in both fresh and irradiated fuels was done sporadically using less reliable methods. In this contribution, we report on the systematic radial microstructural examination of irradiated U-Pu-Zr fuels performed using SEM, focused ion beam (FIB) instrument, and transmission electron microscope (TEM). The crystalline phases in irradiated fuels were conclusively identified and the results compared to unirradiated fuels.

9:00 AM
Does the Fuel Fabrication Method Have an Impact on the Fuel Performance Microstructure in Uranium-molybdenum?: *M. Okuniewski*[1]; G. Park[1]; L. Ecker[2]; S. Gill[2]; D. Murray[3]; [1]Purdue University; [2]Brookhaven National Laboratory; [3]Idaho National Laboratory
Uranium-molybdenum (U-Mo) fuels have applications within both research and test reactor fuels, as well as fast reactor fuels. Each of these reactor types requires differing fabrication methodologies, thus resulting in varied microstructures prior to reactor insertion. Specifically, U-Mo fuels are cast and then rolled to produce a monolithic foil, whereas fast reactor U-Mo fuels are simply cast to produce a fuel rod. Therefore, it is of interest to understand how fabrication influences irradiation performance. This research explored low fluence neutron irradiation effects on rolled and cast U–10 wt.%Mo microstructures as a function of dose and temperature. The evolution of phase fractions, lattice parameters, and strain, was determined with synchrotron X-ray diffraction. Electron microscopy was utilized to complement the phase identification, identify decomposition regions, and characterize defects.

9:20 AM
Cancelled: Zirconium Redistribution in a High Burnup U-10Zr Metallic Fuel: *T. Yao*[1]; M. Benson[1]; L. Capriotti[1]; [1]Idaho National Laboratory
Zirconium (Zr) redistribution inside an irradiated U-10Zr (weight %) metallic fuel can significantly change fuel performance and reactor safety margin. Inside a reactor, with increase of burnup, concentric zones form inside U-10Zr fuel with presumably different U matrix phases. Following the temperature gradient from center to rim, the matrix phase changes from gamma to beta and to alpha phase. Gamma phase has the highest Zr content whereas beta phase has the lowest Zr content. The mechanism of Zr redistribution is often attributed to the low solubility of Zr inside beta U phase. This work investigates a U-10Zr fuel irradiated to a local burnup of ~12.4 % atomic percent at the Fast Flux Test Facility. Transmission electron microscopy reveals a nanoscale Zr rich phase redistribution in different zones for the first time to support a better understanding of Zr redistribution in irradiated metallic fuel.

9:40 AM Break

Fundamental Irradiation Damage- Session IV

Wednesday AM **Room: Urban**
November 10, 2021 **Location: Omni William Penn Hotel**

Session Chair: E. Martinez, Clemson University

8:00 AM Invited
Cancelled: Low Temperature Hardening-embrittlement Phenomenon IN 9-14% Chromium Based Ferritic-martensitic and Oxide Dispersion Strengthened Steels: *A. Bhattacharya*[1]; S. Levine[2]; Y. Katoh[1]; S. Zinkle[3]; [1]Oak Ridge National Laboratory; [2]University of Tennessee, Knoxville; [3]Oak Ridge National Laboratory; University of Tennessee, Knoxville
High chromium ferritic-martensitic (FM) steels and ODS steels are promising candidates for the fusion first-wall, and claddings/ducts of sodium-cooled fast reactors [1]. However, a narrow operating temperature window, ~330-550°C, is typically envisaged for FM steel thick-wall structures. The upper temperature limit, which may increase to ~650°C with ODS, is due to poor creep strength. The low temperature hardening-embrittlement (LTHE) phenomenon causing fracture toughness loss imposes the lower temperature limit [1]. Currently, LTHE is not well-understood. Here, a phenomenological overview of LTHE is presented to better understand the operating limits for FM steels, using which some alloy design guidance is presented. In addition, the susceptibility of ODS steels to hardening-embrittlement is presented based on compelling new neutron irradiated data from ORNL. Research sponsored the U.S. Department of Energy, Office of Fusion Energy Sciences under contract DE-AC05-00OR22725 with UT-Battelle LLC. [1] S. J. Zinkle et al., Nucl. Fusion. 57(9) (2017) 092005

TECHNICAL PROGRAM

8:40 AM

Cancelled: Decoupling Thermal and Irradiation Effects on Clustering and Chemical Redistribution in 14YWT ODS: *A. Sen*[1]; M. Bachhav[2]; J. Wharry[1]; [1]Purdue University; [2]Idaho National Laboratory

The objective of this study is to understand the roles of temperature and irradiation on nanocluster stability and grain boundary chemistry in 14YWT oxide dispersion strengthened (ODS) steel. ODS steel is being considered for advanced nuclear reactor structural and cladding material. Studies have attempted to understand nanocluster irradiation behavior, but there remains little consensus on the influence of competing factors of thermal diffusion and irradiation disordering. Moreover, synergistic chemical evolution of grain boundaries and nanoclusters has not yet been considered. Here, we conduct separate annealing and irradiation experiments on 14YWT at 400°C and 500°C to 100 dpa using 4.5-5.0 MeV Fe^{++}. We characterize the nanocluster and grain boundary microchemistry using atom probe tomography (APT). Results suggest nanocluster morphology is driven by irradiation, but a combination of irradiation and thermal diffusion produces grain boundary segregation of clustered species. These mechanisms and their influence on properties will be discussed.

9:00 AM

Dose and Temperature Effect on Dispersoids in Neutron Irradiated Oxide Dispersion Strengthened (ODS) Alloys: *S. Levine*[1]; A. Bhattacharya[2]; J. Poplawsky[2]; A. Lupini[2]; D. Hoelzer[2]; Y. Katoh[2]; S. Zinkle[1]; [1]University of Tennessee; [2]Oak Ridge National Laboratory

Although ODS alloys are among the leading candidates for fusion first-wall/blanket (FW/B) structures, the effect of fusion-relevant irradiation on these advanced materials is still not well-understood. Here, three ODS steel variants (12%Cr 12YWT, 14%Cr MA957, and 20%Cr-5.5%Al PM2000) were neutron irradiated in the high-flux isotope reactor (HFIR) at 300-500°C for ~3.5-80 dpa. Previously we revealed at low temperatures and high doses, transformation of the nano-dispersoids included cavitation, amorphization, and formation of internal "cherry-pit" structures. Here we expand upon the effects of neutron dose and temperature on nano-dispersoid stability using analytical scanning transmission electron microscopy (STEM) and atom probe tomography (APT). Possible mechanisms are presented to explain structure-chemistry evolution of the nano-dispersoids. Research sponsored by the U.S. Department of Energy, Office of Fusion Energy Sciences, under contract DE-AC05-00OR22725 with UT-Battelle, LLC. APT/STEM was conducted at CNMS, which is a DOE Office of Science User Facility. Work supported under UTK's GATE Fellowship.

9:20 AM

The Subtle Effects of Nitrogen on Radiation Effects in Tempered Martensitic Steels: *S. Maloy*[1]; B. Eftink[1]; H. Kim[1]; C. Rietema[2]; E. Aydogan[3]; H. Vo[4]; [1]Los Alamos National Laboratory; [2]Colorado School of Mines; [3]Middle East Technical University; [4]University of California, Berkeley

The Nuclear Technology R&D program is investigating options to transmute minor actinides. To achieve this goal, new fuels and cladding materials must be developed and tested to high burnup levels (e.g. >20%) requiring cladding to withstand very high doses (greater than 200 dpa) while in contact with the coolant and the fuel. Tempered Martensitic Alloys are the leading candidates for these extreme service conditions. Recent irradiations on tempered martensitic alloys show that slight variations in the composition of one tempered martensitic alloy, HT9, can improve resistance to low temperature embrittlement. This material maintained 5% uniform elongation after irradiation to 6 dpa at 290C while all other alloys exhibited less than 2% uniform elongation. To investigate the reasons behind these significant improvements, controlled alloys were produced while systematically varying the nitrogen concentration between 10 and 500 wppm nitrogen. Ion irradiations performed on these alloys showed that model alloys with higher nitrogen show a higher loop density while heats of HT9 with controlled nitrogen content show lower overall void swelling and a higher density of fine G-phase precipitates.These results will be summarized along with their correlations with radiation effects in tempered martensitic steels.

9:40 AM

Defect Cluster Configurations and Mobilities in -zirconium: Implications for Breakaway Irradiation Growth: *J. March-Rico*[1]; B. Wirth[1]; [1]University of Tennessee, Knoxville

A key component necessary for the predictive modeling of irradiation growth strains is a detailed understanding of defect cluster configurations and their expected modes of transport. In this work, we use a modern interatomic potential published in 2020 (the BMD19 potential) to analyze the preferred structures and mobilities of SIA and vacancy clusters. We find that small SIA clusters form configurations that are contained entirely within a single basal plane and, consequentially, migrate exclusively in 2-D within the basal plane. Large clusters form perfect dislocation loops and migrate rapidly in 1-D. Conversely, small vacancy clusters migrate either quasi-isotropically or with a preference for migration along the c-axis; this is in stark contrast to the considerable anisotropy of the monovacancy. Therefore, the inherent difference in the anisotropy of diffusion of defect clusters, rather than point defects, will be a critical component for the accurate modeling of microstructural evolution in irradiated zirconium.

10:00 AM Break

Integrated Phenomena- Session I

Wednesday AM **Room: Allegheny**
November 10, 2021 **Location: Omni William Penn Hotel**

Session Chair: J. Carter, Naval Nuclear Laboratory

8:00 AM Invited

Radiation-decelerated Corrosion of Nuclear Structural Materials in Gen IV Reactor Environments: W. Zhou[1]; N. AlMousa[1]; K. Woller[1]; G. Zheng[1]; Y. Yang[2]; M. Lastovich[3]; R. Schoell[3]; P. Stahle[1]; A. Wilkinson[4]; M. Moody[4]; A. Minor[2]; T. Lapington[4]; F. Hofmann[4]; D. Kaoumi[3]; *M. Short*[1]; [1]Massachusetts Institute of Technology; [2]Lawrence Berkeley National Laboratory; [3]North Carolina State University; [4]Oxford University

The effects of ionizing radiation on materials often reduce to "bad news." Radiation damage usually leads to detrimental effects, including radiation-accelerated corrosion. However, we have discovered a subset of conditions, practically useful for nuclear structural materials, where radiation damage decelerates corrosion. For example, proton irradiation decelerates intergranular corrosion of Ni-Cr model alloys and Ni-rich commercial alloys in molten fluoride salt at 600-700°C. We demonstrate this by showing that the depth of intergranular voids resulting from Cr leaching into the salt is reduced by proton irradiation alone. Radiation enhanced diffusion more rapidly replenishes corrosion-injected vacancies with alloy constituents, playing the crucial role in decelerating corrosion. Analogous results for steels in molten lead will also be shown in this talk. Only such fully coupled experiments can show that irradiation can have a positive impact on materials performance, challenging our view that radiation damage always results in negative effects.

8:40 AM

Mitigating Irradiated Assisted Stress Corrosion Cracking with Minor Refractory Element Modification – A High-throughput Approach Using Compositionally-graded Specimen: *J. Yang*[1]; L. Boring[2]; L. He[3]; M. Song[4]; Z. Jiao[4]; Y. Zhang[5]; D. Schwen[3]; L. Shao[2]; X. Lou[1]; [1]Auburn University; [2]Texas A&M Univeristy; [3]Idaho National Laboratory; [4]University of Michigan; [5]University of Wisconsin

Irradiation experiments and post-irradiation material testing are critical for the new alloy development and qualification in reactor cores. It represents the most costly and lengthy step, and typically follows a one-at-a-time experimental paradigm. This study demonstrates the feasibility of using compositionally gradient specimens, fabricated by laser additive manufacturing, to improve the throughput of stainless-steel composition screening for better irradiated assisted stress corrosion cracking (IASCC) resistance. The low-level doping (<1 wt.%) of minor refractory elements was selected because of its significance on the local atomic level heterogeneity. The study confirmed these elements not only interacted with point defects but also resulted in different grain boundary oxidation, as well as grain-boundary-dislocation interaction. The validity of using compositionally-graded specimens in IASCC evaluation has been demonstrated for two testing methods, constant extension rate test and step load test. The advantages and challenges of using compositionally gradient design for IASCC evaluation will be discussed.

9:00 AM

Determination of Tritium Trapping Mechanisms in the TPBAR Aluminide Coating: *A. Chaka*[1]; B. Schmitt[1]; [1]Pacific Northwest National Laboratory

The 316SS cladding and its iron aluminide coating of the Tritium Producing Burnable Absorber Rods (TPBAR) serve as both a structural pressure boundary and a permeation barrier in order to retain tritium within the TPBAR. Experimental results have determined that tritium is retained in the aluminide barrier region at a concentration several orders of magnitude greater than can be explained by solubility alone, suggesting that other trapping or binding mechanisms are involved. The cladding is subject to both hydrogen and tritium flux, so the binding energies of both need to be determined. We utilize first principles quantum mechanics (density functional theory) in combination with ab initio thermodynamics to determine the free energy of binding for tritium and protium in the aluminum-rich phases of the aluminide coating as a function of temperature and pressure. Both Fe and Al vacancy sites are evaluated as well as interstitial sites.

9:20 AM

Understanding Tritium Permeation in FeCrAl Alloys: A. Hoffman[1]; K. Sakamoto[2]; Y. Garud[3]; X. Hu[4]; F. Cappia[5]; R. Rebak[1]; *R. Umretiya*[1]; [1]GE Research; [2]Nippon Nuclear Fuel Development Co.; [3]SIMRAND, LLC; [4]Oak Ridge National Laboratory; [5]Idaho National Laboratory

FeCrAl alloys are an excellent candidate for accident tolerant nuclear fuel cladding due to their corrosion resistance and good mechanical properties. One potential topic for concern recently has been the hydrogen (and in particular tritium) permeation behavior of these alloys. Because ferritic alloys have the potential for having higher hydrogen permeation the current commercial Zr based alloys, tritium generated in the fuel could be released into the coolant water. This presentation will give an overview of the current work being done to understand permeation behavior in ferritic FeCrAl alloys. Attention will be given to the oxide layers which can be generated from the fuel-cladding interface and the coolant cladding interface. Such oxide layers are presumed to significantly decrease the hydrogen permeation in FeCrAl alloys.

9:40 AM Break

Fuels and Actinide Materials- Metallic Fuels II

Wednesday AM
November 10, 2021

Room: Grand Ballroom
Location: Omni William Penn Hotel

Session Chair: E. Kardoulaki, Los Alamos National Laboratory

10:30 AM Invited

The Challenges of -uranium: Fundamental Understanding of a Past and Future Nuclear Fuel Material: *A. Jokisaari*[1]; B. Beeler[2]; M. Tonks[3]; F. di Lemma[1]; K. Mahbuba[2]; A. Rezwan[4]; Y. Wang[5]; T. Yao[1]; [1]Idaho National Laboratory; [2]North Carolina State University; [3]University of Florida; [4]University of Wisconsin; [5]University of Michigan

Metallic uranium is one of the first materials ever used as nuclear fuel; yet it displays complex irradiation behaviors that are still not well understood today. These complex behaviors make the material challenging to use in modern metallic nuclear fuels, but provides a rich arena to investigate the fundamental, multi-scale mechanisms of irradiation damage. Most open research into the irradiation behavior of uranium ceased during the 1960s, while experimental and computational techniques have continued to progress. We apply modern investigation techniques, such as molecular dynamics, phase field modeling, crystal plasticity, and in-situ TEM experiments, to study the fundamental behaviors of α-uranium with and without irradiation. We investigate the properties of point defects, their collection into extended defects and interaction with microstructural sinks as well as mesoscale phenomena such as grain growth, irradiation growth, and plasticity. Recently gained insights also highlight potential avenues of future work.

