Page 1 of 13

CX Posting No.: DOE-ID-INL-21-030

SECTION A. Project Title: FY-18 to FY-20 LDRD Projects

SECTION B. Project Description and Purpose:

INL uses LDRD investments to accelerate advanced nuclear energy Research, Development, and Demonstration (RD&D), develop integrated fuel cycle solutions, accelerate advanced integrated energy systems, develop advanced materials and manufacturing processes for extreme environments, and improve the security and resilience of cyber-physical systems across critical infrastructure systems. LDRD is a relatively small, but vital DOE program that allows INL and other DOE laboratories to select a limited number of RD&D projects. It works to: 1) maintain the scientific and technical vitality of INL, 2) enhance INL's ability to address future DOE missions, 3) foster creativity and stimulate exploration of forefront S&T, 4) serve as a proving ground for new research, and 5) support high-risk, potentially high-value RD&D. Determining LDRD and other RD&D investments relies on alignment with the Laboratory's science and technology (S&T) initiatives.

The Laboratory ensures that LDRD program goals and objectives are aligned with DOE Order 413.2C, Chg 1, and that the LDRD portfolio is managed with integrity and transparency. All LDRD projects go through a rigorous proposal review and selection process, and ongoing projects applying for renewal are contingent on a progress report review process. These steps ensure that LDRD investments are continually aligned with INL's vision, mission, and S&T initiatives, and are technically sound, innovative, cutting-edge RD&D projects.

INL's five strategic S&T initiatives are described below:

Nuclear Reactor Sustainment and Expanded Deployment. INL works to develop and qualify new nuclear fuels, design and enable testing and demonstration of a microreactor by early 2024, and leads the National Reactor Innovation Center (NRIC). INL's efforts contribute to enabling the U.S. to regain and sustain leadership in advanced reactor technologies.

Integrated Fuel Cycle Solutions. INL develops integrated fuel cycle solutions to sustain the current reactor fleet and enable its expansion and replacement with advanced reactors.

Advanced Materials and Manufacturing for Extreme Environments. INL focuses on advanced materials and manufacturing solutions for use in extreme environments, including advanced nuclear reactors, integrated energy systems, defense systems, and space applications. INL, often in partnership with industry, seeks to discover and advance materials that must function in extreme environments for instrumentation and energy technologies.

Integrated Energy Systems. INL researches and demonstrates methods to harness and use a variety of forms of nuclear energy products (radiation, heat, and electrons) in conjunction with energy products from other clean-energy sources to accelerate the deployment of an economy based on clean, reliable, and sustainable energy.

Secure and Resilient Cyber-Physical Systems. INL advances automated-control solutions for vital systems and critical infrastructure through its control systems cybersecurity capability. INL's threat analysis and consequence-based risk prioritization with embedded, component, and system security RD&D for critical process technology develops automated threat responses and resilient systems that limit the physical effects of cyberattacks.

LDRD investments offer the potential to achieve INL's five S&T initiatives by focusing on its long-term objectives and key S&T drivers. Additionally, strategic investments enable researchers to conduct early-stage exploratory research to foster innovation through collaborative RD&D, while providing science and engineering opportunities for students and postdocs. The FY-20, FY-19, and FY-18 LDRD research projects are summarized below:

<u>FY-2020</u>

138: Demonstrate Viability of Accelerated Fuel Qualification Approaches - NS&T (C600)

The two leading contenders in accelerated fuel system qualification are Idaho National Laboratory (INL)'s Fission Accelerated Steady-state Testing (FAST) and General Atomics (GA)/Oak Ridge National Laboratory (ORNL)'s Accelerated Fuel Qualification (AFQ), recently funded through a Department of Energy Funding Opportunity Announcement (DOE FOA) award. AFQ starts small, irradiating large numbers of spherical fuel particles under diverse conditions to develop inputs for mechanistic fuel behavior models. The FAST approach irradiates a sizable number of scaled down integral fuel pins to accelerate burn up by a factor of up to 10 and is more suited for characterizing fuel performance at engineering scales.

The proposed action aims to show that accelerated fuel qualification is possible by increasing fuel enrichment and reducing size to accelerate burnup. This LDRD produces test articles for a ceramic fuel system to give data demonstrating the viability of the approach for a range of fuel forms. The LDRD will establish scaling relationships for fuel pins (both solid and consolidated geometries) and test articles. Analysis work is required to verify that appropriate geometries can be fabricated for ceramic fuel systems and to allow follow on work supporting the scaling relationships that can be applied to fuel system design.

The proposed research aims to achieve accelerated burnup of uranium carbide (UC) fuel utilizing INL's FAST approach and to validate results from GA and ORNL's AFQ and fuel performance modeling. The first two years of this laboratory-directed research and development (LDRD) focus on fabricating and

Page 2 of 13

CX Posting No.: DOE-ID-INL-21-030

modeling UC pins with GA serving as a potential contracted supplier of UC fuel and consultant. The third year performs the final preparation for irradiation insertion, focusing on fabrication and certification of specimens for irradiation.

This project will be located at the Experimental Fuels Facility (EFF) and the Fuels and Applied Science Building (FASB) for fabricating samples. GA will fabricate UC fuel. The proposal will use nitric acid and ethanol. Uranium metal will be down blended to the target enrichment and will be delivered to GA. The enrichment level and amount is yet to be determined. Project activities will generate hazardous and low level waste (LLW) (ethanol, acid (nitric), losses from U arc melting). Exhaust will be emitted through the facilities suspect exhaust system and pass through HEPA filters.

145: Coordinated Examination of Microstructure and Thermal Properties of Gamma Uranium-Zirconium Alloy in Volumetric Space – MFC (U500)

This project characterizes the gamma phase region of the uranium-zirconium (U-Zr) system and produces critical experimental data needed for the developing mechanistic understanding of metal fuel performance. Using a combination of laser flash analysis (LFA), the thermal conductivity microscope (TCM), and transmission electron microscopy (TEM), all equipped with a furnace or heating stage, the project will characterize solid volumes of U-Zr alloy with respect to Zr composition, phases present, crystal orientation, grain sizes, bulk thermal conductivity, local thermal conductivity, and Kapitza resistance across grain boundaries. The proposed action will irradiate U-Zr alloy in the Neutron Radiography Reactor (NRAD) and conduct examinations to understand the irradiated high temperature microstructures and thermal properties of U-Zr. This experimental data is needed to validate the potentials used in molecular dynamics (MD) and phase field simulations focused on modeling the radial thermal conductivity across a fuel segment. These lower length scale models will be used to populate large scale fuel performance models to support fuel qualification for use in new reactor designs.

