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CONTENTS

FIGURES

ADVANCED FUELS CAMPAIGN

MATERIAL RECOVERY AND WASTE FORMS DEVELOPMENT

NUCLEAR TECHNOLOGY RESEARCH AND DEVELOPMENT TECHNICAL MONTHLY NOVEMBER FY18

ADVANCED FUELS CAMPAIGN

ADVANCED LWR FUELS

LWR Fuels

- **[LANL]** Single crystals of U_3Si_2 were grown at various crystal rotation and pull rates to establish the best parameters for growth of crystals with diameters ≥5 mm (Figure 1). Crystals were pulled from the melt using a modified Czochralski method. U_3Si_2 single crystals will enable more fundamental property studies for this proposed high density fuel providing data to develop and inform physics-based fuel performance models. (D. Byler)

Figure 1. Growth of a U_3Si_2 crystal in a modified Centorr Tri-arc system. For reference, the diameter of the electrode on the left and right hand sides is 2.4mm.

- **[LANL]** A publication titled, "Mechanical Properties of Uranium Silicides by Nanoindentation and Finite Element Modeling," was accepted for publication in JOM (U. Carvajal-Nunez, M.S. Elbakhshwan, J.T. White, N.A. Mara, and A.T. Nelson). The manuscript presents hardness and elastic property data for U3Si, U3Si2, and USi. These data are analyzed in comparison to microhardness measurements collected using traditional means. A finite element model is utilized to calculate the yield stress of U3Si2 by fitting the load-displacement curves obtained. This data and critical assessment of published hardness data will be important in interpretation of initial post irradiation examination data collected for U3Si2 in the coming months. (U. Carvajal-Nunez)

- **[LANL]** A publication titled, "Determination of elastic properties of polycrystalline U3Si2 using resonant ultrasound spectroscopy," was accepted for publication in the Journal of Nuclear Materials (U. Carvajal-Nunez, T.A. Saleh, J.T. White, B.A. Maiorov, and A.T. Nelson). The elastic properties of U3Si2 at room temperature were measured via resonant ultrasound spectroscopy. These results, the first such data obtained for high purity, well characterized polycrystalline material, are assessed against historic values and more recent predictions obtained through density functional theory or other first principles approaches. A numerical model to assess thermal stress in an operating fuel was evaluated using these previously unavailable values. The thermal stress evolved in U3Si2 was compared to UO2 to facilitate an estimation of the probability of crack formation in U3Si2 under representative light water reactor operating conditions. These results suggest that even with its brittle nature, the reduced thermal gradients facilitated by the improved thermal conductivity of U3Si2 greatly minimize the chance of fuel fracture. The availability of elastic property data for U3Si2, the first available, allows for improvements in implementation of U3Si2 mechanical behavior into fuel performance codes and benchmarking of ongoing modeling and simulation efforts. (U. Carvajal-Nunez)
- **[LANL]** A series of two companion manuscripts titled, "U3Si2 Behavior in H2O," were accepted for publication in the Journal of Nuclear Materials (A.T. Nelson, E.S. Wood, A. Migdosov, J.T. White, and C.J. Grote). The first, "Part I: Flowing Steam and the Effect of Hydrogen" reports thermogravimetric data for U3Si2 exposed to flowing steam at 250-470°C. Additionally the response of U3Si2 to flowing Ar-6% H2 from 350-400 C is presented. Microstructural degradation is observed following hours of exposure at 350°C in steam. U3Si2 undergoes pulverization on the timescale of minutes when temperatures are increased above 400°C. This mechanism is accelerated in flowing Ar-H2 at the same temperatures. The second, "Part II: Pressurized Water with Controlled Redox Chemistry," examines the behavior of U3Si2 following exposure to pressurized H2O at temperatures from 300-350°C. Testing was performed using two autoclave configurations and multiple redox conditions. Use of solid state buffers to attain a controlled water chemistry is also presented as a means to test actinide-bearing systems. Buffers were used to vary the hydrogen concentration between 1 and 30 parts per million hydrogen. The submission summarizes the results of these conditions on fuel integrity, and presents new data supporting hydriding as a dominant mechanism governing pulverization of this material under reducing conditions. The data presented in these publications provides critical data on the response of U3Si2 under exposure to water, steam, and hydrogen and elucidates a critical vulnerability for this fuel when used in light water reactor applications (A. Nelson).
- **[LANL]** An initial assessment of the thermal diffusivity of UB2 and UB4 pellets that were sintered to high densities (>90% TD) via SPS in RPI (June 2016) was carried out. The thermal diffusivity of these samples was measured up to 1000°C and is shown in Figure 2. It was found that the thermal diffusivity for both uranium boride pellets was increased, when compared to the diffusivity of UO2. The thermal diffusivity of the UB2 sample showcased the larger increase with respect to UO2. Further thermal diffusivity measurements up to 1600°C are planned and will be carried out in the near future to confirm the preliminary data shown here and assess the accident tolerance of UB2 and UB4. (E. Kardoulaki)

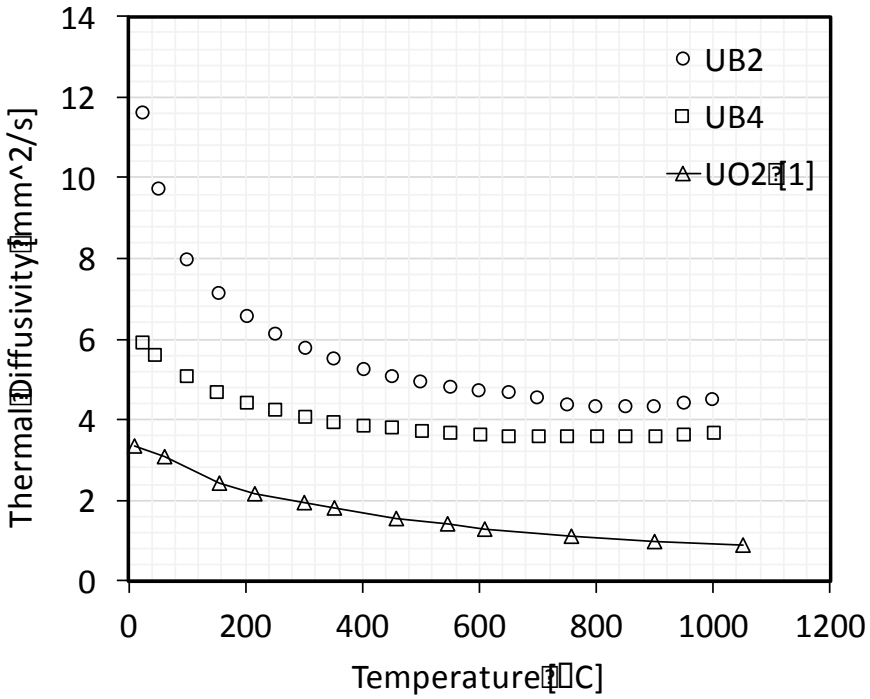


Figure 2. Thermal diffusivity as a function of temperature up to 1000°C for UB_2 (circles) and UB_4 (squares) samples along with reference thermal diffusivity data on UO_2 [1] (triangles).

References

[1] J. Fink, "Thermophysical properties of uranium dioxide," *J. Nucl. Mater.*, vol. 279, no. 1, pp. 1–18, 2000.

- **[ORNL]** Gadolinium has been added to the sol-gel feedstock broth as both a sesquioxide and as Gd(NO3)36H2O (gadolinium nitrate hexahydrate). When added as an oxide, theoretical densities were well below the benchmark kernel densities. On the other hand, when added as a hexahydrate, increasing Gd content results in increasingly higher kernel theoretical density as illustrated in Figure 3 below. Gadolinium nitrate hexahydrate has been successfully added to the sol-gel solution up to ~0.05 heavy metal fraction. Somewhere between 0.05 and 0.10 Gd heavy metal fractions, the solution separates into two immiscible phases. (K. Terrani)

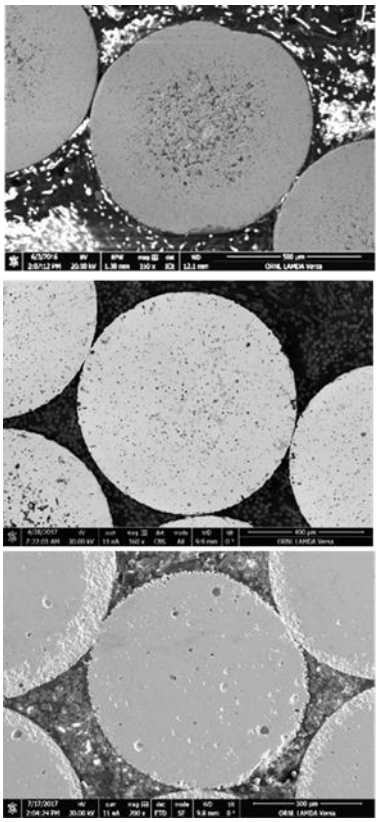


Figure 3. Increasingly higher kernel theoretical density illustration.

LWR Core Materials

- **[LANL]** Two L3 milestone reports were met this month. Room temperature and elevated temperature tensile testing was performed on rods of two FeCrAl alloys (B136Y3 and C35M4). Data showed good ductility in both alloys while some inclusions were observed. Ion irradiations were performed on these alloys at 300°C to doses up to 70 dpa. The microstructure was characterized after ion irradiation quantifying the increased dislocation loop density using TEM. (S. Maloy)
- **[LANL]** Ring pull tests were performed on tubes of three generation I FeCrAl alloys. Results showed a good measure of ductility and excellent reproducibility. Testing was performed rings with a straight cut and a gauge length. These results were summarized in a report to meet a L3 milestone. (S. Maloy)
- **[LANL]** The manuscript titled, "Oxidation Kinetics of Ferritic Alloys in High-Temperature Steam Environments," (S.S. Parker, J.T. White, P. Hosemann, and A.T. Nelson) was accepted for publication in JOM. The publication presents the results of high temperature (800-1200°C) isothermal steam oxidation studies performed on a range of commercial alloys. Unlike optimized FeCrAl compositions that have been specifically engineered with resistance to steam oxidation and irradiation tolerance in mind, the focus of this study was characterization of traditional Fe-Cr and Fe-Cr-Al systems. These alloys were not expected to resist degradation under steam to the same extent as optimized FeCrAls. However, industrial experience in manufacturing, joining, or potential ease of licensure may make these alloys attractive for limited applications. The oxidation kinetics and microstructures evolved by commercial alloys are generally inferior to optimized FeCrAl (C26M). The data provided by this document augment the existing FeCrAl literature and elucidate the behavior of non-optimized alloy compositions under environments relevant to accident tolerance. (A Nelson).