11:10 AM

Impact of Zirconium Concentration Variation on Metal Fuel Constituent Redistribution: *T. Rahn*[1]; F. Di Lemma[2]; T. Trowbridge[2]; L. Capriotti[2]; A. Aitkaliyeva[1]; [1]University of Florida; [2]Idaho National Laboratory

Constituent redistribution in metal U-Pu-Zr fuels is a complex process driven by gradients in temperature and chemical potential, which produce radially-distributed phase fields, each with different material properties and behaviors. The location and composition of the phase fields evolve dynamically as swelling, fission gas release, and sodium infiltration alter the thermal conductivity of the fuel. Gaps in understanding of these processes limit our ability to model higher-level behaviors such as fuel-cladding chemical interaction and perform design and safety analyses with confidence. To study constituent redistribution in metal fuels, we selected three U-Pu-Zr fuel pin with varying Zr compositions (6-14 wt%) from X441 experiment for postirradiation examination (PIE), which included both non-destructive and destructive analyses. In this contribution, we discuss the results from optical metallography and scanning electron microscopy and compare new PIE results to historical data.

11:30 AM

Electron Probe Microanalysis of Fuel from EBR-II Experiment X441A: Effects of Varying U:Pu:Zr Elemental Ratios: K. Wright[1]; T. Rahn[2]; L. Capriotti[1]; *A. Aitkaliyeva*[2]; [1]Idaho National Laboratory; [2]University of Florida

Three samples from the EBR-II X441A experiment were selected for electron probe microanalysis (EPMA) to determine how varying U:Pu:Zr ratios affects constituent redistribution and fuel cladding chemical interaction (FCCI), and to provide a comprehensive, modern quantitative analysis for model development. The Na-bonded, D9-cladded, irradiated metallic fuel samples experienced burnup ranging from ~9-11.5% fissions per initial metal heavy atom and were all cut from the x/L = 0.65 section of the fuel rod. Samples A814 (U-19Pu-14Zr) and A812 (U-19Pu-10Zr) show similar radial elemental redistribution profiles; however, in the rod's center, A814's U concentration is about 20% lower and its Zr concentration approximately 20% higher than observed in A812. There is no significant Pu profile difference. Sample A814 shows non-uniform FCCI around the fuel periphery, with fuel and cladding constituents migrating further and at larger concentrations on one side compared to the opposite side. Results from all three samples will be presented.

Fundamental Irradiation Damage- Session V

Wednesday AM
November 10, 2021

Room: Urban
Location: Omni William Penn Hotel

Session Chair: J. Trelewicz, Stony Brook University

10:30 AM Invited

Radiation Effects and Thermal Stability in Ferritic Steels and High Entropy Alloys: *E. Aydogan*[1]; O. El-Atwani[2]; K. Iroc[1]; A. Ozalp[1]; S. Maloy[2]; Y. Kalay[1]; [1]Middle East Technical University; [2]Los Alamos National Laboratory

There is a worldwide need of nuclear energy due to the increase in the world's population and the desire to reduce greenhouse gasses from burning of fossil fuels. However, nuclear energy systems operate under high temperatures and stresses, chemically corrosive environments, and high neutron fluxes. Engineered ferritic alloys are one of the best materials for high temperature and extreme radiation environments. Moreover, new material system of refractory high entropy alloys (RHEAs) have demonstrated great promise. In this study, thermal stability and radiation resistance of nanostructured ferritic alloy (NFA), 14YWT, produced by powder metallurgy methods and TiZrHfNbTa RHEAs produced by vacuum arc melting and additive manufacturing techniques have been investigated. Recently, we have shown that NFAs and RHEAs are extremely stable up to >1000 ˚C and they show almost zero swelling under high dose irradiation.

11:10 AM

Effect of Damage Rate and Cascade Size on ' Precipitate Stability in Fe-15Cr: *K. Thomas*[1]; Z. Jiao[1]; G. Was[1]; [1]University of Michigan

Fe-Cr ferritic-martensitic (F-M) steels are candidates for nuclear reactor structural components due to their high resistance to swelling and corrosion. However, these steels are susceptible to Cr-rich α' precipitate formation at low to intermediate temperatures in thermal and irradiation environments. In this study, the effects of damage rate and cascade size on α' precipitate stability is determined using a steady state α' precipitate population formed by 2 MeV proton irradiation at 1x10-5 dpa/s to 1 dpa at 400˚C. Samples were then subjected to further irradiation, varying the damage rate and cascade size using self-ion, proton, and electron irradiation up to 10 dpa at 400˚C. Atom probe tomography (APT) analysis was used to assess precipitate size, number density, volume fraction and Cr content. Results are used to determine the ballistic dissolution factor and to unfold the roles of cascade size and damage rate on α' stability.

11:30 AM

A New Statistical Approach for Atomistic Calculations of Point Defect Formation Energies in Multicomponent Solid-solution Alloys: *Y. Zhang*[1]; S. Masengale[1]; A. Manzoor[2]; C. Jiang[3]; D. Aidhy[4]; D. Schwen[5]; [1]University of Wisconsin-Madison; [2]University of Wyoming ; [3]Idaho National Laboratory ; [4]University of Wyoming; [5]Idaho National Laboratory

Understanding thermodynamic properties of defects is critical for developing multicomponent alloys for nuclear energy applications. Calculating formation energies of point defects in multicomponent alloys requires calculating chemical potential of each alloying element, which induces additional computation cost and extra uncertainty. This talk presents a new, statistical approach for calculating point defects formation energies in multicomponent alloys. The proposed approach can give the statistical distribution of point defect formation energies without separate calculations for chemical potentials, which can still be derived in a self-consistent manner. It is found that, capturing the distributions of formation energies is of critical importance for estimating thermal equilibrium point defect concentrations. The approach is demonstrated using density functional theory calculations for ternary FeNiCr alloy and molecular dynamics simulations for binary UZr alloy as well as a five-element high-entropy alloy. It is straightforward for alloys with any number of alloying elements.

11:50 AM

Effect of Helium Injection Rate on Cavity Microstructure in Dual Ion Irradiated T91 Steel: *V. Pauly*[1]; S. Taller[2]; Z. Jiao[1]; G. Was[1]; [1]University of Michigan; [2]Oak Ridge National Laboratory

Ferritic-martensitic steel T91 heat 30176 was irradiated using defocused 5.0 MeV Fe^{2+} or 9.0 MeV Fe^{3+} ions up to 100 dpa at 445-460˚C with a constant damage rate of 7×10^{-4} dpa/s with co-injected He^{2+} ions at a rate varying between 0.22 and 4 appmHe/dpa. Transmission electron microscopy was used to characterize irradiation-induced cavities. For the first 35 dpa, the He injection rate was kept constant at 4 appmHe/dpa. After 35 dpa, the He injection rate was either kept constant or reduced to 0.22 appmHe/dpa. The cavity microstructure at 72 dpa with a reduction in He injection rate was similar to the constant 4 appmHe/dpa. Characterization results were combined with a model based on the cavity growth rate equation and the critical bubble model to better understand the impact of varying He injection rate on the nucleation of bubbles and their transformation to voids.

Integrated Phenomena- Session II

Wednesday AM
November 10, 2021

Room: Allegheny
Location: Omni William Penn Hotel

Session Chair: G. Meric, Kairos Power LLC

10:30 AM Invited

Kinetics of SiC Reaction with Water and Oxygen Under Light Water Reaction Conditions: *P. Doyle*[1]; S. Zinkle[2]; S. Raiman[3]; [1]Oak Ridge National Laboratory; [2]University of Tennessee, Knoxville; [3]Texas A&M University

SiCf/SiC composites have been identified as a potential accident tolerant fuel cladding. Among the R&D topics requiring investigation, aqueous corrosion behavior under normal operating conditions requires improved understanding. In the present work, SiC was exposed to high purity pressurized water in a constantly recirculating autoclave environment. Exposures ranged between 288°C and 350°C for times up to 2000 h, with either 1-4ppm O2 or 0.15-3ppm H2 dissolved in the water. Oxygen reacted with SiC with a reaction order of 1 and was initially linear with time until grain fallout became prevalent. No localized attack was observed in the absence of oxygen and uniform dissolution is predicted to be below 4μm/5 years, an acceptable rate. A predictive equation is given and compared to other published data. Recommendations are made for future testing parameters, include sample preparation. Funding was provided by the U.S. Department of Energy Office of Nuclear Energy, Advanced Fuel Campaign.

11:10 AM

Structural Materials Testing for the Westinghouse Lead Fast Reactor: *M. Ickes*[1]; P. Ferroni[1]; [1]Westinghouse Electric Company

Westinghouse continues to develop the Lead Fast Reactor (LFR) as its Generation IV reactor concept, with the mission to provide safe, sustainable, and especially economical carbon-free electricity generation to global market. The Westinghouse LFR is a 950 MWt (~460 MWe) pool-type reactor with compact in-vessel heat exchangers and no intermediate heat transport system. The operation of an LFR at temperatures greater than approximately 500°C is challenged by liquid lead corrosion of structural materials. Recognizing that some key components such as the reactor vessel and the primary pumps will operate at cold leg temperature (~400°C), some others will operate at higher temperatures. Investigations into materials integrity under reactor operating conditions to allow operation at higher temperature are therefore an important aspect of LFR development to maximize the economic performance of the LFR. Some key aspects and select results from the R&D campaign supporting the Westinghouse LFR will be presented and discussed.

11:30 AM

3D Reconstruction and Quantification of Oxide Nano-porosity in Zirconium Alloys: *H. Zhang*[1]; A. Couet[1]; T. Kim[1]; W. Howland[1]; [1]University of Wisconsin-Madison

In the corrosion of Zirconium alloy, the oxide grows at a decreasing rate until reaching critical thickness, followed by the sudden loss of the protective property in the oxide and growth of a new cycle of oxide. The oxidizing-induced pores are pathways to oxidizing species in the oxide. TEM is usually used to determine pore density and size. However, due to the size of the pores and the thickness of the TEM samples, some of the pores are invisible in TEM at only one angle. Manually counting pores will also bring some artifacts. We precisely quantify oxide porosity in corroded Zircaloy-4 as function of exposure time and temperatures using manual and machine-learning-based counting. The structure and distribution of pore in different depths are analyzed to study porosity interconnection using 3D pore reconstruction. Then discussed as function of substrate texture to study lattice mismatch vs stress-driven oxide growth.

Fuels and Actinide Materials- Metallic Fuels III

Wednesday PM
November 10, 2021

Room: Grand Ballroom
Location: Omni William Penn Hotel

Session Chair: A. Aitkaliyeva, University of Florida

1:30 PM Invited

Constructing Multi-component Diffusion under Irradiation in U-Mo Alloys: *B. Beeler*[1]; G. Park[2]; M. Okuniewski[2]; Z. Mei[3]; S. Hu[4]; [1]North Carolina State University; [2]Purdue University; [3]Argonne National Laboratory; [4]Pacific Northwest National Laboratory

Under the United States High-Performance Research Reactor (HPRR) program, a number of research reactors are planned to undergo a conversion to U-Mo monolithic fuel. The accurate prediction of fuel evolution under irradiation requires implementation of correct thermodynamic and kinetic properties into fuel performance modeling. One such property where there exists incomplete data is the diffusion of relevant species under irradiation. Fuel performance swelling predictions rely on an accurate representation of diffusion in order to determine the rate of fission gas swelling and local microstructural evolution. In this work, molecular dynamics simulations are combined with rate-theory calculations to determine the radiation-enhanced diffusion of U, Mo, and Xe as a function of temperature and fission rate. In combination with previous studies on intrinsic diffusion and radiation-driven diffusion in U-Mo alloys, this study completes the multi-component diffusional picture for the U-Mo system.

2:10 PM

Three-dimensional Characterization of Pore Evolution in High-burnup U-Mo: A. Figueroa[1]; D. Murray[2]; P. Kenesei[3]; *M. Okuniewski*[1]; [1]Purdue University; [2]Idaho National Laboratory; [3]Argonne National Laboratory

Low-enrichment monolithic uranium-molybdenum-based fuels are of interest due to their potential to replace high-performance research and test reactors in conjunction with global nonproliferation efforts. Swelling in uranium-molybdenum in monolithic and dispersion fuel applications undergo a two-part swelling behavior, with an initial linear swelling rate followed by a subsequent increase in swelling due to irradiation-induced grain refinement. Understanding the porosity development as a function of fission density in this increased swelling rate regime is critical to understand the swelling behavior properly. This work investigates four separate locations on an edge-on miniplates that experienced a burnup between 5-10E21 fissions/cc. Analyzing the porosity in three dimensions utilizing micro-computed tomography creates a better understanding of porosity development as a fission density and rate function. This understanding is crucial for mechanistic modeling of fuel swelling in this increased swelling regime.

2:30 PM

An Investigation of FCCI Using Diffusion Couple Test between UMTZ Alloys and Cladding: *W. Zhuo*[1]; H. Wu[1]; M. Benson[2]; J. Zhang[1]; [1]Virginia Tech; [2]Idaho National Laboratory

Two U-rich alloys containing additives Mo, Ti, Zr are proposed as fuel candidates, the alloys are U-1.5Mo-1.5Ti-7Zr (UMT7Z), and U-2.5Mo-2.5Ti-5Zr (UMT5Z) in wt.%. To investigate their fuel-cladding chemical interactions (FCCIs), the diffusion couple tests were performed between the fuel alloys and the cladding at 600°C. The as-cast fuel alloys and the pre-annealed alloys (annealed at 600C for 168h) were used for comparison because their microstructures and phases were different according to the scanning electron microscope (SEM) characterizations. The cladding materials were Fe and HT9. In those diffusion couples using as-cast alloys, Zr-rind was found at the fuel interfaces. The reaction product UFe2 was found at the HT9 side but not at the Fe side. The interface interaction of those diffusion couples using pre-annealed alloys is expected to be different from that of the as-cast alloys.

2:50 PM
Transmission Electron Microscopy of the Uranium-22.5 Atom% Zirconium System Following Casting, Cold-working, and Annealing: W. Williams[1]; *M. Okuniewski*[2]; F. Di Lemma[3]; T. Yao[3]; [1]Idaho National Laboratory/Purdue University; [2]Purdue University; [3]Idaho National Laboratory
Transmission electron microscopy was performed on uranium-22.5atom% zirconium samples in as-cast, cold-worked, and post-annealed conditions. Samples were characterized through bright field, dark field, energy-dispersive X-ray spectroscopy (EDS), and selected-area electron diffraction (SAED). Phase morphology and bulk microstructure were measured throughout the material processing steps to quantify the evolution of the a-U and d-UZr2¬ lamellar structure. The solubility of Zr in the a-U phase was measured, by semi-quantitative EDS, to be <15atom%. Additionally, EDS identified that the d-UZr2 phase consists of ~66atom% Zr. Zirconium rich (U-80atom% Zr) inclusions were also identified through imaging and EDS. The crystal structure of each phase, including Zr inclusions, was identified with SAED. The SAED of the bulk microstructure indicates deformation-induced grain subdivision following cold-working, as well as recrystallization and growth during annealing. Zirconium inclusions were also observed to undergo a stress-induced phase transformation from a hexagonal to face-centered cubic crystal structure.