This project will be located at MFC in FASB, the Analytical Laboratory (AL), Irradiated Materials Characterization Laboratory (IMCL), and in Idaho Falls at the INL Research Center (IRC). The proposed actions use nitric acid for cleaning metal uranium feedstock and alloy samples; isopropanol, ethanol, and acetone for cleaning of alloy samples; and metallic gold. Metallic depleted uranium will be used to cast alloys of varying uranium/zirconium compositions for testing samples. The project will generate mixed LLW (MLLW).

149: Proton Recoil Effect on Light Output in Fast Neutron Scintillators - MFC (U510)

This proposal examines proton buildup in high density polyethylene (HDPE) Fast neutrons produce proton recoil interactions that interact with scintillator materials to generate visible light photons that can then be read with a digital camera. Recent measurements have demonstrated feasibility of performing fast neutron imaging with the neutron beams at INL's NRAD Reactor. This project includes a parametric study to optimize fast neutron scintillator screens by varying the converter and phosphor thicknesses, phosphor composition, and grain size. This project will also investigate fundamental science issues between the theoretical performance and experimental measurements of fast neutron screens. The development of higher resolution scintillator screens would bolster INL's fast neutron imaging capabilities for post-irradiation examination activities.

The project is located at NRAD and Technical University at Munich (TUM). Small quantities of radioactivity will be released, and radioactive and nonradioactive waste will be generated at NRAD only.

168: A New Approach to Cathode Interface Structure/Activity with Transient Kinetics – EES&T (B623) Research uses density functional theory (DFT) modeling in combination with artificial intelligence (AI) algorithms to predict compositions with advanced physical (mechanical, electronic, chemical) properties. Computational results for reactivity and passivation at model defect sites will be used to understand experimental results.

The project is located at EIL. The project uses lithium acetate, nickel acetate, manganese acetate, cobalt acetate. These are mixed together in ball-mill machines, then calcinated under oxygen flow conditions for synthesis. Milligram to gram amounts of Li(Ni_xMn_yCo_z) will be generated as solid waste. Small amount of CO₂ emissions will be generated.

193: Real-time axial neutron flux profile measurement at the Advance Test Reactor Critical Facility - EES&T (B633)

Real-time characterization of irradiation facilities is necessary to improve the utilization of the core capabilities of test nuclear reactors. Advanced sensors can significantly reduce time and cost of experiments, improve our understanding of the experimental environment, and enable verification and validation of simulation and modeling methods. The proposed action fabricates and deploys a prototype real-time axial neutron flux monitor, leveraging proven technologies, to characterize the transient that occurs in the small B positions at the Advanced Test Reactor Critical facility. These measurements will be compared to simulation results to identify biases in past and future modeled data that cause discrepancies in irradiation experiment results.

This research will be performed at TRA-678, TRA-1627, and TRA-670. Various solvents and buffer agents will be used with 93% enriched uranium dioxide powder to perform electrodeposition of uranium onto small neutron sensor components. Low-level liquid radioactive waste will be generated in the form of enriched uranium solution that will be used for electrodeposition.

197: Control System for Hydrogen Retention Problem in Microreactors - NS&T (C650)

This LDRD develops metal alloy hydrides with high hydrogen binding energies. The project (i) computationally develops and physical demonstrates alloy hydrides which minimize hydrogen transport and maximize its retention, (ii) measures microstructures and material properties of the developed alloy hydride(s), and (iii) investigates the possible effects of irradiation on these critical properties by performing a small set of screening ion irradiations. First principles techniques will be used to down select the best option for pure and alloy-based hydrides based on hydrogen binding energy and thermal-elastic properties. The density functional theory (DFT) and ab initio molecular dynamics (MD) simulations will explore materials with the optimum hydrogen binding

CX Posting No.: DOE-ID-INL-21-030

energy and thermal properties with the additions of various elements to improve hydrogen behavior. Down selected candidates will be subjected to screening ion-irradiations and post-irradiation property measurements.

The project is located at the MFC Research and Collaboration Building (RCB), Center for Advanced Energy Studies (CAES) in Idaho Falls, ATR Safety and Tritium Applied Research (STAR) facility, and IRC with contributions from Idaho State University (ISU) and the Massachusetts Institute of Technology (MIT). Chemicals will be used for cleaning samples and polishing (acetone and colloidal silica solutions). This project will generate industrial waste. No air emissions or water discharges are expected. Metallic alloy components and quartz materials are planned to be purchased for this project.

206: Advanced Computational Modeling and Experimental Determination of the Thermophysical Properties of Molten Salt Systems applicable to Molten Salt Reactor Design – NS&T (C420)

A significant knowledge gap exists in the data for the fundamental properties relevant to fuels and coolants for molten salt reactors (MSRs) that needs to be addressed to expedite the technical readiness level of MSR design concepts. The proposed project aims to experimentally and computationally determine fundamental thermophysical properties for molten alkali/alkaline earth metal chloride and fluoride systems. The proposed research develops an experimentally validated computational framework and applies it to a range of temperature and chemical compositions. The ab-initio Molecular Dynamics (AIMD) technique allows for quantum mechanical-based calculations to be performed at non-zero temperatures and can thus model the many-body effects of species, leading to the interpretation of chemical and thermophysical properties of a given system. Leveraged by the computational results, experimental data will be determined within reactor operating temperature ranges, and extremes. Due to the hygroscopic and corrosive nature of molten salts, specialized atmospheres, tools, and instrumentation are needed.

The project is located at the Energy Innovations Laboratory (EIL) in Idaho Falls, the Fuel Manufacturing Facility (FMF) at MFC, Engineering Development Laboratory (EDL), and Water Chemistry Laboratory (WCL). Chemicals to be used will be chloride and fluoride salts of Na, Mg, Li, and K. UCl₃ and PuCl₃ will be used by mixing with other chloride salts for thermal property studies. The UCl₃ and PuCl₃ will be handled in radiological facilities. LLW and TRU waste will be generated from this project. Less than 50g of TRU waste will be generated. Furnaces and balances were purchased for this project.