- **[ORNL]** A manuscript titled, "Effects of Laves phase particles on recovery and recrystallization behaviors of Nb-containing FeCrAl alloys," was published in Acta Materialia in November, 2017 (volume144, pp. 716-727, 2018). It proposed an alloy design to control grain size of FeCrAl alloy during thin-wall tube production process through the formation of second-phase particles. One related article investigating the recrystallization texture is currently under internal review process at ORNL, and preparation of another article summarizing impact toughness of FeCrAl alloys is currently in progress. (Z. Sun, Y. Yamamoto)
- **[ORNL]** Production of Gen. II wrought C26M FeCrAl alloy tubes (Fe-12Cr-6Al-2Mo base) for PWR fuel cladding is currently in progress. Total ~34 ft. length of the master bars has been provided to Century Tubes, Inc., and the gun-drilling process of all master bars has been completed. The tube drawing process will be initiated in December 2017. The expected delivery date is now March, 2018. (Y. Yamamoto)
- **[ORNL]** SiC tensile bars subjected to an in-pile creep test in the Halden reactor have been transferred from the reactor to the LAMDA laboratory at ORNL. Post-irradiation strain measurement of the tensile bars (Figure 4) has been conducted by measurement of distances between engraved marks on the specimens (Figure 5) using an optical microscopy to calibrate the in-situ strain measurement. The analysis found irradiation creep strain was ~6×10-4 following irradiation at 300°C to 0.1dpa under applied tensile stress of 100MPa. Further analysis will be conducted to predict the creep behavior under different applied stress level and temperature/dose conditions. (Y. Katoh)

Figure 4. Appearance of irradiated SiC tensile bar.

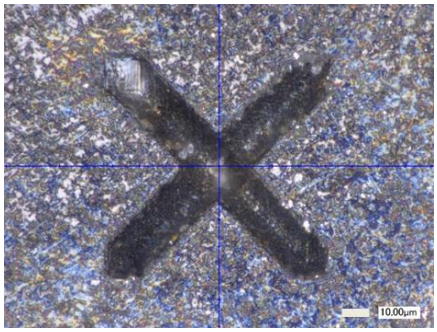


Figure 5. Engraved mark on the irradiated SiC tensile specimen. Distance of the engraved marks were used to measure the creep strain.

- **[ORNL]** ORNL has been asked to present an invited talk titled, "Post-irradiation examination of SiC tubes neutron irradiated under a radial high heat flux," T. Koyanagi, Y. Katoh, G. Singh, C. Petrie (ORNL) C. Deck (GA) and KI. Terrani (ORNL). (K. Terrani)

LWR Irradiation Testing & PIE Techniques

- **[INL]** The Accident Tolerant Fuels 2 (ATF-2) Sensor Qualification Test (SQT) experiment began irradiation on October 6, 2017 during Advanced Test Reactor (ATR) cycle 162A and is scheduled to finish on December 7, 2017. Design, analysis, and fabrication of "low risk" ATF-2 (Fuel Test)

components is in progress. ATF-2 fuel pin components are being machined and weld development is in progress. (G. Hoggard)

- **[INL]** Rodlets from ATF-1W (U3Si2 – Zirlo) were sectioned for optical microscopy and chemical analysis. The results from this microscopy will be the first optical microscopy on LWR condition neutron irradiated U3Si2. (J. Harp)
- **[INL]** Preparations were also made to qualify an in-cell pycnometer to measure the density of irradiated ATF fuel. Preliminary wiring has begun and it was confirmed that the existing feedthrough will work for the current system. Phase 1 and 2 qualification are expected to be completed in December. (J. Harp)

LWR Fuel Safety Testing

- **[INL]** Requirements for inclusion into the test plan and Transient Prescription predictive analysis were determined. The timeline and personnel availability were firmed up to perform these activities. (D. Dempsey)
- **[INL]** Design of the Data Acquisition system is progressing allowing procurement of prototyping equipment and long lead equipment to begin. Assembly of the DAS is also beginning as procured equipment arrives. (J. Schulthess)
- **[INL]** Drawings were completed for the design of the Multi-SERTTA hydro test equipment that will support multiple configurations of equipment. Drawings have also been reviewed and approved. (J. Schulthess)
- **[INL]** All fabricated components of the Multi-SERTTA prototype have been crated and placed in recoverable storage for future use. (J. Schulthess)

LWR Computational Analysis & Fuel Modeling

- **[BNL]** New cross-section libraries have been generated for the reference UO2/Zr fuel at hot-full-power (HFP). They include all model refinements (control rod self-shielding, pin powers) and were obtained with Triton lattice fuel assembly code in SCALE6.2.2 code package. Manual cycle-by-cycle depletion with PARCS is underway. The objective is to obtain credible equilibrium BOC/MOC/EOC conditions to use as the initial conditions for accident analysis with the TRACE systems code.

  The sequence will be replicated for U3Si2 fuel with SiC/SiC or coated Zircalloy cladding. The PARCS three-dimensional core model will be recompiled to incorporate the most recent properties for the fuel and cladding. Using updated kinetics parameters from the refined full core analysis representative accidents will be simulated using the TRACE PWR plant model to evaluate the coping time of different ATF designs against the standard UO2/Zr fuel. Sensitivity analysis will be performed to assess the impact on the coping time from inherent plant response, potential component failures and emergency actions. (A. Cuadra, L.-Y. Cheng)
- **[INL]** The focus of the modeling effort is being placed on the as run analysis of the ATF-1 experiments with the emphasis on pre and post irradiation analysis of the experiments and the capability to model fission gas generation and release, swelling etc. (P. Medvedev)
- **[ORNL]** Recent work on the fuel performance simulation of FeCrAl cladded fuel rods has targeted the behavior of the cladding under transient conditions. In order to show the impact of using FeCrAl cladding over Zircaloy, similar behavioral models must be implemented for the FeCrAl cladding. This work consists of improvements to the current plasticity (linear strain hardening) model to incorporate a variable strain hardening parameter. Work is also being done to conduct a parametric analysis on fuel rod conditions during a loss of coolant accident. Here, the temperature boundary

conditions and fuel burnup are varied to compare the differences between the Zircaloy and FeCrAl cladding for a range of situations. A manuscript titled, "Fuel performance simulation of iron-chrome-aluminum (FeCrAl) cladding during steady-state LWR operation," R.T. Sweet, N.M. George, G.I. Maldonado, K.A. Terrani, and B.D. Wirth, has been accepted for publication in Nuclear Engineering & Design. (B. Wirth)

Industry FOA

- **[INL]** Fabrication drawings are in for approval for the Fuel Fabrication for Westinghouse LFR task. (P. Wells)
- **[INL]** Procurement of the Tr-Arc Furnace was initiated, as well as the sintering furnace. (P. Wells)

ADVANCED REACTOR FUELS

AR Fuels

- **[INL]** Work has continued on characterization of the extruded Zr sheathed U-6Zr and U-10Zr rods. Based on radiographs, both radial and longitudinal sections were taken along the lengths of the rods. Samples were taken at the approximate beginning of the fuel (immediately after the header), in the center section, and toward the tail section (right before the footer). In addition to these sections, because the U-6Zr was inadvertently extruded with the footer going first copper was entrained internal to the zirconium liner. Metallographic samples were taken at this location as well as at a large void found within the U-6Zr rod towards the tail section. Characterization has been initiated. Figure 6 below shows an optical image of the center section of the U-10Zr rod.

  When the U-6Zr and U-10Zr extrusion billets were cast, both billets were cast into a slightly oversized Y2O3 coated graphite mold and machined to final diameter for insertion and sealing into the zirconium can. An additional U-10Zr billet was cast at that time, however, the billet was cast directly into the zirconium can which had been loaded into the graphite mold. This integrally canned billet was ultrasonically examined for shrinkage voids which may lead to debonds between the fuel and the zirconium can. Testing indicated that there were no debond regions between the fuel and can, however, because due to equipment and development limitations, no effort was made to determine if voids were present in the fuel portion of the billet. This billet can now be cut to length and be prepared for extrusion with minimal processing. (R. Fielding)

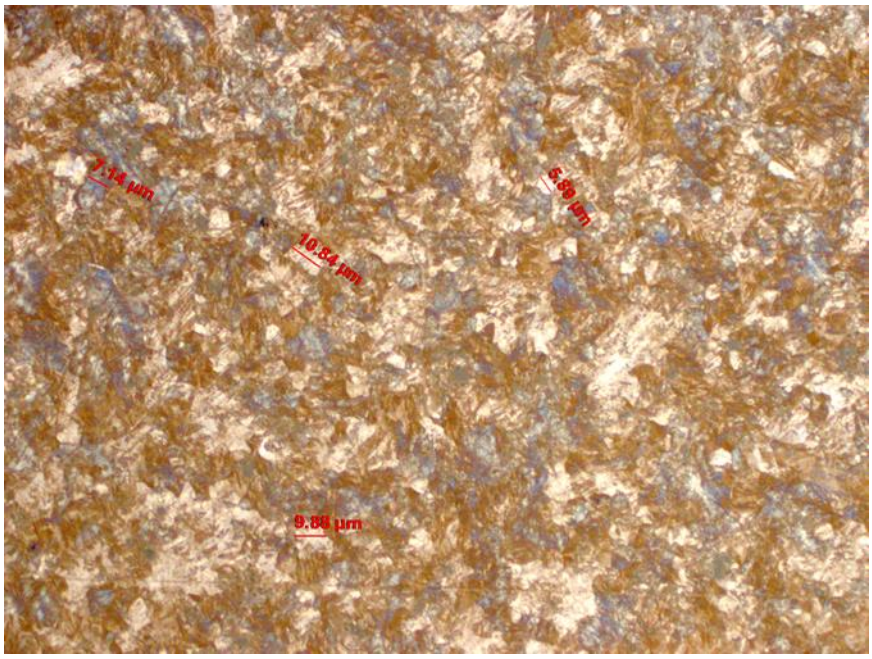


Figure 6. Radial microstructure of the extruded Zr canned U-10Zr rod.

- **[INL]** As part of the MOX work led by Dr. Seongtae Kwong, a new tungsten carbide die was procured and delivered. Using the custom made die should aid in increasing the final sintered density and structural integrity of the MOX pellets. Unfortunately, one of the die punches was chipped. The punch has been returned to the vendor for re-work. (R. Fielding)
- **[INL]** Optimized fuel work has progressed, led by Dr. Michael Benson. Two metallic fuel additives, tin and palladium, are being investigated for their effectiveness to control FCCI, as well as the first mixed additive system, using tin and antimony. Analysis of two diffusion couples, U-10Zr-4Sn against a lanthanide mix, and against iron, have been analyzed by scanning electron microscopy (SEM). Analysis of the data is underway. The SEM analysis of the as-cast and annealed microstructures of U-10Zr-2Sn-2Sb and U-10Zr-2Sn-2Sb-4Ln has been completed. Analysis of the data is underway. (R. Fielding)
- **[INL]** The diffusion couples U-20Pu-10Zr-3.86 against iron, and U-20Pu-10Zr-3.86-4.3Ln against iron, have been moved to EML and prepared for SEM analysis, which is scheduled for January. The alloys U-20Pu-10Zr-4Sn and U-20Pu-10Zr-4Sn-4Ln, which were cast last fiscal year in FMF, have been sectioned for analysis. The sections are being moved to the analytical laboratory for diffusion couple experiments, and to EML for as-cast SEM characterization. (R. Fielding)
- **[INL]** The following journal article was submitted and is under review: "Microstructural characterization of annealed U-12Zr-4Pd and U-12Zr-4Pd-5Ln: Two fuel alloys addressing cladding interactions," M. T. Benson, L. He, J. A. King, R. D. Mariani, J. Nucl. Mater., in review. (R. Fielding)
- **[INL]** An assessment of the thermal expansion data for the fuels handbook was conducted. According to phase diagrams, room-temperature U-Zr alloys should contain two phases. Single crystals of both phases have anisotropic thermal expansion (i.e., they expand or contract by different amounts in different crystallographic directions when heated). Thermal expansion of polycrystalline samples is dependent on microstructure (including phases actually present, crystal sizes, and preferred orientations, which may be significantly influenced by low levels of impurities such as dissolved oxygen), particularly when the samples contain more than one phase or have phases with anisotropic thermal expansion. It is therefore not clear how much of the difference between the results of Saller et

al. and of Basak et al. can be explained by differences in samples, and which (if either) is a good representation of the thermal expansion of an actual U-10Zr fuel.