3:10 PM
First-principles Study of the Interfaces between Gamma-U and Uranium Carbide: Z. Mei[1]; B. Yei[1]; A. Yacout[1]; *B. Beeler*[2]; [1]Argonne National Laboratory; [2]North Carolina State University
To understand the effect of uranium carbide formation on the mechanical properties of UMo alloy fuel, we investigated the interfaces formed between bcc gamma-U metal and uranium carbide using first-principles density-functional theory calculations. Two representative interfacial plane orientations, i.e., U(110)/UC(100) and U(100)/UC(100), were investigated for different potential terminations of UC. Calculations show that both lattice mismatch and interfacial bonding play crucial roles in determining the interfacial stability and adhesion strength of the gamma-U and UC interfaces. The effect of Mo alloy in gamma-U metal and non-stoichiometric of UC on the adhesion strength of gamma-U/UC interfaces were investigated. We studied the effect of the defect concentration and their locations with respect to the interface on the interfacial stability. Finally, the predicted interface models of gamma-U/UC interface were used to simulate the fracture toughness of gamma-UMo/UC interfaces.

3:30 PM Break

Fundamental Irradiation Damage- Session VI

Wednesday PM **Room: Urban**
November 10, 2021 **Location: Omni William Penn Hotel**

Session Chair: Z. Jiao, University of Michigan

1:30 PM Invited
Radiation Enhanced Diffusion (RED) and the Coupled Effects of Irradiation and Corrosion in Fe_2O_3: K. Yano[1]; A. Kohnert[2]; A. Banerjee[2]; D. Edwards[1]; E. Holby[2]; T. Kaspar[1]; H. Kim[2]; S. Taylor[1]; Y. Wang[2]; *B. Uberuaga*[2]; D. Schreiber[1]; [1]Pacific Northwest National Laboratory; [2]Los Alamos National Laboratory
The extreme environments present in a nuclear reactor do not occur in isolation – they are often coupled. In particular, the defects produced by irradiation have the potential of changing the rates and even mechanisms of corrosion. Here, we examine radiation-enhanced transport in a model oxide – Fe_2O_3 – and use that insight to develop a model of coupled irradiation and corrosion. Fe_2O_3 films with isotopic tracer layers are deposited, irradiated with ion beams, and characterized via atom probe tomography to determine the extent of RED. These results are compared to an atomistically-informed mesoscale model of transport to identify mechanisms responsible for RED. Once validated, the model is used to explore the potential impact of irradiation on the corrosive growth of Fe_2O_3 scales. We find that irradiation can increase growth rates by orders of magnitude and that the growth rate becomes non-monotonic with thickness, a consequence of different regimes of radiation damage evolution.

2:10 PM
Radiation-induced Segregation in Nanocrystalline FeCrNi under Concurrent Grain Boundary Movement: *A. Rezwan*[1]; Y. Zhang[1]; [1]University of Wisconsin Madison
Irradiation of crystalline materials modifies the microchemistry and microstructure, including solute segregation towards defect sinks such as grain boundaries (GBs), known as radiation-induced segregation (RIS). Unlike coarse-grained alloys, where GBs are nearly static, RIS in nanocrystalline is accompanied and affected by concurrent grain growth, either thermal or irradiation induced. This talk presents a phase-field study of concurrent RIS and grain growth in austenitic Fe-Cr-Ni. It is found that the overall RIS is grain size-dependent and increases with increasing grain size. The segregation profile is asymmetrical, with Cr depleted behind and enriched in front of a moving GB. This leads to a heterogenous Cr distribution, depleted in growing and enriched in shrinking grains. These findings highlight different effects of RIS in nanocrystalline alloys than those in their coarse-grained counterparts.

2:30 PM
Suppressing Irradiation Instabilities in Nanocrystalline Tungsten through Grain Boundary Doping: *J. Trelewicz*[1]; W. Cunningham[1]; K. Hattar[2]; Y. Zhu[3]; D. Edwards[4]; [1]Stony Brook University; [2]Sandia National Laboratories; [3]University of Connecticut; [4]Pacific Northwest National Laboratory
Targeted doping of grain boundaries stabilizes nanostructured materials against thermal coarsening, which provides a pathway to advanced alloys containing a high density of defect sinks. However, the impact of dopants on irradiation damage processes in interfaces represents a knowledge gap in radiation-resistant alloy design. In this study, we probe the coupling between microstructural evolution and irradiation damage in nanocrystalline W-20 at.% Ti using complementary in situ and ex situ ion irradiation experiments. Compared with a nanocrystalline W film, the W-Ti alloy is shown to exhibit smaller defect loops and a delayed saturation dose with a period of irradiation induced grain growth during the transient damage accumulation regime. Application of a thermal spike grain growth model reveals that the microstructure in the W-Ti alloy plateaus to a much finer grain size relative to predictions for pure W, indicating that doping for enhanced thermal stability also stabilizes the material against irradiation-induced instabilities.

2:50 PM
Correlating Properties of Irradiation Produced Nanoscale Superlattices with Irradiation Condition Parameters: *A. Schneider*[1]; Y. Zhang[1]; J. Gan[2]; [1]University of Wisconsin Madison; [2]Idaho National Laboratory
Void superlattices have been known to form in materials under irradiation for decades. Although the exact mechanisms of such lattice ordering remain debated in the literature, recent theoretical and experimental studies have clarified the role of one-dimensional self-interstitial atoms diffusion in the superlattice formation process. Based on the framework developed in earlier modeling works, the present study aims at providing a deeper understanding of the dependance of several key superlattice properties on irradiation conditions, by combining theoretical analysis and Kinetic Monte-Carlo simulations. The results suggest that superlattice properties such as the lattice constant, ordering, and critical dose and temperature limit of formation are clearly correlated with irradiation condition parameters such as dose rate and temperature. The correlations elucidated by theory and simulations provide deeper insights regarding superlattice formation and constitute a valuable step towards the development of tailor-made meta-materials.

3:10 PM
Study on Role of Irradiation Induced Vacancies and Voids on Strain-induced Martensitic Transformations by Molecular Dynamics: *C. Yang*[1]; Y. Pachaury[1]; A. El-Azab[1]; J. Wharry[1]; [1]Purdue University
Strain-induced martensitic transformations can improve the strength and ductility of face centered cubic metals and alloys. Defects such as vacancies, dislocation loops, and voids – often introduced by irradiation – activate martensitic transformations over a wider range of conditions than the pristine material. However, the mechanisms underlying irradiation-enabled martensite transformations remain unclear. In this work, molecular dynamics simulations study the effect of vacancies and voids on strain-induced transformations. Single vacancies have no resolvable effect on the transformation because they reduce the stacking fault energy by a relatively insignificant margin and do so only if the vacancy is located on the stacking fault plane. Voids, however, activate the martensite transformation through shear strain accumulation around the void due to dislocation pileup. The larger the void, the more pronounced this effect. Mechanisms identified here are consequential to the deformation behavior of porous, nanoporous, irradiated, and hydrogen- or helium-charged steels and FCC alloys.

3:30 PM Break

Integrated Phenomena- Session III

Wednesday PM
November 10, 2021

Room: Allegheny
Location: Omni William Penn Hotel

Session Chair: M. Short, Massachusetts Institute of Technology

1:30 PM Invited
Irradiation Creep and Fatigue Observed via In-situ Electron Microscopy: *K. Hattar*[1]; E. Lang[1]; S. Dillon[2]; [1]Sandia National Laboratories; [2]University of Illinois, Urbana-Champaign
To predict the lifetime of any current or future component in a fission reactor with any degree of certainty requires a fundamental understanding of the materials response to coupled extreme environments. Many recent studies have highlighted that the response of material to two independent sequential harsh environments does not dictate the response to the same environmental exposure when they are simultaneous. We have developed an in-situ Scanning Electron Microscope (SEM) and a Transmission Electron Microscope (TEM) to elucidate the nuances of materials response to these coupled environments. In-situ TEM examples on quantitative room temperature irradiation creep, creep at 1200 °C, high temperature irradiation induced creep, and high cycle fatigue will be presented. Finally, recent efforts to explore coupled liquid, stress, temperature, and radiation environments in both TEM and SEM will be highlighted.SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

2:10 PM
Wear and Friction Behavior of Fuel Pebbles in Molten Fluoride Salt: G. Meric[1]; *L. Vergari*[2]; J. Quincey[3]; R. Scarlat[2]; T. Merriman[4]; M. Hackett[1]; [1]Kairos Power LLC; [2]University of California Berkeley; [3]Kairos Power/Oregon State University; [4]Tribology Associates
Kairos Power's fluoride-salt-cooled, high-temperature reactor (KP-FHR) technology uses a novel combination of existing technologies to achieve unique levels of economy, safety, flexibility, modularity and security for nuclear power production. The KP-FHR is a pebble-bed design that relies on TRISO fuel particles embedded in a graphite-like pebble as a fuel form. During online refueling and operation, fuel pebbles are continuously circulating through pebble handling systems and the core. Characterizing the friction and wear behavior of pebbles as they roll and slide against structural component surfaces and against each other is important for accurate modeling of the core behavior and to predict pebble wear and wear dust production. This talk will present tribology data and microstructural characterization for graphite sliding against 316H stainless steel and graphite in inert gas and in molten fluoride salt. The results exhibit the lubrication effect of fluoride salts.

2:30 PM
Thermal Gradient Effect on the Helium and Intrinsic Defects Transport Properties in Tungsten: *E. Martinez Saez*[1]; D. Maroudas[2]; D. Perez[3]; N. Mathew[3]; B. Wirth[4]; [1]Clemson University; [2]University of Massachusetts; [3]Los Alamos National Laboratory; [4]University of Tennesse
Materials in a fusion reactor are expected to withstand stringent conditions, with high heat and particle fluxes that will create strong gradients of temperature and concentration of diverse species. Defects and He migrate in the presence of the afore-mentioned gradients. We use nonequilibrium molecular dynamics to study the transport properties of He, and self-interstitials in the presence of a thermal gradient in W. We observe that in all cases, the defects and impurity atoms tend to reside in the hot regions of the system. The concentration profile results in an exponential distribution, in agreement with irreversible thermodynamics. We compute the heat of transport for each species resulting in negative terms, indicating that the mass flux is opposite to the heat flux. These results have important implications to plasma-facing materials in fusion environments. We demonstrate that the steady-state profiles when the mass-heat coupling is considered varies significantly from the decoupled case.

2:50 PM
Dependence of Sink Strength Effects on Defect Evolution in Dual-ion Irradiated Additive-Manufactured HT9: *P. Xiu*[1]; N. Sridharan[2]; K. Field[1]; [1]University of Michigan; [2]Lincoln Electric
Additive-manufacturing (AM) is attracting attention in the nuclear materials community for the fabrication of ferritic-martensitic steels due to the flexibility of composition and geometry control of structural components during the build. In this study, the dual-ion-irradiation responses of three conditions of AM-HT9 are evaluated including the as-built (ASB) from the direct-energy-deposition as well as two other conditions from the same build with different post-build heat-treatments (ACO3 and FCRD). The test matrix includes varying irradiation dose from 16.6 dpa to 250 dpa at 445°C, and varying temperatures from 400°C to 480°C with constant injected helium appm/dpa ratio of 4. Significant disparity of radiation responses among the three conditions of AM-HT9 is observed, with ASB condition exhibiting much more retarded defect evolution including Ni-rich clusters and cavity swelling compared to ACO-3 and FCRD. This is probed by discussing the effects of sink strengths in these alloys tailored by AM and heat-treatment processes.

3:10 PM Break

Advanced and Novel Materials- Session I

Wednesday PM **Room: Urban**
November 10, 2021 **Location: Omni William Penn Hotel**

Session Chair: S. Zinkle, University of Tennessee

4:00 PM Invited
Overview of Fuel System Options for Nuclear Thermal Propulsion: *K. Palomares*[1]; D. Burns[2]; H. Gerrish[3]; [1]Analytical Mechanics Associates; [2]Idaho National Laboratory; [3]NASA Marshall Space Flight Center
An in-space propulsion technology, nuclear thermal propulsion (NTP) has the potential to enable faster interplanetary transit times compared to traditional chemical propulsion methods due to its capacity for high specific impulse (900+ s) and thrust (~5 – 250 klbf). Because of these performance attributes, NTP is currently an advanced propulsion technology under consideration by the National Aeronautics and Space Administration (NASA) for future crewed Mars missions. The performance of NTP systems is directly contingent upon the development of a robust fuel form capable of withstanding high power densities and operation in a hydrogen environment at temperatures in excess of 2500 K. NASA, supported by the Department of Energy, is leading the development of NTP fuels and reactor materials under the space nuclear propulsion project. This presentation will overview development needs for fuels in NTP systems, historic and current fuel system options, and their remaining challenges prior to successful implementation.

4:40 PM
Grain Growth and Mechanical Properties of Nano ZrO2 Oxide Dispersion Strengthened Mo30W: *N. Gaffin*[1]; K. Palomares[2]; J. Milner[3]; C. Ang[1]; S. Zinkle[1]; [1]University of Tennessee - Knoxville; [2]Analytical Mechanics Associates Inc.; [3]NASA Glenn Research Center
Molybdenum alloys are ideal candidates for the metal matrix of a cermet based nuclear thermal propulsion system due to their high melting points, hydrogen compatibility, low neutron absorption cross-section, and good strength retention at high temperatures. A molybdenum alloy with 30 wt% tungsten (Mo30W) has been produced by consolidating pre-alloyed powders using spark plasma sintering. Given the high operating temperature of an NTP system (above 2500 K), run away grain growth can be an issue. Oxide dispersion strengthening with nano zirconium dioxide (ZrO_2) is being considered to both strengthen the material and to pin grain boundaries at high temperatures. Pure Mo30W and samples with 1.5 and 10 wt% ZrO_2 have been fabricated. These samples will undergo heat treatments up to 2200 °C (2473 K) to compare the change in grain growth. Both hardness and compressive strength testing will be conducted to determine the strengthening effect of the YSZ additions.

5:00 PM
A Study of the Corrosion Behavior of Cold-sprayed 304L Stainless Steel for Dry Storage Canisters: *R. Chiang*[1]; H. Naralasetty[1]; V. Bhattiprolu[2]; C. Roper[2]; P. Allison[2]; L. Brewer[2]; V. Vasudevan[1]; [1]University of Cincinnati; [2]University of Alabama
Dry storage canisters to store SNF are mainly fabricated from 304L SS. Under certain conditions of humidity, temperature and salt chemistry, their weldments are known to be susceptible to localized corrosion and SCC. Cold spray is emerging as a promising technique for repairing pits and cracks. In this investigation, the corrosion behavior of cold-sprayed 304L was compared to the baseline 304L substrate using DLEPR and EIS. Additionally, changes to the corrosion behavior after heat treatment (recrystallization and sensitization) and with the mechanical surface treatments of LSP and UNSM was also investigated. Characterization of the microstructure was conducted using SEM, EBSD, EDS and TEM. The results indicate a notable difference between the cold-sprayed 304L and baseline material with significant impacts from the heat treatments on the corrosion behavior. The specific complexities as effected by the cold spray process, heat treatment and surface treatment will be presented and discussed.