208: Novel nanoindentation testing of creep properties for iron-chromium-aluminum alloy - MFC (U520)

This project aims to develop an innovative method of rapidly assessing creep of nuclear materials using a combined approach of small-scale testing and accelerator-based technologies. To accelerate thermal creep tests, this LDRD project develops a new testing capability at INL which utilizes a model-assisted small-scale testing approach. Then project uses small-scale tensile specimens and accelerator-based technologies at the Michigan Ion Beam Laboratory at the University of Michigan and the Reactor Materials Testing Laboratory at Queen's University. The data collected will help develop and optimize advanced thermal and irradiation creep models to assist in rapid qualification of new reactor materials. The project investigates Iron-Chromium-Aluminum (FeCrAI) and iron based high entropy alloys (HEA). The proposal also leverages material irradiations of FeCrAI on-going in ATR, which will be available for investigation in 2019 to 2021.

The proposed research leverages INL's collaborative University network, which may include but not limited to the University of Michigan, Queen's University for their expertise in experimental proton irradiation and in-reactor creep expertise, and the University of California, Berkeley for their expertise in small-scale mechanical testing. INL will prepare the materials then send them to universities for in-situ irradiation creep experiments at university proton accelerator facilities. No waste will be generated at off-site (university) locations. The project utilizes facilities at INL, including INL's MOOSE modeling capability and experimental testing and characterization capabilities at IMCL. The tasks of this program include:

- 1) Thermal creep assessment of as-manufactured material using innovative small-scale testing
- 2) Irradiation creep experiments using accelerator technology
- 3) Thermal creep assessment of as-irradiated material from accelerator irradiations and ATR irradiations using innovative small-scale testing
- 4) Develop and optimize advanced thermal and irradiation creep models.

209: Advanced Manufacturing of Heat Pipes with Connectivity to Thermoelectrics - EES&T (B120)

This LDRD project addresses key science questions underlying the development an integrated heat pipe-heat exchanger-thermoelectric platform. Through the use of digital design techniques and advanced manufacturing, thermoelectrics can be directly mounted onto a heat exchanger integrated with a heat pipe for increased efficiency and performance. This project focuses on improved performance of system interfaces through advanced manufacturing. Additive manufacturing (AM) allows for the fabricating heat pipes with performance enhancements, such as microchannels, grooves, arteries, or functionally graded porosity, which are difficult, expensive, or impossible to achieve with traditional fabrication techniques.

This project is located at IRC, CAES, and Boise State University (BSU). This effort uses slurries comprised of photoresins loaded with metal or ceramic particles. Photoresins will be the only form of waste from this project. Minor amounts of photoresins may be released into the sinks/drains when 3D printer parts are rinsed in water. No waste will be generated at BSU, and all university work will be computational. Organics from the furnace will be exhausted through the building exhaust.

211: Intensified characterization and analysis of energy storage system to support integrated energy systems - EES&T (B640)

Page 4 of 13

CX Posting No.: DOE-ID-INL-21-030

To accelerate the adoption of lithium-ion battery (LIB)-based energy storage systems (LIBESS) to support future energy supply and infrastructure needs, more intelligent functionalities of the LIBESS to support this intensified electrification in the energy supply are needed. More intelligence in the functionality of the LIBESS requires better understanding of how to improve the performance, durability, reliability, and safety of the LIBESS in the operation. A better battery control and management (BCM) strategy and methodology is also needed. This proposal uses INL's Battery Diagnostics and Prognostics (BDP) capability as an enabling tool for failure analysis so failure mode and effect analysis (FMEA) can be quantitative (in contrast to today's practice in industry, where FMEA is semi-quantitative or qualitative).

This work uses the following INL capabilities:

- · Principle-based state-of-charge (SOC) and state-of-health (SOH) determination and model
- ·Cell variability study and analysis
- •Cell degradation and failure analysis
- ·Cell to pack integration and analysis

The project identifies degradation mechanisms and path dependence to identify and quantify component and system level performance variations and environmental impacts. The project uses high performance computing (HPC) to conduct data analytics, e.g., data tagging, filtering, and qualification, and using artificial intelligence (AI) and machine learning (ML)-based analytics to quantify results.

The experiment is being performed at IRC for battery testing by INL personnel only. Idaho State University will complete data regression using artificial intelligent techniques. No physical activity will be performed on site. The project usesrechargeable lithium batteries. Both Industrial and Hazardous waste will be generated. Industrial waste will be generated in the form of lab washwater, scrap metal, wipes, rags, personal protective equipment (PPE), and similar material. Hazardous waste will be generated from spent solvents, electrolytes, some spent batteries, and scrap metal. Emissions may be discharged to the atmosphere due to evaporation of solvent. Lab washwater will be discharged to the Idaho Falls Sewer System in accordance with limits established in the city sewer regulations.

216: Development of an Innovative Testing Framework to Assess Crack Initiation Assisted by Corrosion-Fatigue - MFC (U520)

Assessing material susceptibility to cracking from irradiation assisted stress corrosion cracking (IASCC) and corrosion fatigue is a growing concern within the nuclear industry and has been identified by the Nuclear Regulatory Commission (NRC), Electric Power Research Institute (EPRI), and other industry experts as a knowledge gap of high significance for the nuclear community. INL has heavily shielded state-of-the-art IASCC testing capabilities, and there are similar low activity facilities within the United States (e.g., The University of Michigan and Pacific Northwest National Laboratory), yet there are no facilities currently capable of assessing irradiation assisted corrosion fatigue of materials in a simulated corrosive environment like that of a boiling water reactor (BWR) or pressurized water reactor (PWR) within the United States. To demonstrate this technique, this research develops an innovative corrosion-fatigue testing framework capable of testing multiple specimens at a time providing a cost-efficient and accelerated routine to obtain statistical analysis of materials behavior. Furthermore, the proposal investigates the susceptibility of non-irradiated austenitic steel to crack initiation assisted by corrosion-fatigue.

The project is located at IF-688 EIL B-106 and testing will be done in accordance with LI-682. Acetone and ethanol may be used for cleaning specimens and testing autoclaves (small amounts applied to lint free cloth for wiping down components). Waste generated include general office supplies and cleaning supplies. New fixtures for the novel test method will be fabricated in INL machine shops. During operation, exhaust gases containing hydrogen will be diluted with inert gas below 4%H and the mixture directly vented to the outside via a laboratory exhaust duct. For example, if the hydrogen gas flow rate is 50 sccm, an air flow rate of at least 1250 sccm air will be used to keep the mixture fraction of hydrogen below 4%.