All data show an increase in thermal expansion with increasing temperature and an abrupt change in sample length related to phase transitions between ~950 and 1000°C. (Figure 7). Data labeled "Heat treat B" and "Heat treat E" is from Saller et al. 1956. All samples were induction melted, solidified, re-melted, cast, forged, hot-rolled, annealed, cold-rolled, annealed a second time, and heated at 800°C for an hour. Heat treat B samples were then furnace cooled from 750 to 500°C. Heat treat E samples were furnace cooled to 670°C, annealed at that temperature for an hour, and furnace cooled to room temperature. Data collected during heating and cooling show good agreement. No information about impurities was provided. The line labeled "Touloukian" is a polynomial fit to the data of Saller et al. The line labeled "Basak" is a polynomial fit to the data of Basak et al., from a sample that was melted and solidified, then machined. It had 450 ppm C, 60 ppm N, and 580 ppm O. Concentrations of both C and O are high enough that they may affect material properties. C. Papesch)

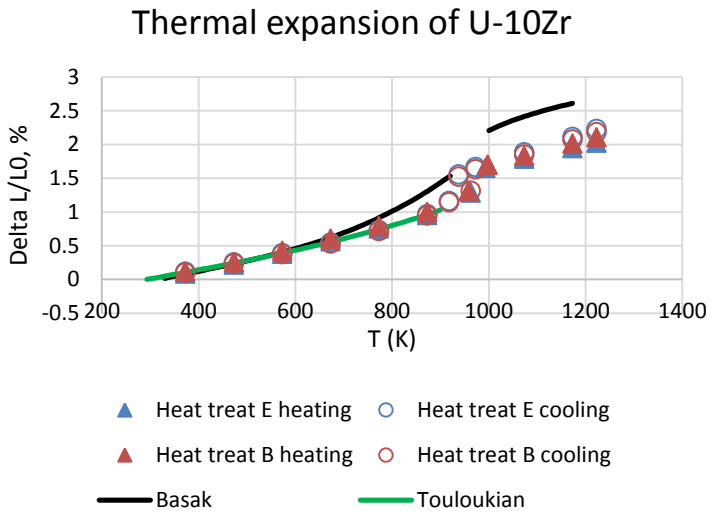


Figure 7. Thermal expansion data.

- **[INL]** A review paper was drafted for JNM on the physical properties of U-10Zr as a result of all the work done to write the Handbook. It is currently out for INL review. (C. Papesch)
- **[INL]** A presentation on the content of the Fuels Handbook was given by Dawn Janney at the Innovative Fuels Expert Group meeting in early November, conducted by the OECD-NEA organization, in France. (C. Papesch)
- **[INL]** Work on optimized fuel compositions continues. DSC testing has begun on three compositions of U-Pu-Zr with Pd and MTZ added. An investigation of new crucible materials for use in measurement of specific heat capacity for high-Pu bearing materials was conducted. It was shown with measurements of standard materials that MgO crucibles are a candidate for these measurements. Using MgO instead of Y2O3 or Al2O3 may reduce the sample interaction with the instrument and reduce error in thermophysical property measurements. (C. Papesch)

AR Core Materials

- **[PNNL]** The first experiments on observing the fate of injected ion redistribution have been completed, and the data have been analyzed. A journal publication on the topic will be prepared over the next several months. (M. Toloczko)

- **[PNNL]** Draft reports for the completion of several milestones have been written. These will be finalized over the next several weeks. (M. Toloczko)
- **[LANL]** Rods of 14YWT received from CEA under the bilateral agreement were hydrostatically extruded to ~10 inches in length. Microhardness was performed on these tubes and the microstructure was characterized using EBSD. (S. Maloy)
- **[ORNL]** The remaining half of the 1 mm thick 14YWT plate is being prepared for the second friction stir welding (FSW) that will attempt to produce a butt joint. Special precautions are being taken to determine how to cut the 1 mm thick plate sample into two halves and then clamped to minimize the bending stresses that may form during the FSW run. (D. Hoelzer)
- **[ORNL]** The user proposal titled, "The Role of Friction Stir Welding on Generating Residual Stresses in a Thin Plate of 14YWT," (IPTS-19909.1) submitted in October 2017 to the ORNL Neutron Sciences User Office was accepted and awarded 4 days of beamtime at the HB-2B beam line at the Neutron Residual Stress Facility at HFIR. The planned experiments will study residual stresses in the stir zone of a butt joint that will be produced by friction stir welding (FSW) in the 1 mm thick 14YWT plate. These results will be significant in determining how much residual stresses are caused by FSW by comparing with results from the previous Neutron Science User proposal that determined residual stresses up to ~380 MPa formed during hot rolling of the 14YWT plate to the 1 mm thickness. (D. Hoelzer)
- **[ORNL]** An oral talk titled, "High-Temperature Creep of MA957,"' was given at the 18th International Fusion Reactor Materials Conference (ICFRM-18) held in Aomori, Japan on November 5-10, 2017. The results covered in the talk were supported by the NTRD program. The highlight of this talk included the recent sample of MA957 that only accumulated ~0.25% creep strain after exposure for ~61,000 h at ~825ºC and 70 MPa. This sample did not fail since the creep test was terminated. However, these results provide evidence that advanced ODS ferritic alloys can be pushed to operating temperatures of 800ºC and stresses of 70-100 MPa. (D. Hoelzer)
- **[PNNL]** As part of the program to fabricate tubing from difficult-to-fabricate materials, MA956 and 14YWT are being extruded and pilgered to final dimensions. Two thick-wall hollow tubes of 14YWT have been extruded and are staged for pilgering. Prior to pilgering, it will be advantageous to perform some straightening. The straightening will take place in order to facilitate the pilgering process, and a tool or fixture has been procured to facilitate the straightening process. The fixture is shown in Figure 8 below, and will be used in conjunction with a Load Frame. The straightening should take place in the next few weeks. (R. Omberg)

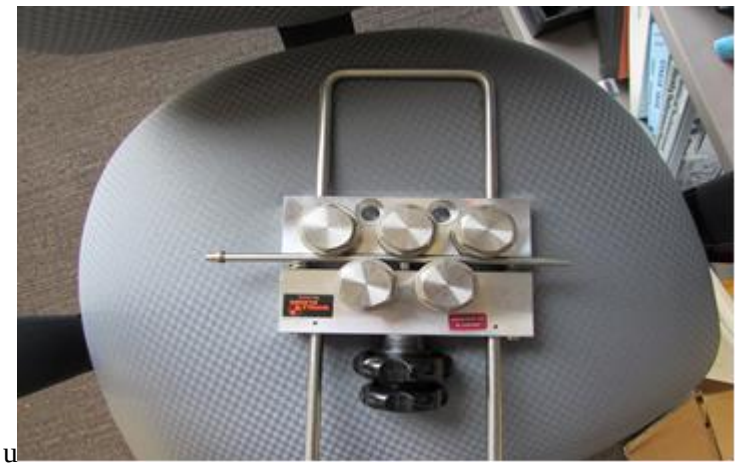
u 

Figure 8. Fixture used to straighten thick-wall extrusions prior to pilgering.

- [PNNL] As part of the effort to improve the fracture resistance of HT9 steels, estimation of plane-strain fracture toughness (KIC) was performed for the two HT9 steels (i.e., those with original composition and with nitrogen addition) in water-quenched condition and two-step tempered conditions. The Hahn and Rosenfield's model for fracture toughness calculation from tensile test data was modified to apply to the HT9 steels. The estimation results confirm the general temperature dependence of fracture toughness in ferritic steels, in which the fracture toughness slowly decreases with test temperature and the decreasing becomes steeper above about 400°C, primarily because of decrease in strength at high temperatures. The results indicate that the nitrogen addition in HT9 steels may not improve fracture toughness, although it will increase ductility. Relatively higher fracture toughness was calculated for the water quenched samples, which indicates that an incomplete tempering condition can result in improved fracture toughness along with increased strength. (T.S. Byun)

AR Irradiation Testing & PIE Techniques

- **[ANL]** In a transient accident, the relocation of molten fuel to the upper gas plenum is one of the important mechanisms to provide negative reactivity to a solid fuel SFR. In particular, bond sodium locked in fuel slugs plays an important role to the molten fuel relocation. Since annular fuel does not have bond sodium, however, different molten fuel behavior is expected in a transient accident. In order to compare the molten fuel behaviors between solid and annular fuels, transient models are under development in advanced test burner reactor (ABTR) core. As the first step, the unprotected loss of flow transient model for SAS4A code with solid fuel was developed and the change of the fuel form to annular fuel is underway. (T. Kim)
- **[INL]** The AFC-IRT experiment Conceptual Design Review was completed. This marks the point in design where we have determined that we have a successful path forward and will now launch into final design activities. (D. Dempsey)
- **[INL]** AFC-3C rodlets were examined by gamma spectrometry. This reveals the distribution of fission products in the fuel and can be used to infer local changes in fission density. (J. Harp)
- **[INL]** Dimensional inspections were completed on AFC-3D revealing little change in the diameter of these rodlets during irradiation. (J. Harp)
- **[INL]** Optical Microscopy was initiated on samples from a fuel pin irradiated in EBR-II that contained minor actinides (X501 G591). A sample of this microscopy is shown in Figure 9 for a cross section taken from about the mid-plane of the fuel column. (J. Harp)

Figure 9. Microscopy sample for a cross section taken from mid-plane of the fuel column.

- **[ORNL]** Specimens from HFIR irradiation capsules have been disassembled in the hot cells at 3525 and transferred to LAMDA for characterization. A work package has been opened at LAMDA for the characterization work and the drum containing the samples was received on 12/6/17. Acceptance of the samples by LAMDA represents a major step forward, as it enables the use of the significant characterization capabilities possessed by that facility. (G. Helmreich)

AR Computational Analysis & Fuel Modeling

- **[INL]** Significant progress has been made in modeling porosity migration in fast reactor MOX fuel. Methods to account for redistribution of fission power due to fuel restructuring have been developed. (P. Medvedev)

CAPABILITY DEVELOPMENT

CX Fuels

- [INL] Assessment of a sputter coater for use with the TCM is ongoing. The sub contract for TCM software fixes and enhancements has been established and the sub-contractor is in the INL badging process. Compatibility testing of stage motors with an argon environment is being conducted in a glove box at the MFC. Results are expected next week. A shim to adjust sample stage heights and incorporate lifting bails has been fabricated and installed. Procurement of extended cables for stage control has been initiated. Mockup testing revealed laser power losses in the optical fiber for the thickness monitor are limiting the coating thickness that can be measured. Switching from a single mode to a multimode fiber and feedthrough offer a substantial improvement. Quotes for a new feed through have been requested from several vendors. (D. Hurley)

For more information on Fuels contact Jon Carmack (208) 533-7255.