5:20 PM
Cold Spray for Repair of Nuclear Power Plant Components: *M. Ickes*[1]; A. Parsi[1]; [1]Westinghouse Electric Company
Cold spray is a materials deposition process in which small metallic particles, or blends of metallic and non-metallic particles, are accelerated using a high pressure gas stream above a critical threshold velocity out of a de Laval type rocket nozzle. and bind to a surface of a suitable substrate upon impact. The temperature of the particles are significantly below the melting point of the impinging particles, giving rise to the 'cold' in cold spray. Westinghouse is developing cold spray technology for a wide variety of applications that benefit from cold spray's ability to apply continuous high hardness corrosion resistant material deposits. These include protection from stress corrosion cracking, repair and mitigation of erosion and corrosion damage in carbon steel piping, and dimensional restoration of components.Key results of Westinghouse's research in cold spray will be presented, with applications focused on repair and mitigation of degradation in nuclear power plant equipment.

5:40 PM
Cancelled: Metal and Amorphous Ceramic Composites for Extreme Conditions: *J. Wang*[1]; K. Ming[2]; B. Wei[1]; M. Nastasi[3]; [1]University of Nebraska-Lincoln; [2]Hebei University of Technology; [3]Texas A&M University
Strong, ductile, and irradiation tolerant structural materials are in urgent demand for improving the safety and efficiency of advanced nuclear reactor. Amorphous ceramics could be very promising candidates for high radiation tolerance since they do not contain conventional crystal defects that are induced in crystalline materials under irradiation. However, amorphous ceramics exhibit 'brittle-like' behavior. We realized the strength-ductility-irradiation tolerance combination of amorphous ceramic composites (ACCs) through tailoring nanosized heterogeneities. Principles for the design of such ACCs are that metal elements should prefer to form nanosized metal-rich clusters in ACCs. Moreover, the phase structure and properties of the heterogeneity can be modified by synthesis and annealing conditions. By averting plastic flow localization and enhancing irradiation tolerance, we impart to ACCs the ability to undergo both uniform plastic deformation and irradiation tolerance, markedly advancing their potential for use in nuclear industry as core structural materials.

Fuels and Actinide Materials- Thermal Properties, UN and UC Fuels I

Wednesday PM **Room: Grand Ballroom**
November 10, 2021 **Location: Omni William Penn Hotel**

Session Chair: T. Allen, University of Michigan

4:00 PM Invited
Utilization Potential for the Molten Salts Thermal Properties Database – Thermochemical (MSTDB-TC) in Operational and Safety Analysis for MSRs: *T. Besmann*[1]; J. Ard[1]; J. Yingling[1]; J. Schorne-Pinto[1]; M. Aziziha[1]; M. Aslani[1]; C. Dixon[1]; M. Christian[1]; A. Mofrad[1]; K. Johnson[2]; J. McMurray[2]; [1]University of South Carolina; [2]Oak Ridge National Laboratory
An extensive thermochemical database, the Molten Salt Thermal Properties Database – Thermochemical (MSTDB-TC), has been developed and continues to be expanded to provide for computing detailed thermochemical states for salt and related systems for MSRs. The MSTDB-TC is designed for stand-alone use with equilibrium calculational software, notably FactSage, or with codes such as the open-source Thermochimica which can be coupled to reactor performance and other applications. In the current work, the use of the database in computing reactor states as a function of burnup and consideration of potential accident analysis such as the determination of key species vapor pressures have been explored.

TECHNICAL PROGRAM

4:40 PM

Determination of Chromium Corrosion Potential in the Na-K-Mg-U(III) Chloride Molten Salt: *J. Yingling*[1]; J. Pinto[1]; J. Ard[1]; T. Besmann[1]; K. Johnson[2]; J. McMurray[2]; [1]University of South Carolina; [2]Oak Ridge National Laboratory

Significant strides in the development of the Molten Salt Thermal Properties Database – Thermochemical (MSTDB-TC) will allow the extensive thermodynamic description of salt systems relevant to the design, operation, and regulation of molten salt reactors (MSRs). Given the essential material compatibility requirements for MSR designs, MSTDB-TC provides open access to reliable thermodynamic models useful for prediction of multi-component phase equilibria and other complex processes like corrosion. Chromium in structural materials presents a particular challenge for its formation of halide compounds in salt systems. In this presentation, new phase equilibria measurements for the Cr-U(III) chloride pseudo-binary and Na-Mg-U(III) chloride pseudo-ternary systems will be reported, and their use in the development of predictive phase equilibria for the Na-K-Mg-U(III) chloride salt system is demonstrated. Additionally, the temperature and composition space favorable to inhibit corrosion with chromium is explored.

5:00 PM

Insights into Prediction of Thermodynamic Properties for Chloride Salts for Generation IV MSRs: *J. Schorne Pinto*[1]; J. Yingling[1]; M. Christian[1]; A. Mofrad[1]; M. Aslani[1]; T. Besmann[1]; [1]University of South Carolina

A crucial issue for the development of molten salt reactors (MSRs) is the lack of thermodynamic information for its main constituents, i.e., fuel and/or coolant. For example, enthalpies of liquid-liquid mixing for uranium and plutonium trichloride with alkali metal chloride systems are limited. However, they are important to reliably model thermodynamic properties required from equilibrium calculations of complex systems present in MSRs. The work reported here supports the development of thermodynamic functions through empirical correlations coupled with numerical modeling to predict the enthalpy of mixing for unexplored AkCl-UCl3 and AkCl-PuCl3 (Ak=alkali element) systems. The results contribute to the development of the Molten Salt Thermal Properties Database-Thermochemical (MSTDB-TC), an open-source compendium for MSR applications.

5:20 PM

Molten Salt Thermal Properties Database-Thermochemical (MSTDB-TC) Status and New Assessment of MF-UF_4 (M = Li, Na, K, Cs) Systems: *J. Ard*[1]; J. Schorne-Pinto[1]; J. Yingling[1]; T. Besmann[1]; J. McMurray[2]; [1]University of South Carolina; [2]Oak Ridge National Laboratory

The Molten Salt Thermal Properties Database-Thermochemical (MSTDB-TC) is a freely licensed resource supporting thermodynamic modeling of MSR-relevant fluoride and chloride salt systems. It continues to be expanded with additional components and higher order systems by the University of South Carolina in coordination with Oak Ridge National Laboratory. The current status of the MSTDB-TC is discussed, including newly added and assessed systems. The MF-UF_4 (M = Li, Na, K) systems have been previously modeled using the modified quasi-chemical model in the quadruplet approximation. However, these models failed to obtain a reliable representation of the liquid phase when interpolated to higher order systems. It was necessary to introduce multiple endmembers for UF_4 to accommodate observed variations in coordination numbers in the melt. A new model was therefore developed for the MF-UF_4 (M = Li, Na, K) systems, and to these has been added the newly assessed CsF-UF_4 system.

Material Properties Evolution- Session I

Wednesday PM **Room: Allegheny**
November 10, 2021 **Location: Omni William Penn Hotel**

Session Chair: S. Maloy, Los Alamos National Laboratory

4:00 PM

Development of a Multicomponent Ideal-solution (MCIS) Free Energy Phase-field Model for Simulation of Nuclear Materials Microstructural Evolution: *C. Bhave*[1]; A. Cheniour[2]; D. Schwen[3]; M. Tonks[1]; [1]University of Florida; [2]Oak Ridge National Laboratory; [3]Idaho National Laboratory

The development of grand-potential (GP) based phase-field models requires an analytical inverse function for the concentration of the chemical components in terms of the chemical potentials. Due to the lack of such an inverse function for multicomponent ideal solution free energy functions, past GP models have required the use of simpler free energy functions, limiting the physical accuracy of the models. In this work, we derive a general inverse function for an ideal solution approximation free energy system with multiple components on a single lattice. This MCIS model is then applied to two problems of interest in nuclear materials evolution – molten salt corrosion of Ni-Cr alloys, and intragranular fission gas bubble growth in UO2. The model predictions are compared against predictions made using the Kim-Kim-Suzuki phase-field model to evaluate model accuracy and computational performance.

4:20 PM

Effect of the Inner Liner on Radial Delayed Hydride Cracking: *A. Colldeweih*[1]; P. Trtik[1]; F. Fagnoni[1]; J. Bertsch[1]; [1]PSI

This work investigates radial DHC in unirradiated Zircaloy-2 cladding material with an inner liner. DHC is induced through a three-point bending test from the outside-in direction. Post DHC examinations were conducted with light optical microscopy (LOM), scanning electron microscopy (SEM), and high-resolution neutron radiography. Metallography analysis has characterized the hydrogen precipitation near and around the crack tip, as well as at the liner/matrix interface in front of the crack tip. Fractography analysis was employed to quantify the crack velocities and determine stress intensity factors in combination with finite element modeling (FEM). Through FEM, stress fields as well as stress intensity factors expected at various stages of crack propagation are calculated. At the SINQ spallation neutron source of the Paul Scherrer Institut (PSI), using the Neutron Microscope detector, radiography provided quantitative information about the hydrogen concentration distribution throughout the sample, specifically at and between the liner/matrix interface and crack tip.

TECHNICAL PROGRAM

4:40 PM

Effects of Heat Treatment, Build Angle and Radiation Type on the Hardness and Microstructure of Inconel 625 and 718 Fabricated via Laser-powder Bed Fusion Additive Manufacturing: V. O'Donnell[1]; M. Andurkar[2]; T. Keya[3]; A. Romans[3]; G. Harvill[3]; *J. Gahl*[1]; S. Thompson[2]; B. Prorok[3]; [1]University of Missouri; [2]Kansas State University; [3]Auburn University

Various Inconel 625 and 718 specimens, manufactured via Laser-Powder Bed Fusion (L-PBF), were investigated for micro and nano-hardness, as well as microstructure, before and after irradiations performed at the University of Missouri Research Reactor Center (MURR). Specimens were exposed to a variety of radiation environments. These included a neutron flux of 6.3x10^13 neutrons/cm²/s in the MURR reactor, an accelerator driven fast neutron flux of 3.0x10^9 neutrons/cm²/s, and a direct proton irradiation in excess of 10^14 protons/cm²/s. The MURR cyclotron facility features a 16.5 MeV GE PETtrace cyclotron situated in a vault, allowing for beam extraction and solid target irradiation as well as fast neutron production. Results indicate that, independent of radiation source/type, all L-PBF specimens harden less due to irradiation relative to the wrought control group. Heat treatments at various time lengths and temperatures were found to produce precipitates in the Inconel alloys that affect hardness and radiation damage.

5:00 PM

Mechanical Testing of Fuel Cladding Tubes: *B. Eftink*[1]; M. Hayne[1]; T. Nizolek[1]; C. Liu[1]; T. Saleh[1]; S. Maloy[1]; [1]Los Alamos National Laboratory

Mechanically evaluating tube material is difficult, particularly in the hoop direction. While tensile samples may be extracted to test along the length of the tube, microstructural anisotropy due to processing means those results do not necessarily represent the tube properties in the hoop direction. Compounding the problem is that common techniques for testing tubes, such as burst tests, are difficult to implement and require large quantities of material. Research will be presented on efforts to refine a ringpull mechanical testing technique using analytical strain calculations and digital image correlation. As a result a test fixture was developed that can accommodate a range of tube diameters while being suited for hot-cell testing environments for activated samples. Test results will be from accident tolerant FeCrAl fuel cladding.

5:20 PM

Accessing High Damage Level Microstructures Using Combined Ion and Neutron Irradiation of a 304L Stainless Steel: *Z. Jiao*[1]; S. Levine[2]; M. Song[2]; C. Parish[3]; G. Was[1]; [1]University of Michigan; [2]University of Tennessee; [3]Oak Ridge National Laboratory

Feasibility of extending the neutron irradiated microstructure to high damage level using ion irradiation was investigated on 304L SS. The alloy was previously irradiated in the BOR-60 reactor to 5.5 dpa at 320°C and was subsequently irradiated with a 9 MeV Ni^{3+} ion beam at 10^{-3}dpa/s to a dose of 47.5 dpa at 380, 400 and 420°C. The irradiated microstructures were compared against those from the neutron irradiated sample at the same dose. Combined irradiation produced a better match of radiation-induced segregation (RIS) profiles compared to the ion-only irradiations. The MIK model revealed that the high sink densities established at 5.5 dpa mitigated dose rate sensitivity of RIS at the grain boundary. While all combined irradiation temperatures failed to reproduce Cu-rich precipitates, combined irradiation at 400°C produced a better overall match of Ni/Si-rich precipitates and RIS observed in neutron irradiated sample.

Advanced and Novel Materials- Session II

Thursday AM **Room: Urban**
November 11, 2021 **Location: Omni William Penn Hotel**

Session Chair: C. Lear, Los Alamos National Laboratory

8:00 AM Invited

Advanced Manufacturing for Novel Material Design and Development: *I. Van Rooyen*[1]; [1]Idaho National Laboratory

Developing critical design criteria for new advanced reactor systems, components, and materials requires an understanding of both fabrication and irradiation environments during normal operating and accident conditions. Next-generation researchers and designers are therefore challenged by demands both to improve performance and to remain competitive by shortening development and commercialization for new nuclear reactors and systems. This provides unique and exciting opportunities for all contributors to this field of study. This presentation will offer a strategic overview on the role of advanced manufacturing during the realization of novel materials using case studies that detail current research for novel gradient and composite cladding and coatings, as well as fuel material systems.

8:40 AM

Additive Manufacturing (AM) of Oxide Dispersion Strengthened (ODS) FeCrAl Using In Situ Oxidation: *T. Austin*[1]; S. Zinkle[1]; N. Sridharan[2]; [1]University of Tennessee, Knoxville; [2]Lincoln Electric

Ultra-high-performance structural materials are needed to improve the safety of current fission reactor designs and meet the demands of the extreme environments proposed in advanced reactor designs. Oxide dispersion strengthened (ODS) FeCrAl alloys offer a possible solution by utilizing finely dispersed precipitates to improve high-temperature strength and irradiation tolerance. ODS FeCrAl suffers from production issues like batch-to-batch variability, long lead-times, and low throughput. This work produces ODS FeCrAl using directed-energy deposition (DED) additive manufacturing (AM) by applying an oxygen-rich atmosphere during production to reduce production costs and time. Two different oxygen addition methods were examined across many processing conditions. Sample characterization demonstrates the ability to significantly increase sample oxygen content, produce near 100% dense parts, and produce fine-scale precipitation. Detailed characterization using TEM, APT, and post-build heat treatments have been done to examine the effects of the varied and complex processing conditions under AM on the morphology of these precipitates.

9:00 AM

Ultra-fine Lattice Wicking Structures Additively Manufactured from Tungsten: *C. Romnes*[1]; J. Bottini[1]; O. Mireles[2]; J. Stubbins[1]; [1]University of Illinois at Urbana-Champaign; [2]NASA Marshall Space Flight Center

Additive manufacturing (AM) is particularly promising for manufacturing complex geometries from tungsten and other refractory metals, which are difficult to form using traditional processes. In this study, tungsten lattices were additively manufactured using various laser energy densities. These lattice structures have promising applications in both fission and fusion systems for heat transfer in applications which require radiation resistance at high temperatures. The goal of the work is to investigate the ability to adjust lattice type and printing parameters to vary the resulting fluid flow and mechanical properties of these lattices. To that end, lattice feature sizes were characterized using scanning electron microscopy and flow tests were performed with water and N2 to characterize the pressure drop across these samples. This work will help inform the development of tungsten lattices for nuclear systems, where tungsten is already of major interest for fusion systems for plasma facing and high thermal load structures.