224: Innovative Materials and Coatings for Sweep Gas Membrane Distillation (SGMD) to Separate Bioethanol from Fermentation Broth – EES&T (B621)

This project prepares new sheets of SGMD membrane by performing a layer-by-layer deep coating of a polyvinylidene difluoride (PVDF) membrane material. The coatings will be 1) polydopamine which will function as a molecular glue, 2) diatomaceous earth which has a functionalizable surface and controlled texture, and 3) 1H,1H,2H,2H-perfluorodecyltriethoxysilane rendering the surface chemically omniphobic. The performance of this material will be compared with a commercially available Versapor membrane as a baseline. The separation testing that was initially done from a pure ethanol water mixture will now be followed by the separation of ethanol from a fermentation broth. All the laboratory-based tasks will be performed at INL Chemical Separations and Demonstration Laboratory.

The location of this project is at EIL. Chemicals to be used include ethanol which will be mixed with water. No radioactive material will be used. Low amounts of hazardous waste will be generated from project activities. A membrane distillation filtration module was purchased for this project.

229: Ion-Solid Interactions in Focused Ion Beam/Secondary Ion Mass Spectrometry: Toward Nanoscale Trace Element and Isotopic Distribution Analysis in Irradiated Materials – MFC (U520)

There is a significant knowledge gap with the multi-ion beam sources on the G4 FIB/SIMS instrument in the open literature. What is known in the literature is that O₂+ ion beam enhances secondary ionization by 2-3 orders of magnitude, because the strong reactivity of O₂ changes the surface chemistry of the sample and promotes positive secondary ion generations. It is also known that O₂ sputtering can cause redistribution of elements, especially along the metal oxide/metal interface that is formed during O2 sputtering.11

Page 5 of 13

CX Posting No.: DOE-ID-INL-21-030

To understand the ionization efficiency of all four ion beams on the G4 FIB/SIMS, this research investigates the following questions: 1) does N2+ give enhanced secondary ion yields compared with O_2 + for some elements due to their differences in reactivity? 2) how does the secondary ion yield of Xe+ and Ar+ beams as a noble gas compare to O_2 + and N_2 + beams? 3) Could some other factors, such as larger mass of the primary ions, be at play to enhance secondary ion yield for non-reactive elements? 4) Do particular primary ions suppress elemental redistribution while still providing enhanced secondary ion yields? In order to answer these questions, the proposed activity measures the secondary ion yield of all primary ion beams on a range of reference material under controlled instrumental setups.

The reference materials used for this investigation need to have a range of complexity for characterization and are representative of the samples routinely characterized at INL. Following these criteria, five types of reference materials are selected: 1) a silicon sample with a layer of Samarium (Sm) implant of known thickness; 2) Xe implanted UO₂ fresh fuel; 3) a HT-9 steel sample with 85% iron, 12% chromium, 1% molybdenum, and trace amount of tungsten, nickel, vanadium and carbon; 4) an irradiated U-20Pu-10Zr fuel sample; 5) hydrided Zr-alloy.

The method used by Hervig et. al. to measure useful yield of the secondary ions in Cameca 3f and 6f SIMS instruments can be adopted for the G4 FIB-SIMS instrument. In that study, the primary beam was tuned so the sputtered atoms were all from a well-defined crater about 65-70µm in diameter with steep walls, for the convenience of calculating the total amount of atoms being sputtered. The transfer optics and contrast aperture were set so that all secondary ions could enter the mass spectrometer. The useful ion yield can therefore be calculated by dividing the amount of detected secondary ions of sputtered atoms calculated based on the sputtered volume, material density and concentration of the element that formed the secondary ions of interest. By replicating the analytical setup for the four different ion beams on the same standard, their secondary ion yield could be compared against each other to look for the optimal beam source for given element/isotope at a given sample matrix and to resolve mass interference issues for certain isotopes through deconvolution of mass spectra from different ion source.

This project is located at MFC, within IMCL and EML. Ethanol will be used for cleaning. Other materials like Silicon, various steels, and zirconium will be used in the microscope. Fresh UO2 and UZr, as well as irradiated UZr will be used for analysis in the instrument. Low level waste will be generated as well as basic office waste.

235: Proof of Principle Experiments for a Pyrochemical Approach to Treatment of Used Advanced Test Reactor Fuel - NS&T (C420)

A novel pyrochemical process for treatment of used Advanced Test Reactor fuel has been identified that involves chemical and electrochemical methods to separate and recover the high-enriched uranium from used Advanced Test Reactor fuel in a purified high-assay low-enriched uranium metal form. The first step in the proposed process involves dissolution of the Advanced Test Reactor fuel – a uranium aluminide-aluminum dispersion fuel in aluminum cladding – in a molten salt system. The objective of this proposal is to perform a rapid demonstration and characterization of this step with a non-radiological surrogate. The demonstration of the critical step would be performed using existing bench-scale molten salt systems at INL facilities. Characterization of salt samples following the demonstration would determine the effectiveness of the proposed dissolution step with surrogate fuel constituents.

The location of the project is located at EDL. Chemicals to be used include Nd, Al, LiCl, LiBr, NH₄Cl, and NH₄Br. Forms of these chemicals will be mixed and heated. The project will generate industrial waste, including steel wool, LiCl, Libr, NdCl₃, NdBr₃, AlCl₃, and AlBr₃.

236: Modeling and characterization of alpha-uranium to accelerate metallic fuels development - NS&T (C650)

To accelerate materials and fuel design and improve fuel performance models, mechanistic (physics-based) models of fuel swelling, fission gas venting and fuel creep are necessary. These models require materials properties information that are not currently available. For example, the alpha-uranium phase exists in U-Zr fuel and significantly contributes to fuel behavior, but many fundamental materials properties and evolution mechanisms of alpha uranium are lacking. Ultimately, the cause of the swelling behavior in alpha-uranium remains unexplained but indicates that the interplay of irradiation defects and mechanical properties must vary.

This research investigates the irradiation-induced microstructure and property changes in alpha-uranium and U-Zr with multiple approaches, including irradiation of single and polycrystalline specimens, multiscale characterization, and multiscale modeling, to accelerate metallic fuel development. The goals of this work are to 1) understand the mechanisms of irradiation damage in alpha-uranium and the effect of interfaces via a combined modeling and experimental characterization campaign, 2) gather high-fidelity mechanical properties data, and 3) develop a microstructure evolution model validated to experimental data and informed by atomistic simulations and experiments.