MATERIAL RECOVERY AND WASTE FORMS DEVELOPMENT

INTERNATIONAL COLLABORATIONS

- **[INL]** Terry Todd participated in the GENIORS (Gen IV integrated oxide fuels recycling strategies) meeting in Prague, CZ November 21-22, 2017. The GENIORS program is an EU framework program developing novel separation methods for recycle of GEN IV oxide fuels. Dr. Todd is on the Scientific Advisory Board for GENIORS and also coordinates the collaborative research between DOE labs (primarily INL, ORNL, ANL and PNNL) and GENIORS. At the Prague meeting, two technical workshops were held, 1) Diglycolamide (DGA) chemistry (an extractant used in many minor actinide separation schemes around the world) and 2) the effects of changing solvent extraction diluents in a process. Dr. Todd presented in the DGA workshop and later gave a seminar at the Czech Technical University. (T. Todd)

PROCESS CHEMISTRY AND INTEGRATION

- **[INL]** P. Zalupski attended the International Solvent Extraction Conference (ISEC 2017) in Miyazaki, Japan. A full conference proceedings paper titled, "Methods for Enhancing the Rates of Dissociation of the f-Element/Aminopolycarboxylate Complex for Efficient Differentiation of Trivalent Actinides from Trivalent Lanthanides in the ALSEP Process," was delivered. (P. Zalupski)
- **[INL]** Nathan Bessen, a graduate student from Colorado School of Mines spent the month of November at Idaho National Laboratory, learning potentiometric and spectroscopic techniques used to determine protonation constants and stability constants. As part of Nathan's efforts to study changes in the coordination chemistry of trivalent actinides (Am3+ through Es3+) the complexation features of Am3+ and Cm3+ by soft-donor ligand were investigated at INL using spectroscopy. (P. Zalupski)
- **[INL]** A new DEHBA irradiation campaign was initiated. Samples are being irradiated neat, and in contact with either 0.1 M or 4 M HNO3, with and without air sparging. These are essentially repeats of previous irradiations, but now at larger volumes to acquire enough solution for solvent extraction work, and repeated mass spec analysis. The major radiolysis product monoethylhexylbutyramide was synthesized by Technocom, and has been received at INL. Its effect on solvent extraction will be evaluated for comparison to work conducted at Marcoule. This is important because INL solvent extraction work indicates that a Pu complexing agent is produced by radiolysis, while CEA work identified no Pu-complexes by mass spec. Monoethylhexylbutyramide is the product most likely to be a Pu complexing agent and it will be directly evaluated in solvent extraction experiments at INL. (B. Mincher)
- **[ORNL]** In the month of November, a more detailed analysis and assessment of operating cost for the membrane-based and CECE process for tritium separation and concentration was performed. The published reports provide some useful information on the energy consumption for the CECE process. However, there is no discussion of the capital cost for the associated equipment such as electrolytic cells and catalyst bed columns. For the CECE process, the major energy usage is associated with the electrolysis of water. This process also involves catalyst exchange to further separate the hydrogen isotopes with the objective of obtained a concentrated HDO or HTO. We used this approach to determine the energy cost for the CECE process. We then compared the results with the energy cost for the membrane-based concentration of tritiated water for an aqueous stream flow rate of 10 L/min. It was observed that the cost associated with the electrolysis of water is relatively high compared to the membrane-based process for the concentration of tritiated water. The delayed milestone report is due by the end of December 2017. (B. Jubin)

- **[ORNL]** The 2018 goals of the project are to provide a path forward for the disposal of the powders that will be generated during the future hot cell demonstration of the pre-treatment process. For this purpose, cermet and grout wastes forms will be tested using surrogate samples of the pre-treated oxide/nitrate powder. A copper based cermet will be tested using WO2 and WO3 powders to simulate uranium oxides. Initially, we will be using a V-blender to mix the tungsten oxide powders with the copper powder and set of dies to cold press green cermet pellets. The green pellets will be then heated to sinter the metallic copper. The objective is to generate a continuous metallic phase that encapsulates the oxide powders. We will vary the mix ratios and processing conditions to determine a reasonable processing window. The equipment is on hand and we are still awaiting some of the reagents. We expect to press the first cermets samples within 1 or 2 weeks. (B. Jubin)

SIGMA TEAM FOR ADVANCED ACTINIDE RECYCLE

- **[ANL]** A paper titled, "Synthesis of hexavalent molybdenum formo- and aceto-hydroxamates and deferoxamine via liquid-liquid metal partitioning," was accepted for publication in Inorganica Chimica Acta. The paper describes the molybdenum speciation in the organic and the aqueous phases under conditions that are relevant to the ALSEP Mo scrubbing step. Additionally, a new method of crystal growth and synthesis based on solvent extraction that allows for isolation of elusive Mo crystals is reported for the first time. (A. Gelis)
- **[INL]** The INL PI traveled to Florida International University to meet with the NEUP collaborator on Am electrochemical oxidation. During this meeting, Prof Dares' next trip to INL (to occur the week of Dec 18) was planned. The PI presented a seminar on Am radiation chemistry to FIU faculty and students. Modeling of redox chemistry in irradiated Am solutions was initiated which incorporates data from longer term irradiations conducted in November to include AmV radiolytic reduction. Being more stable, much higher doses are required to reduce AmV. This has also included long-term data collection for AmV autoreduction at different nitric acid concentrations, to collect data on self-reduction and disproportionation to serve as baselines for the irradiated samples. This work is relying on the molar extinction coefficients that were arrived at through sensitivity analysis in our previous AmVI autoreduction work. (B. Mincher)
- **[PNNL]** The article, "Effect of HEH[EHP] impurities on the ALSEP solvent extraction process," was accepted for publication in the peer-reviewed journal Solvent Extraction and Ion Exchange. In this paper, the acidic extractant, 2-ethylhexylphosphonic acid mono-2-ethylhexyl ester (HEH[EHP]) is characterized with respect to its common impurities and their impact on Am(III) stripping in the Actinide Lanthanide SEParation (ALSEP) system. To control impurities in HEH[EHP], existing purification technologies commonly applied for the acidic organophosphorus reagent is assessed and a new chromatographic purification method specific to HEH[EHP] is presented. The authors of this paper are V.E. Holfeltz, E.L. Campbell, D.R. Peterman, R.F. Standaert, A. Paulenova, G.J. Lumetta, and T.G. Levitskaia. (G. Lumetta)

WASTE FORM DEVELOPMENT AND PERFORMANCE

Electrochemical Waste Forms

- **[ANL]** Samples of the first iron phosphate waste form made with dehalogenated electrorefiner waste salt were examined and subjected to leach tests. These materials are being evaluated as alternative waste forms for salt waste from the electrorefiner. Both quenched glass and glass that had been annealed to represent slow cooling of a full-size waste form were examined. Analyses indicate the salt was not completely dehalogenated prior to vitrification. Figure 10a shows an optical image of the cross-sectioned quenched glass and Figure 10b shows an SEM image of the cross-sectioned annealed glass. Significant amounts of KCl-dominated salt inclusions were observed distributed through both

materials and high Cl– contents were measured in solutions from ASTM C1308 tests with the annealed material. SEM analyses showed an abundance of what appear to be CeO2-dominated inclusions in the glass phase; evaporite crystals of KCl that formed when the sample was polished in water are also seen in the SEM image. Various modifications of the dechlorination process to improve its efficiency are being discussed with collaborators. For example, the efficiency of the dechlorination step will be assessed at different temperatures, hold times, and salt loadings without added iron oxide and without vitrification. (W. Ebert)