9:20 AM

Innovative Elaboration Method of ODS Ferritic Steels Reinforced by Y2Ti2O7 Pyrochlore Phase Oxide: *G. Josserand*[1]; L. Chaffron[1]; P. Giroux[1]; J. Ribis[1]; D. Simeone[1]; T. Gloriant[2]; [1]CEA; [2]INSA Rennes

Oxide Dispersion Strengthened (ODS) ferritic steels are promising candidates as cladding material for 4th Generation Sodium-cooled Fast nuclear Reactors. Conventional reinforcement is achieved by introducing titanium and yttrium oxide Y2O3 during ball milling with matrix steel powder. The dissolution of the oxide leads to an uncontrolled nucleation of complex oxides during the consolidation by hot extrusion. While some Y-Ti-O nano-particles are highly beneficial to the mechanical behaviour of the material, coarser ones – e.g. TiC, TiO2, Y2O3 – make it brittle. An innovative alloy-design approach is developed at CEA. Nanostructured Y2Ti2O7 pyrochlore phase oxides are elaborated by mechanochemical synthesis, and then introduced in ferritic matrix through ball milling. This way prevents from the appearance of deleterious coarse particles. Mechanical tests reveal a significant improvement in ductility and a low anisotropy, while maintaining a sufficient tensile strength up to 650°C. An extended cold-formability is expected from this innovative ferritic ODS grade.

9:40 AM

Strengthening Effects across Ultrasonic Additive Manufacturing (UAM) Interfaces: *M. Pagan*[1]; S. Zinkle[1]; S. Babu[1]; T. Ohmura[2]; [1]University of Tennessee; [2]National Institute for Materials Science

Ultrasonic additive manufacturing (UAM) technology provides the mechanism for creating advanced structural metals with embedded optical fiber sensors for in-situ strain monitoring in demanding environments such as nuclear reactors. The method for creating these complex structures involves bonding dissimilar metals using high strain rate deformation, although the mechanisms involved have yet to be explored before this study. The refined microstructure and strengthening mechanism across these embedded sensor interfaces are explored using nanoindentation and TEM techniques. Various plastic deformation mechanisms are explored at these interfaces. Refined grain structures, vacancy clusters, and elevated dislocation densities are found to be contributing factors to the observed strengthening across the interface, and a hardness superposition principle is used to describe the combination of these effects. A sensitivity analysis provides insight on their relative potential contributions. This study provides valuable insight into defect mechanisms across micron-scale embedded sensor interfaces which is vital to their technical implementation.

10:00 AM Break

Fuels and Actinide Materials- Thermal Properties, UN and UC Fuels II

Thursday AM	**Room: Monongahela**
November 11, 2021	**Location: Omni William Penn Hotel**

Session Chair: N. Abdul-Jabbar, Los Alamos National Laboratory

8:00 AM Invited

Thermal Analysis of Advanced Nuclear Fuels during Simulated Off-normal Events: *E. Sooby*[1]; B. Brigham[1]; K. Montoya[1]; G. Robles[1]; [1]University of Texas at San Antonio

The evolution of commercial reactor fuel forms and development of the next generations of reactors spark a demand to close existing data gaps in the performance of advanced reactor fuel concepts. Commercial fuel vendors are targeting higher uranium density fuels to enhance fuel economy and better accommodate accident tolerant cladding, and the leading designs for small modular reactors are looking toward particle fuel architectures. A number of data gaps and/or inconsistencies exist for these lesser known fuel concepts, including their performance during off-normal events involving oxidant ingress. Presented is the utilization of thermal analysis in precision engineered atmospheres to probe the stability of high uranium density and particle fuel forms during high temperature transients. In each of the studies presented, a combination of thermogravimetric, differential thermal, and evolved gas analysis are employed in a dynamic measurement of the response of advanced nuclear materials to accident conditions and atmospheres.

8:40 AM

Development and Application of a UN Potential to Defect Properties and High Temperature Elastic Constants: *V. Kocevski*[1]; M. Cooper[1]; A. Claisse[2]; D. Andersson[1]; [1]Los Alamos National Laboratory; [2]Westinghouse Electric Sweden

Atomic-scale modeling of thermophysical and defect properties of UN play an important role in establishing improved models, thus having an accurate interatomic potential is crucial for generating reliable data at finite temperatures using molecular dynamic simulations. We report a new interatomic potential for UN, based on a combination of many-body and pairwise interactions, fitted to experimental and density functional theory (DFT) data. We successfully reproduced experimental lattice parameters, thermal expansion, single crystal elastic constants, and temperature dependent heat capacity. The potential also performs reasonably well in reproducing the DFT calculated energy of stoichiometric defect reactions, and defect migration barriers. Furthermore, the potential predicted that a U split interstitial is more stable than a regular interstitial, later confirmed by DFT calculations. The potential was also used to predict UN single crystal elastic constants and elastic properties at different temperatures, showing that UN becomes softer and more compressible with increasing temperature.

9:00 AM

Chemical Interaction and Incorporation of Lead with Uranium Nitride Fuels: *A. Broussard*[1]; K. Yang[1]; J. Lian[1]; [1]Rensselaer Polytechnic Institute

Uranium Nitride (UN) has been identified as a prime fuel candidate for Lead Cooled Fast Reactors and as part of a fuel-cladding-coolant combination consisting of Uranium Nitride, Alumina-forming Austenitic Alloys, and Lead (Pb). Here we report the findings of using spark plasma sintering (SPS) to synthesis Pb-doped UN pellets with different amounts (5 and 10 wt%) and different sintering parameters (temperature and pressure). Characterization of pellets is performed via Scanning Electron Microscopy, Energy Dispersive Spectroscopy and X-ray Diffraction. Results of characterization for Pb-doped UN pellet sintered at 1550°C exhibit evaporation of Pb out of the UN pellet while a pellet sintered at 1450°C displays diffusion of Pb into the UN matrix. Ongoing experimentation is being conducted at lower temperatures to verify this result. Further experimentation is planned to incorporate UN pellets into liquid Pb to simulate a reactor environment and determine if U dissolves in liquid Pb.

9:20 AM
Phase and Thermodynamic Analysis of Uranium Mononitride in High-temperature Steam Light Water Reactor Atmospheres: *G. Robles*[1]; B. Brigham[1]; J. White[2]; E. Sooby[1]; [1]University of Texas at San Antonio; [2]Los Alamos National Laboratory

Uranium mononitride (UN) is investigated here as an accident tolerant fuel candidate for deployment in light water reactors (LWR) due to advantages in uranium density and thermal conductivity when compared to UO_2. Implementation of a fuel with these properties would allow for increased fuel economy, lower fuel centerline temperatures and longer response times during off-normal conditions. However, data for UN exposures to off-normal LWR atmospheres is limited. Presented here are the results from experimental measurements of UN pellets sintered to theoretical densities > 90% and oxidized in high temperature steam and steam+H_2. Experiments were performed under thermal ramp conditions to 1200 °C and isothermal holds at 400 and 500 °C. Thermogravimetric analysis confirmed a dependence on pellet density to the oxidation dynamics under both ramp and isotherms. Characterization techniques include powder x-ray diffraction, scanning electron microscopy, and energy dispersive spectroscopy detailing the oxidation products and degradation mechanisms present following exposure.

9:40 AM Break

Material Properties Evolution- Session II

Thursday AM
November 11, 2021

Room: Allegheny
Location: Omni William Penn Hotel

Session Chair: B. Eftink, Los Alamos National Laboratory

8:00 AM Invited
Mesoscale Simulations of Interactions between Dislocation Loop and Point Defects in bcc Iron: *H. Xu*[1]; Z. Yu[1]; [1]University of Tennessee
Dislocation loops play a critical role in irradiation-induced microstructural evolution of structural materials. Conventional understanding of the interaction between dislocations loops and point defects (PD), particularly at mesoscale, is challenging and limited. In this study, the capture efficiency and bias factor of dislocation loops are determined using a recently developed method based on the lifetime of point defect computed using kinetic Monte Carlo simulations in a model bcc iron system. Bias factors and maximum swelling rate from this approach are compared with both neutron and ion-irradiation experiments and previous theoretical results. The effects of loop densities, loop sizes and temperatures are systematically examined. Comparative analysis of dislocation loop bias and dislocation bias has also been carried out. This approach also applies to many other mesoscale processes and a variety of microstructure features, such as grain boundaries and interfaces.

8:40 AM
Mechanical Response of HT9 and T91 under Dual-ion and Neutron Irradiations: *P. Zhu*[1]; S. Agarwal[1]; S. Zinkle[1]; [1]University of Tennessee, Knoxville
9-12% Cr ferritic/martensitic steels are promising candidate structural materials for Generation IV fission reactors. HT9 and T91 alloys were subjected to dual-ion (9 MeV Fe^{3+} and 3.42 MeV He^{2+}, 445 and 520 °C) and BOR60 reactor irradiations to quantify the possibility of using ion irradiation to simulate neutron irradiation in microstructures and mechanical properties. Nanoindentation hardness testing was performed with Berkovich indenter to obtain information on the bulk hardness of the dual-ion irradiated samples due to limited damage volumes. For the neutron irradiated samples, both nanoindentation and Vickers hardness testing were conducted. An accurate way to extract bulk mechanical properties form nanoindentation data will be used based on our previous study on FeCr binary alloys. The results of TEM characterization of the bubbles and dislocation loops will be summarized, and detailed comparisons will be provided on the predicted (dispersed barrier hardening superposition) vs. measured strength values of the irradiated specimens.

9:00 AM
Rapid Simulation of the Irradiated Microstructure in Flux Thimble Tubes to High Dose Using Ion Irradiation: M. Song[1]; K. Field[2]; C. Topbasi[3]; *G. Was*[2]; [1]Shanghai Jiao Tung University; [2]University of Michigan; [3]Electric Power Research Institute
Flux Thimble Tubes (FTTs) removed from a PWR were subjected to self-ion irradiation to increase dpa to match the 100 dpa peak in the FTT. Ion irradiated microstructures were compared to those created in reactor to determine the extent to which ion irradiation can be used to predict the microstructure evolution in life extension timeframes. FTT samples were taken from regions of the tube with 38 dpa and 74 dpa and irradiated with 8 MeV Ni3+ at 390 and 410°C and a damage rate of ~ 10-3 dpa/s. Ion irradiation of reactor irradiated samples at 410°C resulted in the same size and number density of nanocavities, loops, and clusters, and RIS at 100 dpa as in the FTT section at the same dose with the exception of Ni-Si-Mn cluster dissolution during ion irradiation. Extension of damage to 160 dpa resulted in precipitation at grain boundaries and grain boundary migration.

9:20 AM
Cancelled: Atomistically Informed Cascade Overlap Model to Predict Alloy 800H Microstructure Evolution during High-dose Neutron Irradiation: *S. Morris*[1]; B. Wirth[1]; [1]University of Tennessee Knoxville
High-dose neutron or self-ion irradiation of Ni-base alloys has been shown to produce large quantities of immobile defects, such as interstitial Frank loops. Irradiation experiments have shown the number densities of these defects tend to saturate after doses on the order of a few dpa. However, cluster dynamics modeling substantially overpredicts in these alloys the Frank loop number density at higher doses due to its lack of accounting for cascade overlap effects, which may alter the amount and type of stable damage generated in new cascades, as well as the size or Burgers vector of existing defects. In this work, we use the results of atomistic simulations of cascade overlap in fcc Ni to develop a cascade overlap model suitable for incorporation into cluster dynamics. The model considers changes in cascade-generated damage and changes in size and Burgers vector of existing defects due to cascade overlap.

9:40 AM
Solute Segregation and Precipitation Across Damage Rates in Dual Ion Irradiated T91 Steel: S. Taller[1]; *V. Pauly*[2]; Z. Jiao[2]; G. Was[2]; [1]Oak Ridge National Laboratory; [2]University of Michigan
Dual ion irradiations using 5.0 MeV defocused Fe^{2+} ions and co-injected He^{2+} ions were conducted on ferritic-martensitic steel T91 to 17 dpa in a damage rate range 5×10^{-5} to 3×10^{-3} dpa/s at 445°C followed by characterization using scanning transmission electron microscopy. Ni/Si clusters and radiation induced segregation were quantified using energy dispersive x-ray spectroscopy (EDS) at each condition and compared with the same material in the as-received condition and irradiated in the BOR-60 reactor at 376°C. The density of Ni/Si clusters and magnitude of Ni and Si enrichments were found to decrease monotonically with damage rate. No significant Cr segregation was found with dual ion irradiation. Rate theory calculations suggest the increased recombination at higher ion damage rates reduced the segregation and Ni/Si cluster density compared to BOR-60. This work highlights the importance of irradiation damage rate when using ion irradiation to simulate reactor irradiation.

10:00 AM Break

Advanced and Novel Materials- Session III

Thursday AM **Room: Urban**
November 11, 2021 **Location: Omni William Penn Hotel**

Session Chair: A. Hoffman, GE Research

10:20 AM Invited
Opportunities for Advanced Concepts in Nuclear Fuel Development: *A. Nelson*[1]; [1]Oak Ridge National Laboratory
Advances in the science of nuclear materials have been largely centered on structural materials in recent decades. However, properties and performance of the fissile material (the fuel) ultimately dictate the power output, cycle length, safety margin, and beyond design basis behavior of reactors. Recent advances in manufacturing of ceramic materials, composite structures, incorporation of in situ fabrication diagnostics have the potential to impact how nuclear fuels are designed, fabricated, qualified, and accepted from a quality assurance standpoint. The challenge for nuclear fuels researchers in the coming decade will be efficiently developing new concepts within the broader understanding of nuclear fuel performance and material response to irradiation. This talk will present a range of contemporary efforts in this area including near term opportunities. Finally, the crucial role that accelerated irradiation testing methods including modeling and simulation will play in understanding irradiation performance of these fuel concepts will be summarized.

11:00 AM
Metal Hydride Moderator Development at Los Alamos National Laboratory: *T. Saleh*[1]; A. Shivprasad[1]; C. Taylor[1]; T. Nizolek[1]; J. White[1]; E. Luther[1]; [1]Los Alamos National Laboratory
The use of moderators in advanced reactors can allow for less fuel and result in smaller reactors, which is particularly useful when there are space or weight constraints for the ultimate reactor application or location. Metal hydrides are strong neutron moderator candidates because they contain a high hydrogen density and are phase stable at much higher temperatures than water. This talk will discuss research at Los Alamos National Laboratory studying fabrication techniques and property measurements in a variety of metal hydride moderator materials, focusing on Zirconium and Yttrium Hydrides. Stoichiometry, phase, and fabrication methods and their effect on thermophysical and thermomechanical properties will be presented.