The project is broken down into three processes, fabrication, irradiation, and characterization.

Fabrication will be done at FASB and EFF. Chemicals to be used include ethanol, hydrogen gas, and argon gas. Depleted and high enriched uranium material will be blended by the arc melting technique and subjected to either a powder metallurgy technique or mechanical deformation process (swagging). LLW will be generated from this process. Air emissions will be exhausted into suspect exhaust systems and pass through HEPA filters.

Irradiation will be done at NRAD. Depleted and enriched uranium will be irradiated along with the capsule hardware material exposed which will be titanium, nickel, nichrome wire, and aluminum. Metals from fabrication of capsule and heater hardware will be disposed as LLW. No emissions are expected to occur, however in the event of an experiment failure in the reactor, air emissions will be exhausted into the HFEF suspect cell exhaust system and passed through HEPA filters.

Page 6 of 13

CX Posting No.: DOE-ID-INL-21-030

Characterization will occur at EML and IMCL. The samples will be characterized within confined vacuum systems, including scanning electron microscope and transmission electron microscope.

243: Development of a Streamlined Approach for Burnup and Microstructural Analysis of Nuclear Materials from Nanoscale to Mesoscale - MFC (U520)

Pre- and post-irradiation analysis of nuclear materials can be an expensive and time-consuming endeavor due to the unavoidable processes necessary to gather accurate and precise results. An analysis can take anywhere from a few days to multiple weeks depending on the number of samples, activity of the sample, complexity of the fuel type, and measurement requests. Conventional methods involve surface-based measurements (e.g., Scanning Electron Microscopy, SEM) and destructive analytical techniques (e.g., Inductively Coupled Plasma-Mass Spectrometry). While these methods have their inherent advantages, they also suffer from the inability to rapidly acquire local isotopic information about the fuel sample. This effectively limits the information that can be derived about material performance. These factors prompt the need for an updated approach that improves upon the pitfalls of traditional methods while making notable advances in the analysis of nuclear materials. By merging the unique capabilities of Atom Probe Tomography (APT) with a femtosecond Laser Ablation-Laser Induced Breakdown Spectroscopy-Time-of-Flight Mass Spectrometry (fs-LA-LIBS-TOFMS) technique, we propose to not only increase sample throughput but also provide an avenue to quantitatively evaluate material performance based on three-dimensional isotopic distributions in a specimen. APT offers the unrivaled capability to quantitatively analyze for isotopics on a three-dimensional atomic scale, however, finding the most significant location to analyze can be a burdensome process. LA-LIBS-TOFMS offers many advantages that can complement APT. Through rapid elemental and isotopic mapping of the samples surface at micron resolution, LA-LIBS-TOFMS improves upon customary SEM analysis used to identify locations for Focused Ion Beam (FIB) sampling. To enhance the complementary capabilities of these techniques, we plan to validate a guantitative protocol for LA-LIBS-TOFMS that can be correlated to APT data. Our research aims to improve shortcomings of each method through a joint approach leaning on the concomitant nature of the techniques. Our proposal encourages cross-discipline collaborations which will establish state-of-the-art nuclear material profiling capabilities at the nanoscale to mesoscale. This project will lead to an accelerated approach to research and development while enabling a deeper understanding of nuclear material behavior.

The location of this project is at IMCL, CAES, and AL. No chemicals are planned to be used, however radioactive material will be (UO2, U-Mo, UCO fuel). These are solid samples and very small quantity (less than a nanogram) is used for making specimen for Atom Probe using Focused Ion Beam. Small amounts of radioactive LLW will be generated.

254: Understanding salt chemistry and corrosion control of chloride salts for molten salt reactors - NS&T (C420)

Chloride salts are candidate fuel and coolant for some molten salt reactor (MSR) concepts as they offer potential for sustained operation in a fast neutron spectrum with minimal salt processing, passive safety, and a high-power density. However, molten chlorides present significant corrosion challenges to structural materials at high temperatures, particularly when the salt chemistry is not well controlled. Currently, the corrosion data for relevant metal alloys in chloride salts are very limited, presenting technical risks for MSR design and operation. Specifically, the effects of temperature and alloying elements on corrosion have received only limited studies and yielded inconsistent data. Control of the redox of salt chemistry is known to be critical, but strategies for redox control have been poorly demonstrated.

This proposal aims to provide critical baseline data to understand the salt chemistry and corrosion control of two chloride salts most relevant to chloride MSRs. This activity investigates salt chemistry and corrosion control strategies in NaCl-UCl₃ fuel salt and NaCl-MgCl₂ coolant salt using experimentation and multiphysics modeling.

The location of this project is at FCF, FASB, and EIL (non-rad work at EIL). The chemicals to be used include UCl₃, NaCl, and MgCl₂. The salts are first melted and then some metal samples will be added into the salt melt and exposed to the salt melts for up to 3000 hrs for evaluating the corrosion performance of metal samples. The UCl₃ salt after corrosion will be stored in the glovebox at FCF and disposed of at the end of the project.

262: Improving the Stability and Durability of Aptamer Based Smart-Materials Using Extremophiles - EES&T (B632)

Nucleic acid and peptide aptamers are smart molecules that can dose respond with high levels of sensitivity and specificity to targets molecules ranging from: simple ions to complex whole cells. Even though aptamers are more chemically stable than antibodies, their stability and durability might not be enough for extreme environments or long periods of time. Post-production chemical modifications have been tried to improve stability, but they might compromise sensitivity and specificity. This project proposes a simple but robust solution to improve the stability and durability issues of these flexible smart-molecules. This project will develop standardized biochemical protocols to improve the aptamer's chemical stability so the gained flexibility, robustness and resilience can be translated to smart materials and sensors employed in environmental, advance manufacturing and homeland security applications.

The location of this project is at IRC with collaborations with ISU. Chemicals to be used are DNA and RNA material, Ga salts and a variety of biological buffers. Chemical and biochemical waste will be generated, and all waste will be handled and disposed using ISU established policies and protocols.