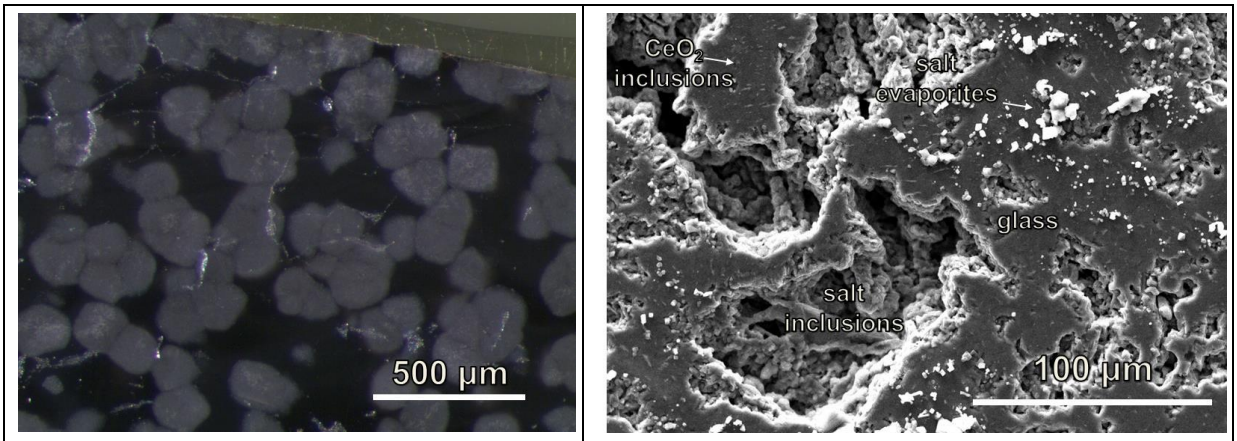


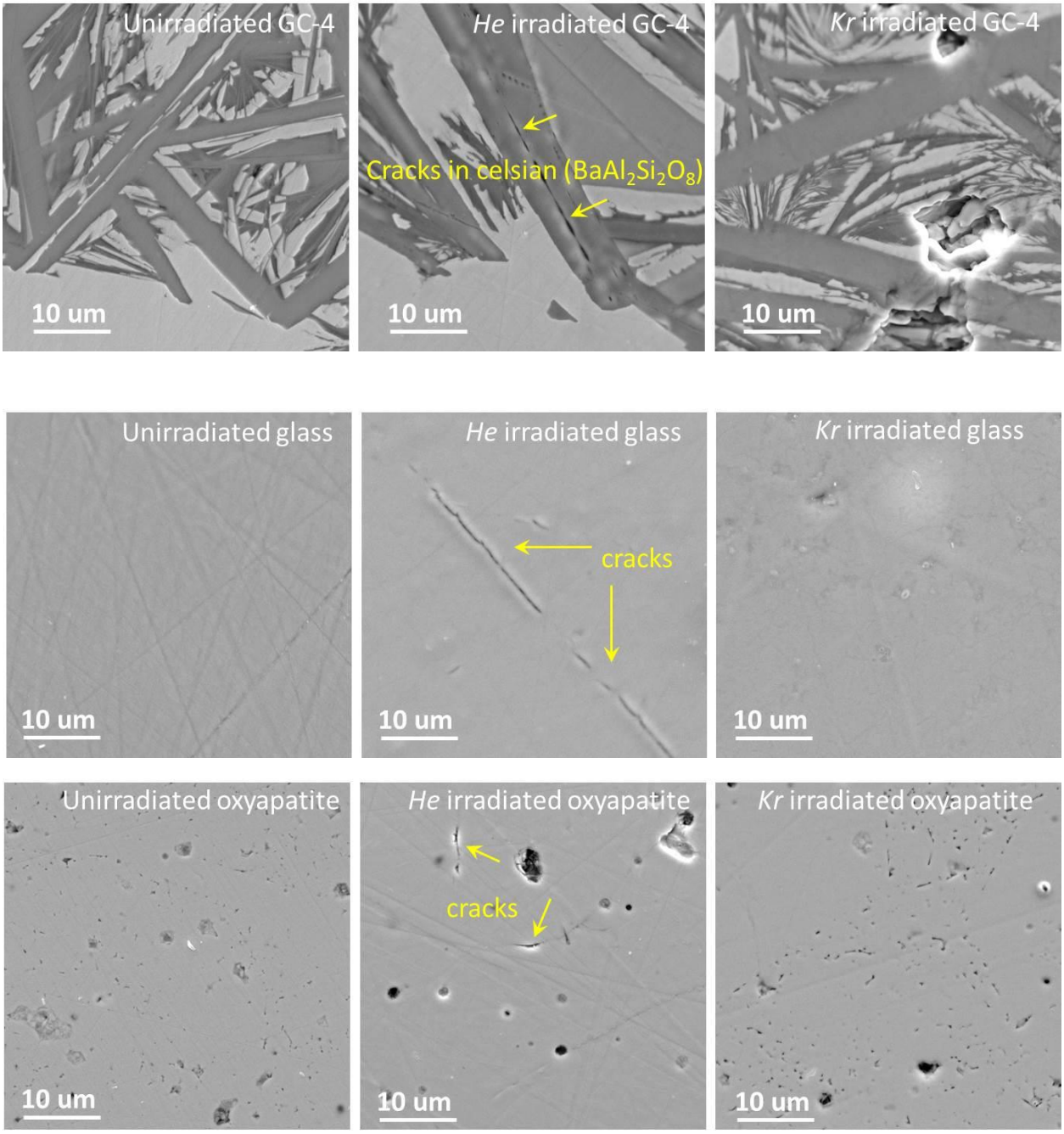
Figure 10. (a) optical and (b) SEM images of polished cross section showing iron phosphate glass matrix with large inclusions of residual salt and small CeO_2 inclusions.

Ceramic Waste Forms

- **[LANL]** Ming Tang attended MRS-Scientific Basis for Nuclear Waste Management Symposium which was held October 29- November 03, 2017, at Sydney, Australia and gave a presentation titled "Radiation stability study of melt processed and hot isostatically pressed multi-phase ceramic waste forms." (M. Tang)

Glass Ceramics Waste Forms

- **[LANL]** Radiation-induced microcrack in multiphase glass ceramic waste form samples, single phase oxyapatite and powellite, and the remainder glass (based on the centroid composition named C1 with the crystals removed after slow cooling), is investigated using ion irradiations including He (alpha) ion beam to simulate helium accumulation and alpha radiation in nuclear wastes and Kr ion beam to simulate alpha decay in nuclear wastes. The SEM images in Figure 11 below show microcracks in He irradiated GC-4, remainder glass, single phase oxyapatite but not in Kr irradiated samples. It suggests that microcracks are induced by He accumulation and alpha radiation. (M. Tang)


Unirradiated GC-4
10 um
He irradiated GC-4
Cracks in celsian ($BaAl_2Si_2O_8$)
10 um
Kr irradiated GC-4
10 um
Unirradiated glass
10 um
He irradiated glass
cracks
10 um
Kr irradiated glass
10 um
Unirradiated oxyapatite
10 um
He irradiated oxyapatite
cracks
10 um
Kr irradiated oxyapatite
10 um

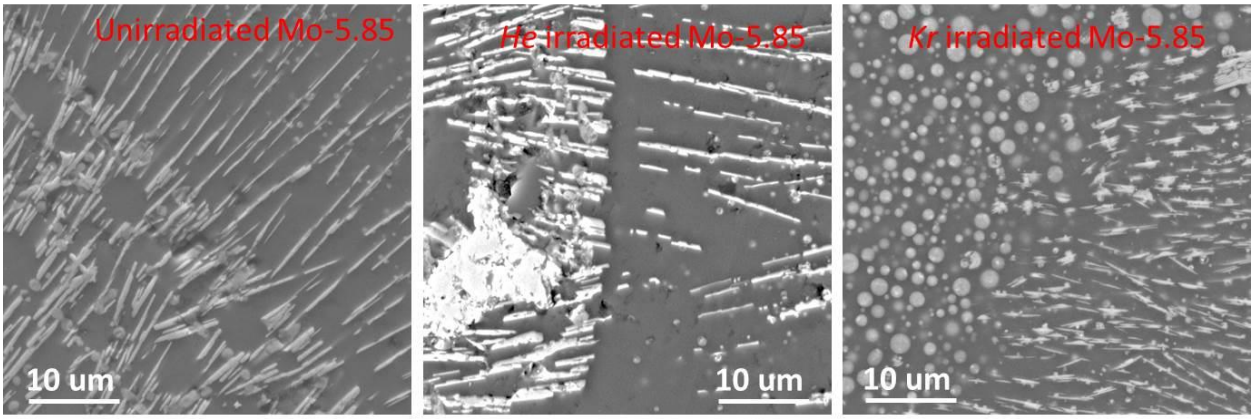


Figure 11. SEM observation of tested samples. From top to bottom: multiphase glass ceramic GC-4, remainder glass, single phase oxyapatite, multiphase glass ceramic Mo-5.85.

- **[SRNL]** SRNL long term multiple-year Phase I and Phase II glass ceramic corrosion tests via Product Consistency Test (PCT) were terminated in November with leachate analyses via ICPES and pH measurements completed. (C. Crawford, P. Smith)
- **[SRNL]** A material flaw (crack) in the drain tube of the CIM was found, which is believed to be the cause of the stuck pour in the CIM. The SRNL path forward is to cut-off the drain tube above the crack leaving enough tube length to continue to operate normally. (J. Amoroso, P. Smith)

Zirconium Recycle

- **[ORNL]** A test plan describing impurities in the ZrCl4 feedstock, test equipment, and procedures for the planned purification tests to be made in Cave B the REDC 7920 facility was prepared for evaluation by REDC reviewers. The equipment will be a glassware reactor and condenser designed for chemical pretreatment followed by re-sublimation of the ZrCl4. The pretreatment procedure is that developed by UTK in their NEUP project, and involves the use of SOCl2 or CCl4 to convert NbOCl3 to either NbCl5 or NbCl4 prior to re-sublimation, and the use of an addition of 5% ZrH2 to the impure ZrCl4 to convert volatile FeCl3 to non-volatile FeCl2 prior to re-sublimation. There is a window of opportunity in the Cave B schedule between mid-December 2017 and the end of March 2018 available to perform the purification tests which are the primary goal for FY 2018. This emphasis and limitations on hot cell availability may cause the milestone to finish the 3rd chlorination test to be delayed. (B. Jubin)

Advanced Waste Form Characterization

- **[ANL]** Analytical results for solutions collected in ASTM C1308 tests with AFCI and LRM glass through about 4 months have been evaluated, but analysis of the ~50 remaining solutions (through about 7 months) will be delayed until mid-December. These tests were conducted to derive parameter values for the ANL Stage 3 model for waste glass degradation. Available results show most tests with AFCI glass have entered Stage 3. These have been analyzed to evaluate the dependence of the Stage 2 rate on the pH and the Al and Si molar concentrations. Analyses of the Stage 3 rate dependencies will be done when results for longer sampling periods are available. Figure 12a and Figure 12b show the correlations of the Stage 2 rates in ASTM C1308 tests conducted at 90 °C with the measured pH (at RT) and with the Al and Si concentrations measured for the test periods used to derive the Stage 2 rate for each test. The three test conditions having the highest Stage 2 rate are those that also have the highest Stage 3 rate. The Stage 2 rates of the other tests show minor influence of the pH and Al and Si concentrations, although the effect of temperature is significant. (W. Ebert)

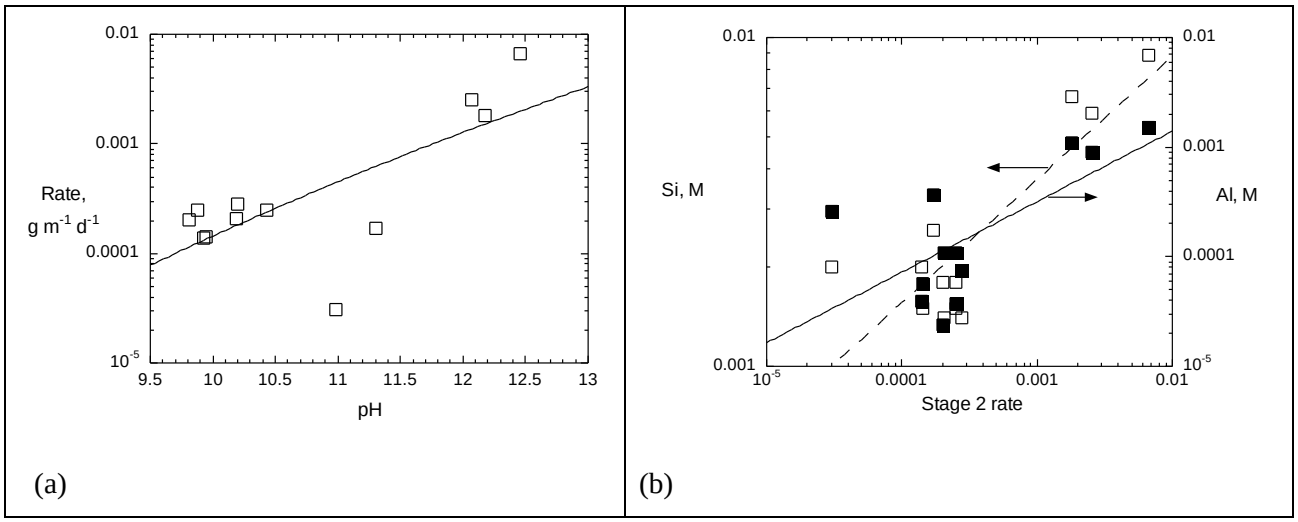


Figure 12. Results of ASTM C1308 tests with AFCI glass tests at 90 °C with (a) the measured pH (RT) and (b) with the measured Al and Si molar concentrations.