11:20 AM
Radiation Tolerance of Capacitive Discharge Resistance Welded 14YWT: *C. Lear*[1]; B. Eftink[1]; H. Kim[1]; M. Schneider[1]; T. Steckley[1]; Y. Wang[1]; T. Lienert[1]; S. Maloy[1]; [1]Los Alamos National Laboratory
Advantages in radiation tolerance, creep resistance, and high temperature strength make oxide dispersion strengthened (ODS) ferritic steels promising materials for extreme conditions. Unfortunately, excess heat and localized melting from traditional fusion welding degrades the dispersed oxide particles responsible for these attributes – making ODS components difficult to join. Recent work with solid-state capacitive discharge resistance welding (CDRW) has produced 14YWT-14YWT joints (caps to thin-walled cladding tubes) without changing dispersoids or microstructure near the weld line. Material from these joints was subjected to self-ion (5.0 MeV Fe2+, 600 dpa, 450 ˚C) and proton (1.5 MeV H+, 0.7 dpa, 300 ˚C) irradiations, with pre- and post-irradiation microstructure characterized using electron microscopy and mechanically tested using nano-indentation. The accumulation of radiation-induced defects (dislocation loops, void swelling) and the stability of the post-CDRW microstructure (grain structure, dispersoids) were evaluated to ensure that the CDRW process does not degrade pre-existing resistance to radiation-induced microstructural evolution.

11:40 AM
Cancelled: In-situ Nanomechanical Characterization of Neutron-irradiated HT-9 Steel: T. Ajantiwalay[1]; *A. Aitkaliyeva*[1]; M. Dubey[2]; Y. Wu[2]; [1]University of Florida; [2]Boise State University
For a safe operation of HT-9 steels as structural material in advanced reactors, a relationship between its irradiated microstructure and mechanical behavior needs to be established. In-situ nanocompression testing inside a transmission electron microscope (TEM) involves a combined analysis of defect microstructure and mechanical properties in real time. Under the application of a uniaxial compressive load, the electron-transparent nano-pillars reveal the morphology and movement of defects. In this study, nano-pillars of different dimensions were fabricated using focused ion beam (FIB) from a HT-9 specimen neutron-irradiated to 4.29 dpa at 469 °C. All these pillars were compressed in a displacement-controlled mode using the PI-95 Picoindenter. The results obtained from the stress-strain curves show that the average yield stress varies with the cross-sectional area of the pillars. The in-situ TEM observation shows several dislocations burst events taking place after yielding as depicted by the sharp load drops in the curves.

Early Career Development in Nuclear Materials - Panel

Thursday AM **Room: Allegheny**
November 11, 2021 **Location: Omni William Penn Hotel**

Session Chairs: K. Field, University of Michigan; M. Okuniewski, Purdue University

10:20 AM
The Early Career Development in Nuclear Materials panel session will provide an outlet for early career researchers, scientists, engineers, and policy makers to interface with, and learn from, six experts and leaders in the field of nuclear energy and materials in a non-technical, career development focused session. The diverse pool of panelists will bring their own unique perspectives and insights towards a range of topics critical to early career development including grant/funding acquisition, career trajectory and pathways, publishing standards and practices, and fostering community and connections.

Fuels and Actinide Materials- Oxide Fuels I

Thursday AM **Room: Monongahela**
November 11, 2021 **Location: Omni William Penn Hotel**

Session Chair: S. Finkeldei, University of California-Irvine

10:20 AM Invited
Atomic Scale Investigation of Thermodynamic and Defect Properties of (U,Pu)O_2 Mixed Oxide: D. Bathellier[1]; *M. Bertolus*[1]; E. Bourasseau[1]; M. Freyss[1]; L. Messina[1]; [1]CEA
One way of increasing significantly the efficiency in designing and qualifying innovative fuels is to enhance the predictive capability of fuel behaviour simulation by developing a more physically based description of nuclear fuels. Basic research approaches combining multiscale modelling and separate effect experiments can bring significant insight into materials properties and key phenomena involved in the evolution of fuels in reactor. We will show the results obtained using state-of-the art electronic structure and empirical calculations on the uranium-plutonium mixed oxide. In particular, the thermal expansion, enthalpy increments and specific heat of (U,Pu)O_2 as a function of Pu content will be presented. The defect properties of(U,Pu)O_2 and the impact of the disorder on the cationic sublattice will also be discussed.This research is part of the INSPYRE project, which has received funding from the Euratom research and training program 2014-2018 under Grant Agreement 754329.

TECHNICAL PROGRAM

11:00 AM
Phase-field Simulations of Fission Gas Bubbles in High Burnup UO2 during Steady-state and LOCA Transient Conditions: L. Aagesen[1]; S. Biswas[1]; W. Jiang[1]; *D. Andersson*[2]; M. Cooper[2]; C. Matthews[2]; [1]Idaho National Laboratory; [2]Los Alamos National Laboratory
U.S. utilities are currently seeking licensing approval to operate UO2 fuel to higher burnups. One significant safety issue that must be addressed to obtain approval is the potential for pulverization of the fuel during a LOCA. It has been hypothesized this is caused by the rapid increase of pressure in fission gas bubbles in the high burnup region of the fuel. To better understand this phenomenon, a novel phase-field model of the fission gas bubble microstructure in UO2 has been developed and implemented in Idaho National Laboratory's Marmot application for phase-field simulation of nuclear materials. During a LOCA transient, simulations of bubbles in the high burnup region showed that bubble size did not change significantly, and the pressure increase due to the transient was calculated and passed to a phase-field model of fracture.

11:20 AM
Thermal Diffusivity of Nuclear Materials at the Miniature Scale: *N. Abdul-Jabbar*[1]; S. Widgeon Paisner[1]; J. White[1]; [1]Los Alamos National Laboratory
To accelerate materials qualification for reactor deployment, a framework has been developed to process and characterize nuclear materials at the miniature scale for irradiation and burn-up experiments at Oak Ridge and Idaho National Laboratories, where specimen geometries are restricted to diameters of ~3 mm and thickness ≈300 µm. The size constraints serve to decouple interrelated materials phenomena that occur in full-scale nuclear reactor testing and will reduce sample radioactivity post-irradiation to avoid costly handling procedures. High-density miniature specimens of pure UO_2, U_3Si_2, and UN have been fabricated by powder metallurgy routes and current efforts have been focused on validating their thermophysical properties. Thermal diffusivity measurements via light flash analysis on UO_2 miniature fuels up to 1000 °C have been demonstrated and additional measurements on U_3Si_2, UN, and reactor cladding materials are currently in progress. The ensuing results will be discussed in the broader context of accelerated nuclear materials testing.

Advanced and Novel Materials- Session IV

Thursday PM	**Room: Urban**
November 11, 2021	**Location: Omni William Penn Hotel**

Session Chair: K. Field, University of Michigan

1:10 PM Invited
Novel Nickel-based Alloys for Molten Salt Fast Reactor Structural Applications: *V. Vasudevan*[1]; [1]University of Cincinnati
Molten chloride and fluoride salt fast reactors (MSR) are under active development because they offer several operational and safety advantages over other types of reactors. Modern designs require structural materials with superior corrosion, creep, thermomechanical fatigue, irradiation damage and Helium bubble and tellurium-induced grain boundary embrittlement resistance to high temperatures of 750-950°C. Nickel-base alloys generally perform better than all other alloys studied to date, though none yet have the set of property requirements to meet these demanding conditions. In this talk, I will report on the development of the next generation of nickel-base alloys for MSRs utilizing an ICME approach combined with a detailed experimental processing, testing, characterization and modeling program. Results of the alloy design strategy, phase equilibria and transformations and evolution of microstructure and high temperature mechanical properties will be presented and discussed. The irradiation and corrosion behavior in molten chloride salt of selected alloys will also be presented. Future directions will be discussed.

1:50 PM
Contextualizing Dispersoid Evolution within Friction Stir Welded and Ion Irradiated MA956: *E. Getto*[1]; N. Nathan[1]; J. McMahan[1]; B. Baker[1]; S. Taller[2]; [1]United States Naval Academy; [2]Oak Ridge National Laboratory
Understanding the co-evolution of dispersoids with the dislocation loops and network is critical for a comprehensive understanding of the response of friction stir welded (FSW) and oxide-dispersion-strengthened (ODS) steels to radiation. Ion irradiations were performed on FSW and ODS Fe-Cr-Al steel MA956 with 5 MeV Fe^{++} ions from 400 to 500°C at doses ranging from 50 to 200 dpa. Characterization was performed primarily with scanning transmission electron microscopy and energy-dispersive x-ray spectroscopy to investigate the Y-Al-O dispersoids, voids and dislocations. The co-evolution of the microstructure was explained as a function of the evolving defect kinetics, utilizing rate theory to calculate point defect concentrations, determine defect partitioning among sinks, and the increasing diffusivity of vacancies. Regardless of temperature, the dispersoids increased in diameter and decreased in number density, which was attributed to an Ostwald coarsening mechanism supported by calculations of the radiation enhanced diffusion and ballistic dissolution.

2:10 PM
Temperature-controlled Friction Stir Welding: A Potential Crack Repair Technology for 304L Stainless Steel Spent Nuclear Fuel-dry Storage Canisters (SNF-DSC): *S. Jana*[1]; I. Charit[2]; K. Raja[2]; M. Bhattacharyya[3]; A. Naskar[2]; [1]Pacific Northwest National Laboratory; [2]University of Idaho; [3]Indian Institute of Technology-Dhanbad
Dry storage canisters for storing spent nuclear fuel rods are usually fabricated from 304L austenitic stainless steels, since it offers excellent resistance to atmospheric corrosion. However, 304L SS is susceptible to pitting corrosion when exposed to chloride containing environments. Chloride-induced stress corrosion cracking (CI-SCC) can lead to early crack nucleation around heat affected zones and fusion weld seams in 304L SS. Thus, it is critical to eliminate any such cracks for a SNF-DSC to perform reliably. In the present study, the feasibility of Friction Stir Welding (FSW), as a low-temperature crack repair method has been explored. Multiple temperature-controlled FSW runs were carried out on 0.5" thick 304L SS plates in a gantry-type machine using a PCBN tool. Weld parameters were optimized to achieve weld temperatures that range from ~700°C to 900°C. The presentation will provide a summary of various characterization details (microstructural, mechanical, electrochemical etc.) of these temperature-controlled welds.

2:30 PM
Thermal Annealing and Irradiation Behavior of Ultrafine-grained and Nanocrystalline FeCrAl Alloys: H. Wen[1]; *M. Arivu*[1]; R. Islamgaliev[2]; [1]Missouri University of Science and Technology; [2]Ufa State Aviation Technical University
FeCrAl alloys are leading candidate materials for cladding of accident tolerant fuels in light water reactors replacing Zircaloy owing to their high temperature strength and corrosion resistance in steam environments. However, FeCrAl alloys suffer from embrittlement after long-time aging at ~500 oC and lower, due to a' Cr precipitation. This phenomenon is detrimental to the structural performance and corrosion resistance. Another major issue for FeCrAl alloys in nuclear environments is the irradiation-enhanced a' precipitation, leading to irradiation-induced hardening and embrittlement. Bulk ultrafine-grained and nanocrystalline metals possess drastically higher strength than their conventional coarse-grained counterparts, and are anticipated to have significantly enhanced irradiation tolerance. In this study, ultrafine-grained and nanocrystalline FeCrAl alloys were manufactured by equal-channel angular pressing and high-pressure torsion, respectively. The thermal annealing and irradiation behavior of these materials were carefully studied. Results indicated that reducing grain size can hinder both thermally induced and irradiation enhanced a' Cr precipitation.

2:50 PM
Finding a Balance in FeCrAl Alloys: Optimization of Alloy Chemistry for Balanced Properties: *A. Hoffman*[1]; V. Gupta[1]; F. Cappia[2]; R. Rebak[1]; [1]GE Research; [2]Idaho National Laboratory
FeCrAl alloys have shown great promise for use as accident tolerant fuel cladding due to their excellent high temperature steam oxidation resistance, good hydrothermal corrosion resistance, and desirable mechanical properties. One concern, however, is the formation of a', a Cr enriched phase which precipitates in Cr bearing ferritic alloys at temperatures around or below 500°C. This presentation will give an overview of GE's development of FeCrAl alloys and future plans to combine experiments and regression analysis using machine learning to optimize alloy chemistry. Considerations of microstructure and chemistry on corrosion, mechanical properties, and phase stability will be discussed. Attention will also be given to the effects of radiation on such properties.

3:10 PM Break

Fuels and Actinide Materials- Oxide Fuels II

Thursday PM
November 11, 2021
Room: Monongahela
Location: Omni William Penn Hotel

Session Chair: M. Okuniewski, Purdue University

1:10 PM Invited
New Microscopic Insights into the Fuel Cladding Interaction Layer of High Burnup Fuel: *S. Finkeldei*[1]; K. Wright[2]; N. Cinbiz[2]; B. Kombaiah[2]; F. Cappia[2]; [1]University of California-Irvine; [2]Idaho National Laboratory
The fuel-cladding interaction layer plays a vital role in nuclear fuel rod performance during off-normal, in particular, transient conditions. Thus, understanding the microstructural features and local chemistry will help to better predict the mesoscale behavior of high burn-up fuels. X-ray maps were collected with an electron probe microanalyzer (EPMA) at the cross section of a high burnup pellet with detailed characterization of the pellet cladding interaction (PCI) layer, revealing the distribution and location of fission products, gases and epsilon particles. EPMA data are complemented with TEM measurements, including orientation mapping via precession electron diffraction technique to gain insights about the chemical and microstructural nature of the PCI and the high burnup fuel which will enable better evaluation and analysis of upcoming TREAT experiments.

1:50 PM
Three-dimensional Characterization of Microstructural Features in Oxide Fuels: *C. McKinney*[1]; A. Aitkaliyeva[1]; [1]University of Florida
Nuclear fuels undergo various microstructural and chemical changes during their lifetime in the reactor. Temperature gradients cause grain restructuring while fission disperses new phases and precipitates throughout the fuel microstructure. Understanding how these features evolve over the lifetime of the fuel is vital as each one has the potential to compromise the safety of the reactor. In this work, we employ focused ion beam (FIB) tomography to study the microstructural evolution. With the incorporation of electron backscatter diffraction (EBSD) and energy dispersive x-ray spectroscopy (EDS), we can study the grain and fission product evolution in oxide fuels. The reconstructions obtained from this study will be used to assess solid and gaseous fission product behavior and their relationship to the local grain structure.

2:10 PM
Modeling the Mechanisms of Fuel Pulverization Using Cluster and Molecular Dynamics: *M. Cooper*[1]; C. Matthews[1]; R. Daum[2]; D. Andersson[1]; [1]Los Alamos National Laboratory; [2]Electric Power Reseach Institute
Reactor operators in the US would like to extend the refueling cycle length in PWRs from 18 to 24 months, which requires an increase in the peak rod average burnup from 62 GWd/tU to 75 GWd/tU. The high burnup structure (HBS) that forms in UO_2 under such conditions is susceptible to fragmentation and pulverization when it experiences a temperature ramp (e.g., during a LOCA). The resultant relocation/dispersal of fuel particles represents a significant safety concern. In this work, we use cluster dynamics to examine the over-pressurization of Xe bubbles through irradiation-enhanced diffusion processes relevant to the cooler temperatures found in the periphery of the pellet, where HBS forms. Then, we employ MD simulations to examine the impact of over-pressurized inter-granular bubbles on the fracture of grain boundaries during temperature ramps, as a proposed mechanism for fuel pulverization. The peak temperature, bubble size, bubble number, and bubble pressure are all examined.