<u>FY-2019</u>

166: Intelligent Additive Manufacturing - EES&T (B120)

CX Posting No.: DOE-ID-INL-21-030

This research develops a better understanding of process parameters and how to optimally model and control them to manufacture materials and components. A combination of modeling and simulation and experimental work will be employed. This effort will take an inverse approach compared with current projects, that is; in place of making a material and adjusting parameters until the desired result is achieved, the conceived material will first be designed, down to the microstructural level, through modeling and simulation of the material constituents and the necessary process parameter inputs, and then created by feeding the parameters and feedstock into the control framework of the additive manufacturing (AM) system. The challenge with this approach is ensuring that the correct processes are monitored and controlled, so the project will incorporate novel in-line diagnostic and monitoring tools. These will allow for refined control of the print and will be used to identify errors and misprints in the process and, through the use of a pared down, surrogate model, adjust process parameters to correct errors when possible. There will be feedback from in-line sensors incorporated into the machine to adjust process parameters during material formation or stop the build process in the event of an unrecoverable build. The initial material studied will be 316L (UNS S31603), a stainless steel with 16% Cr, 10% Ni and less carbon than standard 316 (0.03% max).

The location of this work is at EIL with some minor experimental work at Purdue University. Stainless steel 316 powder will be used in experiments. Industrial waste will be generated from this project. The work being performed at Purdue is mostly computational work. There are some measurements of 3D printed objects, but no waste is expected. Equipment purchased will be computer peripherals such as SD cards, external drives, and monitors.

141: Accelerated Nuclear Materials and Fuel Qualification by Adopting a First to Failure Approach - NS&T (C600)

This activity demonstrates and develops a new approach and framework for shortening the development cycle for nuclear materials by leveraging modeling, high throughput fabrication, and predictive data analytics. The research evaluates a combinatorial methodology seldom used to develop high-entropy alloys (i.e., as a proof-of-principle demonstration for a new class of alloys), leveraging modeling and large-data analysis tools. Employing this approach hinges on the ability to organize, classify, and screen candidate materials and available data utilizing multi-scale modeling and large-data analysis, including deep, recursive, and transfer learning approaches. The approach will begin with combinatorial multi-scale modeling and scale into extensive data analysis to identify candidate compositions for down-selection. The latter will further undergo a first-to-failure testing regime based on defined attributes critical for success from an early stage. Subsequent enhancements and comprehensive testing could focus on a limited number of alloys with less risk, in less time, demonstrating a new approach for material qualification.

The location of this project is at IRC and CAES with collaborations with University of Utah and Rochester Institute of Technology. Chemicals to be used are metal powders which include Fe, Cr, Ni, Mn, Al, Cu, Ti, Mo, Nb, and Zr. Small amounts of metal powder waste will be generated from batching and consolidating. All off-site location work will be characterization and computation and will not generate any waste.

175: Mitigating irradiation assisted stress corrosion cracking by rapid alloy design - NS&T (C650)

This project will employ a rapid alloy design framework for developing reactor structural materials to reduce the development cycles of nuclear materials. This research couples integrated computational materials engineering (ICME), rapid prototyping and fabrication, and out-of-pile testing. The approach will be demonstrated by modeling-assisted design of stainless steels that are resistant to irradiation-assisted stress corrosion cracking. Following the processingstructure-property-performance paradigm for alloy design, the project uses ICME to explore the compositional space for desired properties such as phase stability and irradiation behavior, followed by rapid prototyping and fabrication of composition-graded specimens for reduced experimental cost. Out-of-pile tests - such as proton irradiation and stress corrosion cracking evaluation - will be used in places of in-pile tests to further screen candidate materials.

The project is located at IMCL, CAES and C3 at INL with collaborations with University of Michigan, Auburn University, and University of Wisconsin. No chemicals or radioactive material will be used. Industrial waste will be generated from project activities. At Auburn University, solid waste (metal powder) and liquid waste (etching acid) will be generated. The waste disposal follows the university policy (*A Guide to the Generation, Storage and Disposal of Hazardous Waste at Auburn University*) and chemical wastes are disposed by university's waste management team. There is no waste generated at UM or UW.

178: Coupling of Spark Plasma Sintering with Advanced Modeling to Enable Process Scale-Up – NS&T (C650)

This proposal at INL develops a first-of-its-kind MOOSE-based, multi-scale, multi-physics spark plasma sintering (SPS) modeling and simulation tool that can simulate the thermo-mechanical-electrical aspects of the fabrication process which can then be paired to phase-field and other sub-models to predict resulting microstructure to develop "Freya": a validated, first-of-its-kind numerical algorithm and software to optimize specific manufacturing parameters in the SPS process on both the micro and macro scales.

There is a need for accurate modeling and simulation tools geared specifically to predict the SPS process encompassing the multiple variables involved in the fabrication method. Such simulation tools will be developed by INL based upon the MOOSE-framework and will be validated using experiments carried out in MFC's SPS system. Process scale-up would be possible by expanding simulation capabilities and exploring tooling design to address multi-sample sintering. Expansion of the SPS process to multi-sample sintering will facilitate its use in combinatorial work flows for new materials research. This project is not limited to a single material or area of materials science but can benefit multiple areas of materials research including armor-based materials fabrications, traditional nuclear fuels, energy storage materials, and advanced monolithic fuel forms for nuclear thermal propulsion applications.

The project is located at IRC and CAES. Simulation and modeling work will be conducted at Purdue University and C3. Ethyl alcohol will be used to clean the graphite punches and dies used in the electrical field assisted sintering machine. Waste to be generated include KimWipes, polishing paper, and any

Page 8 of 13

CX Posting No.: DOE-ID-INL-21-030

damaged graphite dies and punches. Some water used in polishing the graphite dies and punches will be sent to the sewer. Equipment purchased will be a Data Acquisition Control (DAC) system for the Dr. Sinter machine at CAES.

183: Constituent redistribution in nuclear fuels - MFC (U170)

The objective of this work is to build and demonstrate an apparatus capable of generating a temperature gradient (radial or axial) in a nuclear fuel pin, and to couple the results with modeling efforts. Out-of-pile testing is a crucial component of understanding fuel behavior. Compared with a reactor experiment, an out-of-pile experiment takes weeks or months, instead of years, and does not have the post-irradiation fuel handling requirements. To be as effective as possible, out-of-pile testing needs to reproduce reactor conditions as closely as possible. To this end, control of the temperature gradient is being incorporated into the experiments to allow simulation of the temperature gradient found in nuclear fuel during irradiation and will also allow simulation of off-normal events.