- **[ANL]** Electrochemical tests to measure the reductive-dissolution rate of AgI as a function of imposed surface potential representing the solution redox potential (Eh) and pH have been completed. The test results were documented in report NTRD-MRWFD-2017-000196. These tests are being conducted to develop a test method to support the design of durable radioiodide-bearing waste forms that is relevant to performance under disposal conditions. For example, Figure 13 shows the dependence of the AgI reductive-dissolution current density (j) on the cathodic over-potential (η) to be essentially constant in alkaline solutions as

$$j = j_0 \frac{C_O(0,t)}{C_O^*} e^{\frac{\alpha F \eta}{RT}} = a^* e^{b*\eta} \quad ,$$

such that the dissolution rate can be expressed using a simple rate law with a constant b term and weakly pH-dependent a term. Previous tests have shown the same rate law to apply in acidic and neutral solutions. (W. Ebert)

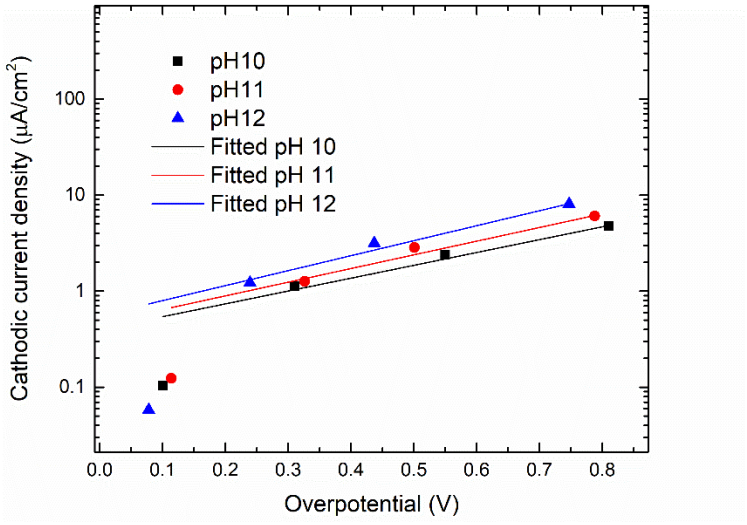


Figure 13. Summary of electrochemical measurements of AgI reductive-dissolution rates in alkali solutions.

- **[ANL]** An environmental glove box is being constructed to minimize air contamination in the next series of electrochemical tests in which various $FeSO_4$ solutions will be used to control the solution Eh and impose the electrochemical potential at the AgI surface rather than a potentiostat. Other electrochemical methods are being used to measure the chemical dissolution rate. (W. Ebert)
- **[PNNL]** An invited talk titled, "Glass corrosion and nuclear waste disposal: Using the study of ancient glass to evaluate long term effects," was given at the International Symposium on Glass Degradation in Atmospheric Conditions in Paris, France. The trip was entirely paid for by the organizing committee, and the research of the community focusing on the preservation of glass artifacts and art was extremely valuable. Often dealing with glass compositions that are much less durable that glass waste forms, the variations in extent due to composition was obvious. Some of these samples have direct relevance to current efforts to improve models of glass dissolution over the long term. Several contacts were made to look at collaborations to characterize particularly well-constrained corroded artifacts. (J. Ryan)
- **[PNNL]** The GRAAL (Glass Reactivity with Allowance for the Alteration Layer) model, developed at CEA, was designed to yield a square root dependence on time of the boron release. As reported in a previous monthly report, this is not always the case in static tests of the corrosion of borosilicate glasses and the introduction of a power factor p in GRAAL's second equation (Eq. 1), which controls the growth of the alteration layer, can significantly improve agreement between model results and experimental measurements. This equation is defined as

$$\frac{dL_{hydr}}{dt} = \frac{r_{hydr}}{1+\left(\frac{L_{hydr} r_{hydr}}{D_{gel}}\right)^{p}} - \frac{dL_{diss}}{dt} \qquad \text{Eq. 1}$$

- where L_{hydr} and L_{diss} are the thicknesses of the alteration and dissolved layers, r_{hydr} is rate of hydrolysis, D_{gel} is the water diffusion coefficient in the alteration layer, and t is time.
- The optimal value of p required to maximize agreement between model results and the time-dependent solution concentrations measured for each glass in the CJn glass series (Gin et al. JNCS 358 (2012) 2559) as well as SON68 was correlated with the glass composition. A value of p = 3.0 was found to be most suitable for the glasses containing both Ca and Al (CJ3 and CJ4), while p = 2.6 was more appropriate if Ce was present in the glass (CJ5, CJ6, and SON68). For glasses without Ca (CJ2 and CJ7), the optimal fit to the data followed the original GRAAL model with p = 1.0. In the absence of Al, glasses containing Ca and/or Zr were not as easily characterized (CJ8 and CJ9). When the residual rate of these glasses was plotted as a function of their optimal p value, a correlation emerged (Figure 5). These findings point to Ca as an important glass component in influencing diffusion

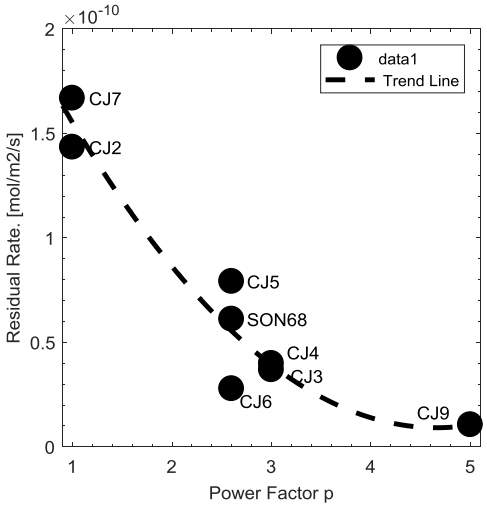


Figure 14. Residual rate taken from Gin et al JNCS 358 (2012) 2559 plotted versus the p value determined in this study. The trend line is for visualization purposes.

through the alteration layer and, in turn, controlling the residual alteration rate. (S. Kerisit)

DOMESTIC ELECTROCHEMICAL PROCESSING

- **[ANL]** Work continued on final reports on the Echem process data gap study and the development of a co-deposition cathode scheduled for issuance at the end of December and January, respectively. Argonne National Laboratory hosted technical experts from the Japan Atomic Energy Agency (JAEA) to discuss nuclear fuel cycle technology development activities at Argonne supporting the Office of Nuclear Energy, Nuclear Technology Research and Development Program. The discussion between JAEA and Argonne staff focused on the results of the recent fuel cycle options study, separations and waste form technology development, advanced nuclear fuel manufacturing, and current US – Japan collaborations in fast reactor analysis. JAEA staff were provided tours of some of the laboratories at Argonne being used for separations and nuclear fuel research and development. (W. Ebert)

SIGMA TEAM FOR OFF-GAS

- **[INL]** A second long-term iodobutane adsorption test is planned to start as soon as flow meter calibrations are complete, early in December. Results of the recently completed first iodobutane adsorption test shows that breakthrough was achieved in at least the first two of four silver Aeogel sorbent beds, as planned in order to determine the maximum practical capacity of the sorbent for those test conditions. (N. Soleberg, A. Welty)
- **[INL]** A Level 4 milestone M4NT-18IN030107015, "Integrated test system design and test plan, support," to support ORNL in preparation of a test plan was completed on schedule November 30, 2017. This test plan was for single component and integrated testing for wet scrubbing and chemisorption of dissolver offgas system iodine. The use of wet scrubbing may enable more practicable iodine chemisorption (needed to achieve the necessarily high decontamination factor) by removing a significant portion of the iodine upstream the chemisorption step.(N. Soelberg, A. Welty)
- **[ORNL]** In 2016, an initial engineering evaluation and design of the off-gas abatement systems required for a hypothetical 1000 t/y UNF reprocessing facility treating 5 yr cooled, 60 GWd/tIHM UNF was completed. One of the key findings of that report was that the consumption rate of silver-based iodine sorbents in the dissolver off-gas primary iodine capture bed is very high, resulting in very frequent remote filter replacements and may warrant the evaluation of alternative methods to capture the bulk of the iodine. This report is intended to describe the design of an experimental system that can be used to examine the use of aqueous scrubbing to remove the bulk of the iodine from the DOG stream prior to a silver-based solid sorbent that would be used to provide the final iodine capture or polishing step. This report also provides a description of the initial series of tests that are proposed for this system. The distribution of the associated report competed milestone M4NT-18OR030107022 on schedule. (B. Jubin)
- **[ORNL]** The milestone to complete the Phase 1B CH_3I tests was originally delayed due to facility shutdowns and required system modifications. It is now further delayed as the CH_3I feed system will require redesign to ensure reliable delivery. These issues were identified during completion of other milestones, in particular the Level 2 VOG effort, which also used the CH_3I feed streams. The compact Stirling Shuttle freezer unit should be delivered in late December. This will allow the direct introduction of controlled quantities of CH_3I via a bubbler operated at -20 to -40°C or low if desired. (B. Jubin)
- **[ORNL]** Pretreatment of 1 *M* scrubber solutions was concluded and the samples were sent for analysis of total Ru content by ICP-MS. RuO_4 is unstable in the 1 *M* NaOH scrubber solutions used during testing to capture gaseous RuO_4. It may exist as $NaRuO_4$ or as RuO_2 precipitate. To ensure

that the total measured Ru content was not biased by Ru precipitation out of solution, the solutions were pretreated prior to ICP-MS analysis of total Ru content. This pretreatment step was not anticipated, but was necessitated following the observation of precipitate formation after test completion. This additional work has pushed out the completion of the report on this work. These results have been received and the milestone report is partially drafted. (B. Jubin)

- **[ORNL]** Testing of an iodine and tritium removal system for advanced tritium pretreatment continued. Analysis of caustic iodine trapping solutions was completed and reflected very low iodine recovery in the trapping solutions. The test system was disassembled and it was observed that a piece of the test system equipment had substantial internal corrosion. Selected portions of the system were smeared for tritium content and it was found that tritium was co-located with the corrosion products. Two corroded fittings were removed from the system, leached in 1 *M* NaOH, and the leach solution sent for iodine and tritium analysis. (B. Jubin)
- **[PNNL]** A level five milestone M5NT-18PN030107033, "Supply Ag^0-Functionalized Silica Aerogel to ORNL," was completed for DOE-NE project "Development of Ag^0-functionalized silica aerogel for capturing and immobilization of radioiodine from reprocessing off-gas." A total 200.5 g of Ag^0-functionalized silica aerogel granules was produced at PNNL through functionalization of temperature strengthen silica aerogel. The granules were larger than 0.85 mm and had a bulk density of 492 kg/m^3. The sorbent exhibited iodine sorption capacity of 445.8 ± 4.7 mg/g after exposure to iodine vapors at 150°C for 66h. This indicates a silver concentration of 378.9 ± 4.0 mg/g, assuming a full utilization of silver during this test. The material was shipped to Oak Ridge National Laboratory for further sorption testing in various off-gas streams. (J. Matyas)
- **[PNNL]** 50 grams of best performing MOF was synthesized using a solvothermal synthesis to test at INL. Experiments are in progress to convert the powder sample to engineered particles in progress. (P. Thallapally)

FLOWSHEET DEMONSTRATIONS

- **[PNNL]** The first CoDCon flowsheet test was performed in November. Figure 15 presents a schematic illustration of the flowsheet tested. The solvent extraction portion of the experiment was divided into two parts. In Part 1, the solvent consisting of 30 vol% TBP dissolved in *n*-dodecane was loaded with U and Pu. In Part 2 of the experiment, the Pu was stripped from the U/Pu loaded solvent with U(IV) in such a way that a fraction of the U followed the Pu into the U/Pu nitrate product stream. The U and Pu concentrations in the aqueous outlet from stage 1 were monitored with the UV/vis and Raman systems so that adjustments could be made to the fresh TBP solvent flowrate at stage 1 to adjust the U/Pu product stream to the desired mass ratio of 2.33 (7/3). Preliminary results suggest that U/Pu nitrate stream from the solvent extraction flowsheet was higher in Pu content than planned, but that the U/Pu ratio was maintained with 3% of the mean value throughout the experiment. Modified direct denitration of the U/Pu nitrate solution is planned for December, along with more in-depth analysis of the experimental results. (G. Lumetta)