2:30 PM
Cancelled: Experimental Characterization of the Chemical Behavior of Cs, I and Te in UO2: *M. Rochedy*[1]; V. Klosek[1]; C. Riglet-Martial[1]; C. Onofri-Marroncle[1]; D. Drouan[1]; P. Bienvenu[1]; I. Roure[1]; M. Cabié[2]; L. Amidani[3]; M. Hunault[4]; J. Lechelle[1]; M. Pinault-Thaury[5]; [1]CEA, DES, IRESNE / DEC; [2]Université Aix-Marseille, CP2M; [3]HZDR; [4]SOLEIL; [5]Université de Versailles St Quentin en Yvelines, GéMAC
Studies are undertaken to better understand Iodine-Stress Corrosion Cracking (I-SCC) of Zircaloy cladding due to Pellet-Cladding Interaction (PCI) in transient conditions [1]. The efficiency of iodine at producing SCC varies with the chemical iodide compounds in interaction with the cladding [1, 2]. In irradiated UO2 fuel, iodine speciation is determined by the (Cs-Mo-I-Te)-UO2 chemical system [2]. In the present study, simulated fuel samples were prepared by implanting UO2 pellets with Cs, I and/or Te. The samples were thermally treated in carefully controlled (T, pO2) conditions and characterized using SIMS, TEM, EELS and XAS techniques. Relevant (T, pO2) phase diagrams were computed to design the tests and interpret the observations. Results regarding the Cs-UO2, I-UO2, (Cs-I)-UO2 and (Cs-I-Te)-UO2 systems are presented and discussed considering thermochemical equilibria and fission products interactions with microstructural defects. [1] P. Konarski et al., JNM, 519, 104-120 (2019)[2] L. Desgranges et al., JNM, 437, 109-414 (2013)

2:50 PM Break

Material Properties Evolution- Session III

Thursday PM
November 11, 2021
Room: Allegheny
Location: Omni William Penn Hotel

Session Chair: T. Byun, Oak Ridge National Laboratory

1:10 PM Invited
IASCC Initiation Testing of ex-PWR Baffle-former Bolts: *M. Ickes*[1]; L. Dong[2]; G. Was[2]; [1]Westinghouse Electric Company; [2]University of Michigan
Irradiation-assisted stress corrosion cracking (IASCC) is an issue that has caused degradation of pressurized water reactors (PWRs), and is managed by costly inspection and replacement activities at nuclear power facilities. Type 347 stainless steel baffle-former bolts have been affected by IASCC at several US PWRS recently, however little IASCC initiation data exists on materials taken from such bolts. To address this gap in data, miniature 4-point bend specimens were extracted from the baffle-former bolts at the Westinghouse Churchill Site hot cell facility and tested in simulated PWR conditions at the University of Michigan. As the US nuclear industry is considering replacing lithium hydroxide additions with potassium hydroxide additions in the PWR coolant, equivalent specimens were tested in either potassium hydroxide or lithium hydroxide in an attempt to determine if there was any difference in IASCC initiation behavior between the two environments.

1:50 PM

Mesoscale YellowJacket: A Phase-field Model for Microstructure Dependent Corrosion of Ni-Cr Alloys by Molten Fluoride Salts: *C. Bhave*[1]; M. Tonks[1]; D. Schwen[2]; D. Andersson[3]; J. McMurray[4]; [1]University of Florida; [2]Idaho National Laboratory; [3]Los Alamos National Laboratory; [4]Oak Ridge National Laboratory

Corrosion of Ni-Cr alloys proposed for use in the containment of molten salts is a major challenge in the commercial utilization of molten salt reactor (MSR) technology. This corrosion damage is sensitive to the microstructure and results in severe microstructure evolution. In this work, an electrochemical phase-field model is being developed for capturing selective depletion of Cr from grain boundaries of the alloy and the resultant formation of sub-surface voids. A study of the effect of alloy microstructure and composition on the corrosion rate and microstructure evolution is performed. This model was implemented under the mesoscale YellowJacket project using the Multiphysics Object-Oriented Simulation Environment (MOOSE), an open-source finite-element framework. The results of this research will be used to form Reduced Order Models (ROMs) for engineering scale models.

2:10 PM

Atom Probe Tomography Study of Elemental Segregation and Precipitation in Ion-irradiated Advance Austenitic Alloy A709: *D. Piedmont*[1]; X. Liu[2]; H. Kim[3]; F. Garner[4]; L. Shao[4]; T. Sham[5]; J. Stubbins[1]; [1]University of Illinois at Urbana-Champaign; [2]Idaho National Laboratory; [3]Los Alamos National Laboratory; [4]Texas A&M University; [5]Argonne National Laboratory

A709 is an advanced austenitic alloy for structural applications in advanced reactors because of its high-temperature strength, corrosion resistance, and creep properties. Previous studies investigated the microstructural evolution at relatively low doses and swelling behavior at high doses. This work quantifies the dose dependence of the elemental segregation and precipitation behavior at high doses so that it could be linked with other microstructural changes, such as void swelling and the formation of network dislocations. Atom Probe Tomography (APT) was used to investigate A709 after ion-irradiated by 3.5 MeV $Fe2^{+}$ ions at an irradiation temperature of 575°C to peak dpa of 100, 200, and 400. Therefore, this work addresses the need to accurately measure the compositional difference of the matrix at different doses; critical to understanding the radiation-induced segregation and precipitation of A709. As well, the possible interconnection between elemental segregation and void swelling, an aspect not well studied, is investigated.

2:30 PM

The Role of Alloying Species on Radiation Tolerance of BCC Fe Binary Alloys: *P. Warren*[1]; C. Clement[1]; C. Yang[1]; Y. Wu[2]; J. Wharry[1]; [1]Purdue University; [2]Boise State University and Center for Advanced Energy Studies

The objective of this study is to understand the effect of alloying species on irradiation tolerance in BCC Fe. BCC Fe forms the basis of radiation-tolerant steels for advanced nuclear structural and cladding applications, but little is known about how alloying species affect irradiation tolerance. Here, model binary alloys Fe-9Cr, Fe-2P, Fe-2.3N, and Fe-1.25Mo (at%) were irradiated to 8.5 dpa by 4.5 MeV Fe^{++} ions at 653 K. Transmission electron microscopy (TEM) evaluated the irradiated microstructures, and nanoindentation evaluated mechanical properties. The Fe-P alloy had a dense dispersion of radiation-induced defects including nanoclusters and dislocation loops, while the other alloys had a lower density of larger loops and dislocation lines. Molecular dynamics simulations confirm a higher defect density in Fe-P. This is attributed to the strong trapping of point defects such as self-interstitial atoms (SIAs) by undersized P atoms. Results are discussed in the context of atomic size factors.

2:50 PM Break

Advanced and Novel Materials- Session V

Thursday PM	**Room: Urban**
November 11, 2021	**Location: Omni William Penn Hotel**

Session Chair: V. Vasudevan, University of North Texas

3:30 PM Invited

MAX Phases for Nuclear Applications: *K. Lambrinou*[1]; [1]SCK-CEN

This lecture focuses on the accelerated development of MAX phase materials for Gen-II/III light water reactors (LWRs) and Gen-IV lead-fast reactors (LFRs). The MAX (Mn+1AXn) phases are nanolayered ternary carbides/nitrides, where M is an early transition metal, A is an A-group element, X is C or N, and n = 1, 2, 3. Conventional nuclear material development involves many cycles of production, neutron irradiation and post-irradiation examination until the property requirements of the end application are met. This approach is time-consuming and costly, discouraging industrial investments in innovative materials. The accelerated materials development approach, however, ensures that design, production, and performance assessment are interconnected, expediting the deployment of novel nuclear materials. Two applications are considered: (a) pump impellers for Gen-IV LFRs, and (b) accident-tolerant fuel (ATF) cladding materials for Gen-II/III LWRs. Tests done in static & flowing liquid LBE, PWR water & steam, ion irradiations at 350-800C to 40 dpa.

4:10 PM

Cancelled: Exploring the Radiation Response of Innovative Accident Tolerant Fuel Candidate Concepts Based on High-entropy Alloys: *M. Tunes*[1]; V. Vishnyakov[2]; S. Maloy[1]; O. El-Atwani[2]; [1]Los Alamos National Laboratory; [2]University of Huddersfield

An envisaged solution to establish accident tolerance on Light-Water Reactors (LWRs) Zr-based alloy nuclear fuel assemblies is to deposit a suitable coating onto the cladding material. This coating must primarily be resistant to oxidation facing steam at both operational and accident conditions such as loss-of-coolant (LOCA), but in order to preserve its relevant oxidation and tribological properties, they should also exhibit resistance to energetic particle irradiation. The development of accident tolerant fuel candidate concepts based on innovative high-entropy alloys (HEAs) will be presented with focus on their radiation response assessed using light- and heavy-ion irradiations with in situ TEM within the operational temperature envelope of LWRs. The radiation response of HEA-based coatings will be compared with conventional materials (e.g. TiN films) showing that HEAs are capable of resist high-doses without significant changes in matrix phase and with suppressed nucleation and growth of extended defects like voids and bubbles.

TECHNICAL PROGRAM

4:30 PM
High Throughput Study of Hardening and Void Swelling in Ion Irradiated Compositionally Complex Alloys: *B. Queylat*[1]; M. Moorehead[1]; P. Nelaturu[1]; M. Elbakhshwan[1]; D. Thoma[1]; M. Bachhav[2]; D. Morgan[1]; A. Couet[1]; [1]University of Wisconsin, Madison; [2]Idaho National Laboratory
Development of next-generation nuclear reactors, operating at higher temperature and under extreme environments, requires the development of new alloys for claddings, internals, and structural materials. Compositionally Complex Alloys (CCAs) are a relatively new class of alloys that has shown promising properties under extreme environments. However, considering the extremely large compositional space of CCAs, manufacturing, characterizing and studying the effects of irradiation on their properties using conventional methods is not compatible with the deployment timeline of these reactors. In this study, we have combined innovative high-throughput CCAs processing method, using additive manufacturing and high-throughput ion irradiation at high temperature and high dose, coupled with automated characterization methods to measure void swelling and hardness evolution of a wide composition space of the Cr-Fe-Mn-Ni system as function of dpa. Preliminary results and importance ranking order based on Cr-Fe-Mn-Ni properties and void swelling/hardening performance metrics will be presented using a Random Forest Regressor algorithm.

4:50 PM
Discerning the Effects of Solute Additions in FeCrAl on Dislocation Dynamics under Irradiation Using a Machine Learning Object Detection Algorithm: *P. Patki*[1]; M. Shen[2]; Y. Yaguchi[2]; J. Haley[3]; D. Morgan[2]; K. Field[1]; [1]University of Michigan; [2]University of Wisconsin; [3]University of Oxford
Machine learning object detection algorithms have become an increasingly popular choice in detecting, quantifying, and tracking of discrete objects in microstructures allowing the analysis of objects of interest with increased accuracy with no sacrifice in time. In this study, we use the You Only Look Once (YOLO) algorithm to detect black dots formed in FeCrAl systems with varying Cr and Al concentrations during Transmission Electron Microscope (TEM) in situ ion irradiations. The TEM in situ ion irradiation videos were analyzed for four alloys irradiated at 320°C up to 2.5 dpa using YOLO. This study will present the effects of solute additions on the size and density of the black dots formed on a per video frame basis and show a detailed analysis of individual defect dynamics including defect growth and mobility including trajectories using the established analysis framework.

Fuels and Actinide Materials- Oxide Fuels III

Thursday PM	**Room: Monongahela**
November 11, 2021	**Location: Omni William Penn Hotel**

Session Chair: M. Cooper, Los Alamos National Laboratory

3:30 PM Invited
Calculation of Irradiation Enhanced Diffusivities Using Centipede: C. Matthews[1]; M. Cooper[1]; R. Perriot[1]; C. Stanek[1]; *D. Andersson*[1]; [1]Los Alamos National Laboratory
The transport of defects in the supersaturated defect environment in irradiated nuclear fuel drives much of the important performance aspects of nuclear fuel. Calculations of defects have traditionally relied on rate theory to estimate defect concentrations to provide meaningful information to fuel performance simulations, albeit with limited scope, and subsequently, poor comparison to experimental measurements. Led by early indications that larger clusters could enable enhanced fission gas diffusion during irradiation, the cluster dynamics code Centipede has been developed to incorporate the hundreds of defects that must be tracked in order to account for the impact of large defect clusters. Through the utilization of an extensive database of atomistic calculations, the mechanistically calculated irradiation enhancement of fission gas in UO2 has been shown to compare favorably with experimental measurements. Centipede has been further refined using machine learning and has been applied to advanced fuels for which data is absent.

4:10 PM
Defect Clustering in UO_2 Doped Systems Studied Using XAS and Neutron Scattering: *A. van Veelen*[1]; J. White[1]; T. Ulrich[1]; S. Widgeon Paisner[1]; T. Saleh[1]; [1]Los Alamos National Laboratory
Uranium Dioxide (UO_2) is the dominant fuel that powers nuclear reactors. UO_2 fuel microstructure, in particular grain size, is known to affect both creep and fission gas release behavior which improves fuel lifetime and stability. Several additives have been recognized to enhance grain growth, of which Cr has been put forth by industry. The addition of Cr increases the grainsizes from 10 (± 3 µm) to 35 (± 5 µm). The dissolution of Cr into the UO_2 lattice is strongly dependent on temperature and oxygen potential during sintering. Cr doping results in lattice contraction due to the introduction of structural defects. Additionally, Cr can potentially be accommodated on the uranium site at low temperatures and low concentrations. We used state-of-the-art X-ray Absorption Spectroscopy combined with X-ray and Neutron Diffraction to study the defect structures of Cr-doped and undoped UO_2. We will discuss the Cr-doping effects on the UO_2 defect chemistry.

4:30 PM
Dislocation Loop Evolution in Fluorite Oxides: *M. Khafizov*[1]; S. Adnan[1]; J. Ferrigno[1]; K. Bawane[2]; T. Yao[2]; M. Jin[3]; C. Jiang[2]; L. He[2]; D. Hurley[2]; [1]Ohio State University; [2]Idaho National Laboratory; [3]Pennsylvania State University
We report on a combined experimental and modeling study focusing on dislocation loop evolution under irradiation in fluorite oxides. UO_2, ThO_2 and CeO_2 were irradiated using a few MeV protons. Dislocation loops were characterized using transmission electron microscopy (TEM). A rate theory (RT) model is implemented to describe evolution of stoichiometric loops. Analysis of TEM results using RT model suggests that loop growth over 400-800 °C temperature range is governed by mobility of cation interstitials, whereas their nucleation is impacted by mobility of cation interstitials and anion defects. It was found that migration barrier for cation interstitials is proportional to the melting temperature of this oxides and migration barriers for other defects are consistent with atomic level simulations of defect energetics. This analysis provides a method to predict point defect concentrations, which impact the physical properties of these compounds, in particular thermal conductivity.

4:50 PM
Cancelled: Grain Growth Kinetic Models for Accident Tolerant Oxide Fuel: *T. Ulrich*[1]; J. White[1]; D. Frazer[2]; [1]Los Alamos National Laboratory; [2]Idaho National Laboratory
Increasing demand for clean energy requires continuous improvement of the operating nuclear reactor fleet. For the last six decades, it has been demonstrated that increasing the grain size of UO_2 has improved fission gas release behavior and is expected to increase the viscoplastic behavior of the fuel at operating temperatures. However, UO_2 grain size increased by the addition of dopants complicates decoupling of dopant and large grain size effects. This work is aimed at developing a method that enhances the grain size of undoped UO_2, which could be used as a reference for fission gas behavior in enhanced UO_2 accident tolerant fuel. By changing the sintering dwell time and atmosphere, a 3 fold increase in grain size was achieved compared to standard UO_2 manufacturing methods. These results will be discussed relative to the respective commercial dopants.This work was funded by the Department of Energy's Accident Tolerant Fuel Campaign.