The location of this project is at FASB and Virginia Tech. Diamond suspensions will be used for sample polishing prior to SEM analysis. The samples are fuel alloys, and are uranium based (depleted). The samples will be put into a modified zone refiner for temperature gradient studies, followed by SEM analysis. LLW will be generated from this project. Air emissions will flow through the zone refiner and will be discharged after passing through the required HEPA filters for suspect gas. LLW will be disposed of using Virginia Tech procedures and managed by their Nuclear Materials Officer.

186: Light Element Analysis of Nuclear Fuels by Electron Probe Microanalysis (EPMA) – MFC (U520)

This proposal aims to develop a cost-effective in-house method to quantify the carbon and oxygen concentration in uranium-based nuclear fuel by means of electron probe microanalysis. Because electron probe microanalysis can analyze the actinide elements and fission products, this method will facilitate the correlation of these light-element parameters to the microstructural and compositional evolution of nuclear fuel. This data is vital for thermochemical fuel modeling as fission product diffusion in the fuel is directly related to its chemical form and oxidation state, which in turn influences factors such as thermal conductivity and gas release. Because there is currently little data on the behavior of light elements in nuclear fuel, the work provides the data necessary to link modeling and simulation with empirical fuel behavior.

The location of this project is at IMCL and EML. Chemicals to be used include ethanol and polishing compounds. Depleted and natural uranium will be used. The material is mounted into metallography mounts, polished, and examined through an electron microprobe. LLW will be generated from this activity. Potential radioactive emissions are captured via vacuum from the electron microprobe and routed through the facility suspect exhaust.

201: Seismic and Cost Assessment of Deeply Embedded or Buried Advanced Rectors with Seismic Isolation Strategies - NS&T (C120)

The historical trend in the structural design of nuclear power plants is that they have been founded at or near the ground surface with shallow embedment. The possibility of deeply embedding or burying safety-critical structures of advanced reactors has gained considerable attention in the past decade. This idea stems from the technical view that deeply embedded or buried (DEB) safety-critical structures have better resilience against external hazards such as earthquake, aircraft or missile impact, and pressure waves due to explosions. There is very limited technical background for assessing the nonlinear seismic performance of DEB advanced reactors with seismic isolators both at the system and component level. This study investigates the opportunities of advanced reactors with seismic isolation systems to; i) reduce economic, technical, and regulatory barriers for their deployment, ii) enhance Idaho National Laboratory's impact on the nuclear energy, and iii) serve as a proving ground for new research and development concepts.

The location of this project is at the Collaborative Computing Center (C3), INL Engineering Demonstration Facility (IEDF), and Purdue University. Glass cleaner will be used, and industrial waste will be generated (concrete blocks).

207: Design and Evaluation of a Nuclear Pumped Laser Detector for Reactor Power Indication – MFC (U701)

Flux in an operating nuclear reactor can be used to pump yttrium aluminum garnet (YAG) lasers. The power output from the laser is proportional to reactor power with a very fast response time. Doping the crystal with uranium or plutonium allows thermal or fast neutron flux to pump the laser. By measuring the difference between un-doped and doped laser output, reactor power and thermal/fast neutron flux can be determined over the range of reactor power of interest to researchers. This work will develop un-doped and uranium doped YAG laser crystals for use in reactor power detection instruments. The crystals will be characterized using gamma and neutron sources in a laboratory setting to determine initial response curves. Crystals will be sized to give proper output over the expected flux for steady state and transient reactor operations in the Neutron Radiography (NRAD) and Transient Reactor Test (TREAT) reactors. Steady state and transient operations will be performed to verify detector response and provide calibration information for the instrument. Expansion of the YAG doping to plutonium bearing material is beyond the scope of the proposed project and is, therefore, not included in this investigation.

This project will be performed at AFF, TREAT, and Purdue University. Single crystal yttrium aluminum garnet (YAG) crystals will be grown at AFF. The crystals will be doped with ~1% neodymium, uranium, or both. Purdue will produce polycrystalline YAG using a different method and similar doping. Purdue is following their processes to dispose of any waste generated during YAG crystal production. After the YAG is cut and polished, it will be put into the TREAT reactor for irradiation. No post irradiation examination is currently planned; however, scope could be added to do PIE at HFEF, IMCL, or AL. Commercially produced Nd: YAG will be used for some of the single crystals. The remainder will be produced from commercially available powders containing yttrium and

Page 9 of 13

CX Posting No.: DOE-ID-INL-21-030

aluminum oxide. For Nd doped crystals, the commercial powders will also contain the Nd. Uranium oxide from INL will be added to grow the U doped crystals. Purdue is using commercially produced powders do produce the poly crystalline YAG. A gold coating will be deposited on the YAG. At the end of testing the YAG samples will become waste. Titanium baskets will be used for the TREAT irradiation. These baskets (DWG 621267, 621435, or 621436) are currently in use at TREAT and may be discarded after use or may be recycled for other experiments. Some waste will be created from the grinding and polishing process for the crystals as well as from the crystal growing process. This waste will be unirradiated and may contain some uranium. Cutting and grinding equipment and inspection equipment will be purchased and installed at AFF.

226: Developing Multi-Scale, Rapid and Comprehensive Post-Irradiation Examination using the Focused Ion Beam Microscope – MFC (U520)

This project designs and demonstrates a prototype multi-scale correlated material characterization platform that will measure microstructure, chemistry, isotopic distribution, thermal properties, and mechanical properties on the same region of interest on the same sample. Further, nanoscale and atomistic scale information from Atom Probe tomography and Transmission Electron Microscopy will be correlated to the large amount of data produced by the FIB and data produced from macroscopic techniques such as optical microscopy and x-ray diffraction.

The FEI Helios plasma FIB in IMCL will serve as the starting point for this project. This instrument is an ideal platform as it currently has an electron backscatter diffraction detector (EBSD), energy dispersive x-ray spectrometer (EDS), a variety of secondary and backscatter electron detectors. In addition, the plasma source allows for large volume serial sectioning which leads to 3D reconstructions of materials.

The instrument setup leaves room inside the chamber on the sample stage for placing micromechanical testing system and an in-situ thermal properties testing system. The micromechanical testing in IMCL is designed to be mounted inside the instrument vacuum chamber on the instrument stage. The thermal properties testing system will be based on the INL developed 3 ω technique.