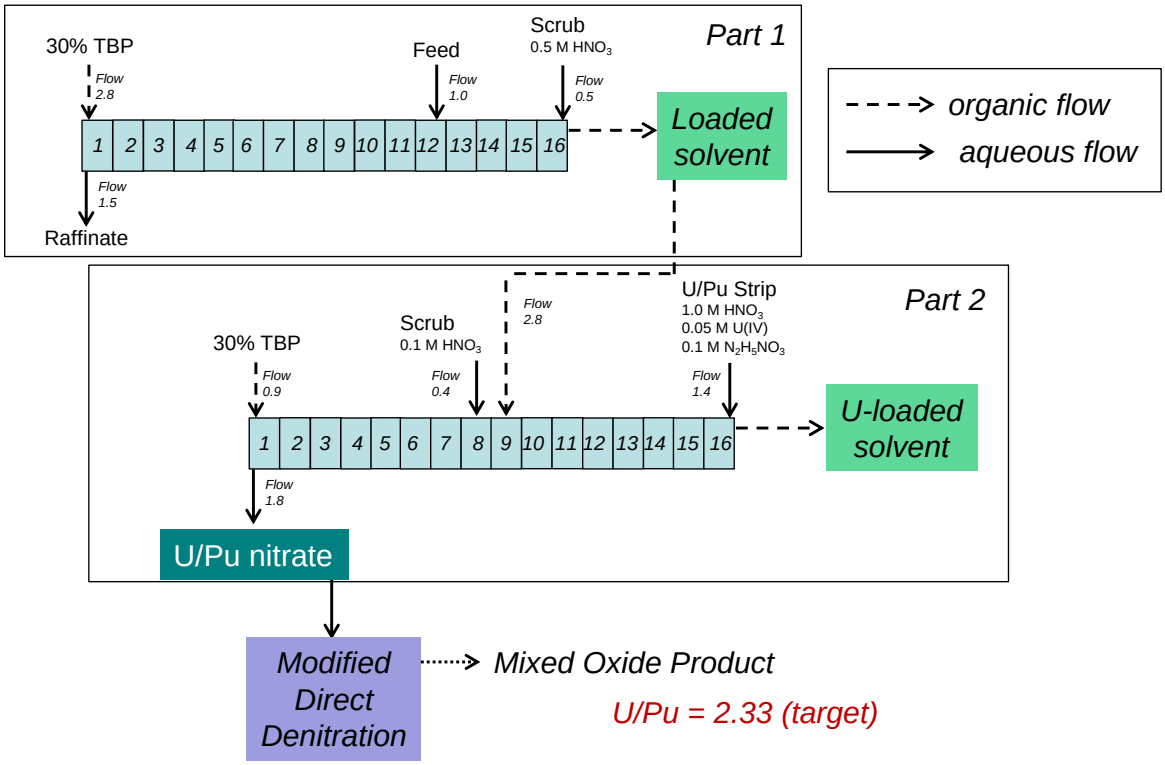


Figure 15. Flowsheet tested in the first CoDCon experiment, the numbers 1 through 16 refer to the individual 2-cm contactor stages.

- **[INL]** The installation of the Material Recovery Pilot Plant (MRPP) began in CPP-653 at the end of November. Premier Technology Inc. is the subcontractor who built the MRPP and will also be doing the installation, which will be ongoing until the end of February. This initial phase of installation involves constructing the Perma-Con enclosure and placing the two main process skids within that enclosure. In addition to this, the Laboratory Instruction for the operation of the MRPP has gone out for initial review. This work control document will be verified during Functional Acceptance Testing of the MRPP and used during the actual test runs. (M. Warner)
- **[INL]** The PI reviewed the test plan for the first CoDCon flowsheet demonstration and traveled to PNNL to observe testing. (J. Law)

For more information on Material Recovery and Waste Forms Development contact Terry Todd (208) 526-3365

MPACT Campaign

MANAGEMENT AND INTEGRATION

Management and Integration

- **[INL]** Mike Miller attended the ANS winter meeting where an early career MPACT researcher, Daniela Henzlova, was presented a Nuclear Technology R&D excellence award for her work on the High Dose Neutron Detector, a new technology that shows promise for product assay from electrochemical processing. As part of the JFCS, Jeff Sanders hosted LANL visitors in preparation for safeguards measurements during the IRT and to coordinate for the December US-ROK-IAEA meeting in Vienna.

CAM & Technical Support

- **[LANL]** Mike Miller (NTD) attended meetings at LANL on Nov. 16 with Advanced Integration and Microcalorimetry WPMs and staff. Discussions were held regarding project status and path forward. Presentations were prepared for the upcoming NE Advisory Committee Meeting.

SAFEGUARDS AND SECURITY BY DESIGN - ECHEM

Modeling and Simulation for Analysis of Safeguards Performance

- **[ANL]** A report has been initiated to describe the electrochemical process model and modelling assumptions that will be used as part of the virtual test bed (M2NT-18AN040104011). A literature review of cathode processing operations was conducted to inform development of a cathode processing unit operation model. Possible coding environments were evaluated for the model for scale-up and equipment selection analysis.

Voltammetry

- **[ANL]** Work on constructing the multielectrode sensor is proceeding according to plan. All of the ceramic parts on the sensor have been completed, and the tungsten electrodes are currently undergoing machining.
- **[INL]** A teleconference was held to discuss the experimental plan and project schedule. Experimenters are preparing to commence two different sets of experiments to address different aspects of the probe design and retest the original probe design with a few modifications based on FY17 research.

Sensor for Measuring Density and Depth of Molten Salt

- **[INL]** A fixture to mount the bubbler in the IRT ER in HFEF had to be designed due to the lack of a mounting port in the ER head plate for the bubbler after the last ER modifications. This month, a prototype of the fixture was manufactured and was delivered. Preliminary testing shows it may be effective at securing the bubbler, however, more testing is needed while applying a side load to the bubbler.

Electrochemical Signatures Development

- **[LANL]** HDND Detector Model MCNP6 simulation results (mesh tally and PHL detector tally) for the 252Cf source and HDND detector model were provided to Daniela Henzlova and Howard Menlove. The team will replicate or perform additional time-dependent experiments to evaluate

HDND response and benchmark simulations. There is the potential of measuring both the neutron and gross gamma simultaneously when using the HDND. Measured data will be of use for benchmarking MCNP6 simulations. The LANL Advanced Integration team was briefed on this matter for possible use in their work. As was discussed in October, FY17 moving-object work to depict radiation behavior in the hypothetical pyprocessing facility model made use of the Advanced Burner Test Reactur (ABTR) metal fuel and the Mark IV electrorefiner (ABTR/MK4). There is interest in use of the Westinghouse oxide fuel, the ANL PEER, and the simplified AFCF pyroprocessing facility as a common model for the advanced integration work leading to the MPACT 2020 capability demonstration milestone. During November, a moving-object neutron model with the HDND detector was created to treat the Westinghouse oxide fuel and the ANL PEER (WFA/PEER) so as to be consistent with the advanced integration work, etc. Differences in the volumes of the fuel dissolution baskets in the Mark IV and PEER models, and differences in the neutron source strengths for the ABTR and WFT models, cause the neutron source for the WFA/PEER to be approximate 1/1000th of that for the ABTR/MK4. Consequently, the HDND response for the WFA/PEER is much poorer than that for the ABTR/MK4. Simulations were made with model adjustments to position the HDND detectors closer to the moving TCATH material. This type of analysis is germane to concept of using MCNP6 radiation modeling to assist with the development and deployment of radiation detectors. Both ABTR/MK4 and WFA/PEER model development and simulation are being carried and detailed in the FY18 report.

ADVANCED INTEGRATION

Advanced Integration (Methods)

- **[LANL]** Continuing to work with Mark Croce with the microcalorimetry sensor to integrate his data with a pyroprocessing flowsheet.

Advanced Integration (Facility Models)

- **[SNL]** A Molten Salt Reactor safeguards model is being developed to expand the breadth of capabilities for the 2020 milestone. We expect to wrap up that development in December and focus on the pyroprocessing safeguards demonstration for remainder of the year.

EXPLORATORY RESEARCH / FIELD TESTS

Microcalorimetry

- **[LANL]** The 256-pixel SLEDGEHAMMER detector module will remain at LANL for testing over the next several months. This will allow us to focus on improving stability and performance of key components of the system. In October, one of the main problems identified was erratic behavior from the FPGA electronics. We determined that this was caused by a problem with a digital clock signal, and were able to fix this problem. This allowed us to begin a series of measurements to evaluate performance at various count rates (from 4 to 60 counts per second per pixel). Data analysis is ongoing. Over the next several months, we will work towards the M3 milestone of achieving reliable high-resolution operation by focusing on improvements in temperature regulation, magnetic shielding, and signal-to-noise ratios. In November, Katrina Koehler focused submitted a paper to the Journal of Low Temperature Physics on the first comparison of a theoretical calorimetric electron capture spectrum with an experimental measurement of Pt-193.

In situ Measurement of Pu Content in U/TRU Ingot

- **[INL]** The furnace and instruments for performing Pu content measurements are ready, and on hold before being transferred into HFEF hot cell due to the schedule change of producing U/TRU ingot under JFCS project.

High Dose Neutron Detector

- **[LANL]** Testing of repaired HDND continues. Scoping trip to INL is planned for December in order to evaluate options and requirements for planned field test of HDND.

For more information on MPACT contact Mike Miller at (208) 526-2813.

Fuel Cycle Options Campaign

CAMPAIGN MANAGEMENT

- **[ANL]** Participated in the 2017 Nuclear Technology Research and Development (NTRD) Annual Review Meeting, in Washington D.C., November 1-3, 2017, to present the Strategic Goals, FY17 Accomplishments, Planned FY18 Activities, and Current R&D Portfolio for the FCO Campaign. Also contributed a write-up for the Transaction Report being compiled on the meeting.
- **[ANL, INL, LLNL]** Continued working on a white paper entitled "DOE Nuclear Technology Research and Development Considerations for Program Strategy," which describes the results of an evaluation of the NE-4 R&D portfolio for completeness and relevance to the current U.S. Administration's R&D budget priorities for maintaining and/or regaining the U.S. leadership in nuclear science and technology R&D to support national security, economic growth, and job creation.

EQUILIBRIUM SYSTEM PERFORMANCE (ESP)

Performance of Fuel Cycle Systems

- **[ANL]** Collected information on the Holos-Generator reactor, which is a small-size gas-cooled reactor targeting a remote area (such as military base). The reactor was designed to use a gas-turbine, be accommodated in a typical container, and deployed by using semi-container trucks or military choppers. The proposed fuel cycle is once-through with LEU fuel (EG01 or EG02).