Material Properties Evolution- Session IV

Thursday PM **Room: Allegheny**
November 11, 2021 **Location: Omni William Penn Hotel**

Session Chair: G. Was, University of Michigan

3:30 PM
Neutron Irradiation Effects on PM-HIP Inconel 625: *C. Clement*[1]; Y. Lu[2]; S. Cheng[2]; M. Dubey[2]; S. Panuganti[1]; Y. Zhao[1]; K. Wheeler[3]; D. Guillen[3]; D. Gandy[4]; J. Wharry[1]; [1]Purdue University; [2]Boise State University/ Center for Advanced Energy Studies; [3]Idaho National Laboratory; [4]Electric Power Research Institute
The objective of this talk is to understand the effects of neutron irradiation on the microstructure and mechanical properties of Inconel 625 (IN625) fabricated using powder metallurgy with hot isostatic pressing (PM-HIP). PM-HIP presents an attractive alternative to traditional manufacturing methods for use in nuclear applications, however its irradiation response must first be understood. IN625 fabricated with PM-HIP and a traditional forging method were neutron irradiated to a dose of 1 displacement per atom (dpa) at 300°C in the Advanced Test Reactor. Post-irradiation examination involved bright field transmission electron microscopy (BFSTEM), atom probe tomography (APT), nanoindentation, and in-hot cell tensile testing. PM-HIP IN625 is less susceptible to void nucleation than its forged counterpart, and it additionally shows less irradiation-hardening and embrittlement. The results of this study are a step forward in demonstrating the viability of PM-HIP materials in nuclear applications.

3:50 PM
Influence of Different Heat Treatments and Ion Irradiation on the Microstructural Evolution and Microhardness of Inconel 625 Fabricated via Laser-powder Bed Fusion: V. O'Donnell[1]; T. Keya[2]; M. Andurkar[3]; A. Romans[2]; G. Harvill[2]; B. Prorok[2]; S. Thompson[3]; *J. Gahl*[1]; [1]University of Missouri; [2]Auburn University; [3]Kansas State University
The microstructure and microhardness of Inconel 625 fabricated via Laser-Powder Bed Fusion (L-PBF) was investigated in as-printed and heat-treated conditions before and after ion irradiations. Direct proton irradiation in excess of 1014 protons/cm^2/s was provided using the cyclotron facility at the University of Missouri Research Reactor Center (MURR). Heat treatment temperatures (between 700 and 1050 °C) and dwell times (1, 5, and 10 hours) were varied. Results clearly demonstrate that the as-printed Inconel 625 microstructure enables the rapid formation of intermetallic and other precipitate phases well in advance of the established wrought time-temperature-transformation (TTT) diagram. Traditional wrought homogenization procedures are not optimal for L-PBF Inconel 625. Hence, a detailed characterization of grain and precipitate evolution with respect to heat treatment and ion irradiation is provided. Results provide insight into the most appropriate heat treatment for L-PBF Inconel 625 for radiation resistance and/or hardness.

4:10 PM
Mechanical Behavior of Additively Manufactured 316L Stainless Steel and SiC before and after Neutron Irradiation: *T. Byun*[1]; T. Lach[1]; M. Gussev[1]; A. Le Coq[1]; X. Chen[1]; D. Collins[1]; G. Vasudevamurthy[1]; K. Linton[1]; K. Terrani[2]; [1]Oak Ridge National Laboratory; [2]USNC
The mechanical properties of additively manufactured (AM) 316L stainless steel (SS) and silicon carbide (SiC) were evaluated before and after irradiation in the High Flux Isotope Reactor to assess the in-reactor performance of AM components. For this research, 316L SS plates were manufactured using the laser powder bed fusion (LPBF) method and SiC disks by a combined process of binderjet 3D printing and chemical vapor infiltration (CVI). Baseline and post-irradiation tensile tests over a wide temperature range of room temperature–600 ˚C were performed for the AM 316L alloy in different post-build heat-treatment conditions, and room temperature flexural strength testing for the SiC disk specimens in different printing orientations. This presentation is to summarize the outcome of these mechanical tests focusing on the irradiation-induced changes. We will also discuss about the statistical aspect of the strength data for both 316L and SiC materials and the size effect in SiC.

4:30 PM
Plutonium Defect Characterization through Mechanical Deformation: T. Jacobs[1]; *C. Yablinsky*[1]; J. Mitchell[1]; M. Gibbs[1]; B. Maiorov[1]; [1]Los Alamos National Laboratory
Mechanical deformation is being used to probe defects related to processing and aging in Pu-Ga (1-7 at pct) alloys ranging from 1 to 11 years of age. Stress relaxation measurements were performed using quasi-static compression tests in conjunction with first principles strengthening mechanisms concepts to provide insight into dislocation-defect interactions related to strength. Strength changes associated with grain size, age, and heat treatment conditions were related to measurable changes in the internal and effective stress components of the flow stress. Internal friction was measured using resonant ultrasound spectroscopy to detect Debye peaks related to mobile defects in d-Pu. Further analysis of the Debye peaks provide the defect activation energy of diffusion and mean residence time, which can help inform material models. Characterization of defects detected by stress relaxation and internal friction will further our fundamental understanding of Pu aging in support of a safe and reliable nuclear stockpile.

Conference Banquet

Thursday PM **Room: Grand Ballroom**
November 11, 2021 **Location: Omni William Penn Hotel**

Session Chair: T. Allen, University of Michigan

6:30 PM Plenary
What's Driving the Acceleration of Nuclear Materials Technology?: *R. Baranwal*[1]; [1]Electric Power Research Institute
Since advanced non-light water reactors (ARs) operate at much higher temperatures than traditional nuclear power plants, design practices now need to account for unique behaviors in material and component properties and in various coolants. Construction materials for ARs need to endure mechanical loads and often extreme environmental conditions for prolonged times while withstanding effects of temperature transients, effects of irradiation damage to material properties, and irradiation-induced swelling. Lessons learned from the deployment of the existing LWR fleet will need to be augmented with new tools such as AI and machine learning as well as new manufacturing methods to facilitate and accelerate the material characterization and qualification process.

Poster Session

Tuesday PM
November 9, 2021

Room: Sky
Location: Omni William Penn Hotel

Quantifying the Impact of an Electronic Drag Force on Defect Production from High-Energy Displacement Cascades in -zirconium: *J. March-Rico*[1]; C. McSwain[1]; B. Wirth[1]; [1]University of Tennessee, Knoxville

Defect production following displacement cascades with PKA energies up to 40 keV is compared between two conditions in -zirconium: 1) considering only nuclear stopping effects and 2) considering simultaneous nuclear and electronic stopping. Electronic energy losses are implemented as a drag force with strength proportional to the energy-dependent stopping power as predicted by SRIM calculations. This adjustment is performed using a new and user-friendly command, "fix electron/stopping", innately available in the LAMMPS software. We find that electronic energy losses result in a 10 – 20 % reduction in the surviving damage produced by high-energy PKAs, and this should be accounted for when considering defect generation rates in mesoscale codes. This method of electronic energy loss implementation predicts nuclear damage energies that are comparable with the SRIM-predicted values when using the full-cascade TRIM calculation, as has recently been recommended to the community.

Cancelled: Evaluation of Water Degradation in Medium Voltage Electric Cables Found in Nuclear Power Plants: S. O'Brien[1]; B. Hinderliter[1]; *M. Elmer-Dixon*[1]; [1]University of Minnesota Duluth

Nuclear power plants use medium-voltage cables to power numerous safety components. Although some are used only in emergency situations, these cables have the same reliability requirements as other cables used in active plant components, and therefore are tested regularly. Testing typically occurs under normal operating conditions and thus does not account for potential water immersion due to accident conditions. Water immersion can lead to a phenomenon called water treeing in regions of the insulation, which over time will permanently degrade the insulation and may lead to cable failure. To better understand water treeing in EPR-insulated cables, finite element analysis was used to simulate various water tree conditions. Specific energy absorption rate (SAR), a measure of insulation degradation rate, was determined at locations along a water tree's growth path to establish when degradation reaches cable failure. Additionally, SAR is directly correlated with a temperature rise, further synergistically increasing the failure rate.

Design of a Test System for Hot Hydrogen-facing Components in Nuclear Thermal Propulsion Systems: *W. Searight*[1]; L. Winfrey[2]; [1]Pennsylvania State University; [2]Pennsylvania State University

Nuclear thermal propulsion is a promising candidate for deep-space crewed missions to Mars given their improved performance over chemical rockets. A pressing issue in NTP development is the testing of high-temperature components at prototypical conditions. To evaluate material performance of moderator elements, a hot hydrogen test loop, capable of producing circulating hydrogen at temperatures up to 1200 ˚C, is under construction at Penn State. This work details the test loop design and development informed by Ansys Fluent to simulate the fluid behavior in the test section. Given that working fluid conditions affect material performance, the potential effects of hydrogen on test materials are evaluated under operating conditions. The design studies performed show laminar flow behavior in the hydrogen and delivered required temperatures to the test section. This work provides the basis for design choices in the test system and correlation of hydrogen behavior in interior components to materials performance.

Cancelled: Quantification of the Resistance to Dislocation Glide in Pre-deformed and Ion-irradiated FeCrAl Alloys Using in Situ Micro-mechanical Testing: *J. Wang*[1]; D. Xie[1]; T. Sun[2]; X. Zhang[2]; L. Shao[3]; [1]University of Nebraska-Lincoln; [2]Purdue University; [3]Texas A&M University

FeCrAl alloys become a competitive candidate for fuel cladding materials because of extraordinary oxidation resistance, excellent corrosion resistance at high-temperature and low parabolic oxidation rate. There is growing interest in FeCrAl alloys for nuclear applications. Correspondingly, the mechanical properties and behaviors of FeCrAl alloys, especially in irradiated state, must be thoroughly investigated. We prepared well-annealed, pre-deformed, and ion-irradiated FeCrAl samples and conducted in situ tension and compression testing in a SEM to evaluate the resistance to dislocation glide at different deformation temperatures. These results provide fundamentals for understanding mechanical behaviors of FeCrAl alloys at macro-scale.

Atomistic Calculations on the Effective Bias of Cavities in BCC Fe: *Y. Wang*[1]; F. Gao[1]; B. Wirth[2]; [1]University of Michigan - Ann Arbor; [2]University of Tennessee, Knoxville

Cavity swelling is an important topic on F-M alloys and recent research reported that the classic thermal criterion of cavity nucleation lost its explanatory power outside the intermediate temperature regimes. Therefore, the bias was introduced for describing the reaction volume of different types of defects with cavities and the results will provide important inputs for cluster dynamics simulation. Molecular statics calculations were performed to determine the interaction radius and effective bias of single SIA/vacancy, di-SIA/vacancy and 7-SIA/vacancy clusters to voids in BCC Fe. Molecular dynamics simulations were conducted to investigate the rotation and migration behavior of SIA clusters with different sizes when interacting with a void. A specific homogenization method was established to describe the capture volume and mimic the one-dimensional diffusion behavior for large SIA clusters. The effective bias of single defects to He bubbles was also investigated with different bubble pressures and bubble sizes.

ACTINIS: Shielded SIMS for Analysis of Highly Radioactive Samples: P. Peres[1]; *M. Pietrucha*[2]; S. Choi[1]; A. Vuillaume[1]; L. Renaud[1]; N. Touzalin[1]; [1]CAMECA; [2]CAMECA Instruments Inc.

Dynamic SIMS (Secondary Ion Mass Spectrometry) proves extremely useful for a wide range of nuclear science applications. ACTINIS is a SIMS instrument designed to perform high precision elemental and isotopic analyses of highly radioactive samples in a safe environment. ACTINIS offers depth profiling with excellent detection limits (ppb to ppm) and high depth resolution; elemental & isotopic information ranging from low mass (H) to high mass species (Pu and beyond); as well as unique sub-µm resolution 2D and 3D imaging capabilities. Studies performed with SIMS on irradiated nuclear fuel focus on three main axes: 1) the nuclear reactions occurring during in-core irradiation which are characterized with isotopic ratio measurements, 2) the physical and chemical behavior of fission products which is evidenced by isotopic mapping, 3) the characterization of fission gases which is carried out through depth profiling measurements.Different applications covered by ACTINIS for irradiated fuel analysis will be presented.

Atom Probe Tomography for Nuclear Materials: R. Ulfig[1]; D. Reinhard[1]; K. Baxter[1]; *M. Pietrucha*; [1]Cameca Instruments Inc.

Atom Probe Tomography (3D imaging mass spectrometer) is the highest sensitivity analytical method identifying up to 80% of the atoms in a volume with sub-nanometer spatial resolution. The time-of-flight mass spectrometer has sufficient mass resolving power to identify individual isotopes of all masses from hydrogen to uranium and beyond with nominally equal sensitivity. Achieving this performance requires specialized specimen preparation, ultra-high vacuum, high-speed pulsing and timing electronics, as well as specialized data reduction techniques. Installations in France and the US have included modifications to facilitate the handling of radioactive materials with the mindset of time, distance, and, shielding.Over the 50 years since atom probe tomography was first demonstrated the technique has been developed to be fast and easy to use. This poster will summarize the technology and methods to achieve such performance with a focus on the contributions that APT has made for nuclear materials.

SKAPHIA: Presentation of the Latest Shielded Electron Probe Micro Analysis (EPMA): A. Robbes[1]; *M. Pietrucha*[2]; M. Lambert[1]; A. Vuillaume[1]; M. Matton[1]; [1]CAMECA; [2]CAMECA Inc.

Electron Probe Micro Analysis (EPMA) is used for material analysis, allowing quantitative mapping of nearly all chemical elements at concentration levels down to few 10s ppm with a spatial resolution of about 1 um. At nuclear facilities, EPMA is mainly being used for nuclear fuel characterization, irradiated materials behavior investigation, post Irradiation examination, and radioactive waste management. CAMECA has been developing dedicated EPMA instrumentation for radioactive samples for more than 40 years and launched SKAPHIA in 2017. We will present its global conception, the loading of hot sample, the safety capacities as well as the maintenance. Technical details to maintain the EPMA efficiency for detection limits of trace elements in the shielded environment will be reviewed. The instrument will be shown at our production facility and also integrated in various possible hotcell configurations. Finally, we'll present different type of applications served by instruments in operation worldwide.

Developing Neural Network Model for Automated Analysis of Radiation-induced Grain Growth in UO2: *X. Xu*[1]; Z. Yu[1]; A. Motta[1]; X. Wang[1]; [1]Pennsylvania State University

In the context of a research project designed to investigate the effect of in-situ Kr ion irradiation on grain growth in UO2, a large number of microscopy images have been generated at a range of temperature and doses. To aid in the processing of this large dataset and to reduce human bias, we developed a U-Net model to automatically recognize grains in dark field transmission electron microscopy (TEM) images and measure the grain sizes. U-Net is a convolutional neural network with a unique architecture that makes it efficient in image segmentation and particle analysis. The use of data augmentation through rotation, zooming, and shearing methods improved the model accuracy from 95% to 97%. The U-Net model successfully reproduced the grain growth kinetics from human experts with a much shorter processing time. The model can be further improved to analyze in-situ TEM videos and grain growth of other nanocrystalline materials.

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