Economic Analysis Capabilities and Assessments

- **[ANL]** A meeting was organized at ANL on November 9 to discuss the grid market analysis tools available at ANL. It was decided that the EDGAR code (Economic Dispatch Genetic AlgoRithms) currently under development will be used by ANL for grid analysis within the FCO campaign.
- **[ANL]** The code development of the algorithm for the cost comparison of different reactors was started, such that the code is developed in a robust and consistent form, easy to debug. The cost model for the reactor containment is almost complete, including unit cost data and geometric calculations for cylindrical containments. A module variation will be added also for rectangular building.
- **[ANL]** The cost model for reactor pressure (and atmospheric pressure) vessels is being reviewed. Additionally, a deeper understanding on steel manufacturing and ingot formation was developed. Data was found for a representative amortization cost for ultra-heavy forging presses, based on the example of a 15,000-ton press installed at the UK Sheffield Forgemasters International. It was calculated that, with a throughput of about 1.7 vessels/year, similar to the throughput of the similar Areva's French facility at Creusot Forge's Chalon St. Marcel, each PWR pressure vessel would have to include about $22 million in facility amortization cost. This consideration helps explain the large cost of pressure vessels (typically between $50 and $100 million).
- **[ANL]** Analyzed the report: "SMR Start to a clean energy future; The economics of Small Modular Reactors", September 14, 2017, and collected a set of high-level information that could be useful for future reference and for potential questions that may need to be addressed by the FCO campaign. By proactively collecting that information, the campaign should be able to progressively (1) learn about those issues, and (2) develop a list of references and data points that could be drawn-upon as needed. Separately, developed a short write-up justifying the total market value claim that was included in a write-up submitted by the FCO campaign to DOE in October.

- **[INL]** Began review of Module B Conversion in the CBR. To support an FY18 deliverable, we will update the module to reflect current trends, data, and trajectories for the outlook on conversion prices. The current review is part of the groundwork in identifying what needs to be accomplished.

Equilibrium System Performance (ESP) Tools Development

- **[ANL]** A list of computation tools used for FCO campaign studies was developed and provided to INL.
- **[ANL]** Several remaining technical issues associated with the NE-COST website were resolved. Additionally, a comprehensive review of the text and explanations of the website was initiated. Performed two test calculations with a lower and higher capital cost of LWR, using the NE-COST web based calculator. Additionally, screenshots of the calculator were shared with other campaign personnel, so that feedback on the current status of the NE-COST website could be received.
- **[INL]** As a part of the work package for analysis of innovative nuclear energy system (NES) technologies, the fuel-cycle concept developed by India, "the three-stage nuclear power program," has been analyzed. Its analysis report is currently under review.
- **[BNL/PSU, ORNL]** An example template for integration of new data into the transmutation data library was prepared for Evaluation Group EG01. This directly supports the key task of adding physics analyses completed under the Evaluation and Screening study and Equilibrium System Performance (ESP) activities into the transmutation data library. A list of issues and questions with the integration of EG01 has also been developed, and we are working to address these. Work has begun to integrate EG29 into the library as a second example. Additionally, a script is being developed to automate integration of cross section data into the transmutation data library template.
- **[SNL]** Finished making the changes to the development site for the Nuclear Fuel Cycle Options Catalog (which is not available to the public) to meet the requirements of SharePoint 2013. Also completed the verification of two fuel cycle options, which are now available on the public Nuclear Fuel Cycle Options Catalog site, and completed cleaning up the database and deleting unnecessary information.

DEVELOPMENT, DEPLOYMENT AND IMPLEMENTATION ISSUES (DDII)

Technology and System Readiness Assessment (TSRA)

- **[ANL]** Participated in weekly conference call to discuss the TSRA for a fast reactor recycling option. Reviewed the report on "Lessons Learned from Trial Application of the TSRA Process to Example Metallic Fuel and Aqueous Reprocessing System, NTRD-FCO-2017-000468," and rearranged the technology readiness level (TRL) questions for tracking based on the DOE TRL guidelines of DOE-STD-1189-2008.
- **[BNL, INL, ANL]** Suggestions for potential modifications to the TSRA process resulting from the trial implementation described in the FY17 level 3 milestone report entitled "Lessons Learned from Trial Application of the TSRA Process to Example Metallic Fuel and Aqueous Reprocessing Systems" by M. Todosow, et al. are being reviewed for possible incorporation in updates to the questionnaires for the Technology Readiness Levels (TRLs) and/or the Systems readiness levels (SRLs) contained in "Technology and System Readiness Assessment Process for R&D Evaluation, FCRD-FCO-2016-000110, June 30, 2016.
- **[INL]** Developing some additional technology readiness level (TRL) questions to ensure that starting an analysis at a TRL other than 1 does not result in aspects of the readiness evaluation not being addressed. This will facilitate the analysis of technologies which enter the evaluation process in a

partially mature state by eliminating the need to start the evaluation at level 1. Refining the grouping of TRL questions into tracks to facilitate focus on specific aspects of readiness and ensure a logical progression of readiness questions is provided.

- **[INL, ANL, BNL, LLNL]** Regularly scheduled telecons have been initiated to discuss and plan the TSRA activities for FY18, including the application of the TSRA process to a complete "promising" fuel cycle. LLNL began participation in bi-weekly TSRA working telecons.

Transition Analysis Studies

- **[ORNL]** A paper has been written for the PHYSOR-2018 conference, and submitted for review. The paper, "Value Added When Using Crossed Sections for Fuel Cycle Analysis", summarizes the findings of the work to date this year.
- **[ANL]** Performed literature review of existing fast spectrum molten salt reactor (MSR) concepts that fit into EG24 and the ability for their mass flow data to be used in fuel cycle dynamic simulations. Half of a dozen candidates were identified but none fit the description exactly. Consequently, currently developing a simple EG24 MSR concept (continuous recycle of U/TRU with only NU feed) using existing MSR fuel cycle modeling tools developed at ANL.
- **[ORNL]** An ORION MSR model was set up with cross sections to simulate a fast MSR. The results look promising, however, many simplifying assumptions have been made to benchmark the model. Some differences exist in the preliminary results from ORION and the reactor physics data and these differences are being actively resolved. The work has also involved the development of a model of a generic fast spectrum molten salt reactor for analysis of equilibrium and transition with this technology. Iterations have been completed to generate the desired outputs and mass flow rates for waste and in-core salt. The same model and assumptions are also being used to generate the recipes and cross sections for the M3 milestone report assessment.
- **[ORNL]** Work has progressed well on the cross section vs. recipes report, due in early February. The methodical approach to evaluate the times when cross sections or recipes are more appropriate has begun to identify a clearer insight into the needs, particularly associated with transition timescales, calculated metrics, and flexibility in the models.
- **[INL]** Finalized the approach to the study on economic transition. The team will prepare a report that evaluates the economic aspects of alternative transition scenarios for EG23 and EG30. In completing the approach, the team is now underway with the analysis of alternative scenarios. This includes simulation modeling in VISION and post-processing, economic analysis.
- **[LLNL]** LLNL provided review and comments on a draft strategy white paper for NE-4 R&D.

Regional and Global Analysis

- **[PNNL]** Joined the OECD/NEA Expert Group on Advanced Reactor Systems and Future Energy Market Needs as the US representative.
- **[PNNL]** In the process of updating GCAM model for FY18 scenario analysis. Collecting data for analysis on renewable energy policy impact. Collecting data on US natural gas prices

Development, Deployment, and Implementation Issues (DDII) Tools Development

- **[INL]** Scoping and evaluating potential upgrades to the VISION model to support upcoming analyses. These include improvements to the recovered uranium management algorithm, rearranging of input and output files to improve workflow, reduce maintenance burden, and efficiently allow for

runs of varying duration. Early investigations into the installation and use of the Cyclus simulator have also been undertaken.

For more information on Fuel Cycle Options contact Temitope Taiwo (630) 252-1387.

Joint Fuel Cycle Study Activities

- The first two U/TRU recovery experiments into liquid cadmium using a galvanic mode of operation were completed including distillation operations. The product of the first experiment was crushed, sampled and sent to the analytical laboratory at MFC for analysis.
- NDA analysis of the U/TRU product was performed in the east radiography station and the Precision Gamma Scanner in HFEF.
- Several successful surrogate castings were completed with uranium zirconium mixtures in the casting/sampling furnace.

For more information on Joint Fuel Cycle Studies Activities contact Mike Goff (208) 526-1999 or Ken Marsden (208) 533-7864.

AFCI-HQ Program Support

UNIVERSITY PROGRAMS

Site: University Research Alliance at West Texas A&M University in Canyon TX, and the following universities: University of Michigan, University of Tennessee, University of California at Berkeley, Massachusetts Institute of Technology, University of Utah, Rensselaer Polytechnic Institute, Washington State University, Colorado School of Mines, University of Nevada at Las Vegas, Clemson University, University of South Carolina, Purdue University, and other universities.

Universities engaged in Nuclear Technology research via URA programs since 2001:

Boise State University
Boston College
Clemson University
Colorado School of Mines
Georgia Institute of Technology
Idaho State University
Florida State University
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North Carolina State University
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University of Tennessee at Knoxville
University of Texas at Austin
University of Virginia
University of Wisconsin
Vanderbilt University
Virginia Commonwealth University
Washington State University

INNOVATIONS IN NUCLEAR TECHNOLOGY R&D AWARDS

Summary Report

- On November 2, the 2017 First Place Innovations Award winners presented their research at the Innovations in Nuclear Technology R&D Awards special session at the ANS Winter Meeting in Washington, DC. The session was chaired by Patricia Paviet, Director of the Office of Materials and Chemical Technologies, DOE Office of Nuclear Technology R&D. The students were presented with their desktop awards and had their pictures taken with Dr. Paviet.
- Six award-winning papers were presented:
  - Complexation Thermodynamics of Oxalate with Hf(IV) for Application to Nuclear Fuel Reprocessing - Mitchell Friend, Washington State University
  - Evaluation of Simultaneous Ion Irradiation and Liquid Metal Corrosion - David Frazer, University of California at Berkeley

- Irradiation-Induced Void Swelling in Pure Copper Characterized Using Transient Grating Spectroscopy - Cody Dennett, Massachusetts Institute of Technology
- Quantitative Analysis of Localized Stresses in Irradiated Stainless Steel - Drew Johnson, University of Michigan
- Selective Partitioning of Ruthenium from Nitric Acid Media - Jason Richards, University of Nevada at Las Vegas
- The Influence of Citrate and Oxalate on $^{99}Tc^{VII}$, Cs, Np^{V}, and U^{VI} Sorption to a Savannah River Site Soil - Dawn Montogmery, Clemson University

- The award winners presenting at the ANS meeting were honored with a lunch after the session. DOE personnel attending the dinner included Patricia Paviet, Director of the Office of Materials and Chemical Technologies.
- University Research Alliance began preparing reimbursements for the winners' travel expenses for the ANS meeting.
- University Research Alliance began preparing materials for the 2018 Innovations Awards.
- University Research Alliance continued to improve the email distribution list in preparation for the 2018 Innovations Awards.

For more information on the University Research Alliance contact Cathy Dixon (806) 651-3401.