The aforementioned characterization techniques may be performed on the same region of interest. Optimizing this workflow may require iterations of detector and/or sample configuration within the instrument chamber. Automation of correlated data acquisition from multiple detectors and testing modes will be another major effort. The project addresses this using custom scripting within the instrument software. MatLab will be used to provide fast and efficient data analysis.

This project is located in MFC - IMCL, EML, and RCB. Ethanol will be used for cleaning, and materials such as silicon, various steels, and zirconium that will be used in the microscope. Fresh UO2 and UZr, as well as irradiated UZr. Will be used for analysis in the instrument. There will also be irradiated steels. All waste will be low-level waste. A small micro manipulator was purchased that goes into the microscope.

234: Dissolution Phenomena of Used Nuclear Oxide Fuel in Molten Salt Systems - NS&T (C420)

This research investigates, demonstrates, and characterizes a technique for dissolution of used nuclear oxide fuel in select molten salt systems. This technique involves conversion of used nuclear oxide fuel constituents into a molten chloride system for use as (1) molten chloride salt reactor fuel or (2) a head-end step to group actinide metal recovery via electrochemical methods. Both conversion options facilitate reuse of used nuclear oxide fuel in fast reactor systems, where transuranic constituents can be burned – as a metal fuel or a molten chloride salt fuel. Dissolution of used nuclear oxide fuel is accomplished by immersing the fuel in particulate form into a molten salt system containing a base chloride salt and a chlorinating agent. Dissolution of the oxide fuel may be assisted by an electric current to effect an actinide chemistry that promotes the formation of transuranic, lanthanide, alkali, and alkaline earth chloride. Noble metal fission products are not converted to chlorides in this system and are consequently removed in an insoluble solid form. Lithium chloride, potassium chloride, or combinations thereof, may be used as the base salt in this system. Specifically, a lithium-potassium chloride base salt might best serve subsequent removal of group actinide metals, while another base salt (e.g., sodium chloride), or salt combination, might be better suited for a molten chloride salt reactor fuel.

The location of this project is at HFEF. Chemicals to be used are LiCl, KCL, UCl3, NaCl, Li, U, Na, and used nuclear oxide fuel. Forms of these chemicals will be mixed and heated. Used nuclear oxide fuel already present at HFEF and will be heated and contacted with molten salt systems. The work will generate about 1500 mL of TRU waste in the form of solid salt ingots.

238: Moving Beyond DPA: A new approach for rapidly quantifying radiation damage - MFC (U510)

Despite more than a half-century of irradiated materials research, a unit for quantifying radiation damage (RD) and the resulting defect populations that govern material properties has not been standardized. The conventional calculation of displacements-per-atom (DPA) is descriptive of dose, not damage, and suffers from imprecise damage efficiency factors and obscures a fundamental mechanistic understanding of RD. A new method is proposed for directly measuring RD of both neutron- and ion-irradiated materials that could supersede or augment the calculation of DPA and unify the manner in which the nuclear materials community quantifies and models RD. This will be achieved by using ultra-fast (~105 kelvin/second) and ultra-sensitive (order of nanojoules/kelvin) nano-differential scanning calorimetry (nanoDSC) to rapidly anneal irradiated specimens and measure the release of stored defect energy (*Wigner energy). Time-accelerated molecular dynamics modeling will predict the theoretical Wigner energy for each defect type, which, when compared with signature peaks measured by nanoDSC, will act like fingerprints for defect identification.

The effects of dose, dose rate, and exposure temperatures on the nanoDSC spectra of neutron- and ion-irradiated austenitic 304 stainless steel and model reactor pressure vessel steels will be investigated. The cumulative energy calculated for the multi-scale defect populations will be compared to the total defect annealing energy measured by traditional DSC. Additionally, the calculated vacancy cluster size distributions for each irradiated sample will be verified with positron annihilation spectroscopy.

Page 10 of 13

CX Posting No.: DOE-ID-INL-21-030

The project is located at EML, IMCL, FASB and at MIT. Chemicals to be used will be solid metal specimens (steel, zirconium). Small segments (micrograms to milligrams) of irradiated foils will be analyzed in instruments. Waste to be generated will be lightly irradiated non-fuel solid metal specimens, including a 0.19 mL Pt/Rh crucible that was in contact with neutron irradiated steel. Additionally, water used in cutting irradiated steel was collected, evaporated, and the residual solids put in a solids waste container. At MIT, use and disposal of radioactive material is regulated by the Radiation Protection Program (https://ehs.mit.edu/radiological-program/radioactive-material-safety/) and the university's Regulated Waste Program (RWP) administered by the Environmental Health and Safety Office (https://ehs.mit.edu/regulated-waste-program/rad-waste/).

189: Electronic and thermodynamic properties of selected uranium compounds at high magnetic fields - NS&T (C610)

This proposal focuses on fundamental understanding of thermodynamic and transport properties of selected UX (X = p-electron element) actinide materials. These materials crystalize in cubic structures and order magnetically at low temperatures. Despite the large experimental and theoretical works carried out, the nature of the f-electrons and their coupling to lattice vibration and magnetic fluctuations are still unclear. This project performs systematic studies of uranium mononitride (UN) and uranium monosulfide (US) crystals, with special attention to uranium monoantimonide (USb). In order to better understand the interplay of many-body physics and other degrees of freedom, such as strong electronic correlations, magnetism, and structural distortions, the research performs detailed magnetic, transport, and thermodynamic, studies of f-electron materials at low-temperatures and high magnetic fields.

The location of this project is at IRC. The project will use GE varnish to glue the sample to the sample holder. The 20mb USb single crystals will be mounted in the sample holder and then measured inside the Physical Property Measurement System (PPMS). Mixed waste will be generated from this project.

213: Evaluating thermal properties of advanced materials - MFC (U510)

Thermal conductivity and specific heat are critical for predicting the fuel temperature during normal and off-normal reactor operation. Currently, only thermal diffusivity is measured via the Laser Flash (LF) technique at INL. The LF technique measures the temperature increase on the rear side of a specimen induced by a laser pulse (flash) on the specimen's front side. The conventional method (a mathematical formula derived by Parker) uses the sample thickness and the time to half maximum to determine thermal diffusivity. This proposal aims to enhance this technique and its capabilities by using the existing experimental facilities at INL, while also developing a data analysis tool for application to new, advanced materials. This will be accomplished by further developing a machine learning based tool and modifying the LF set-up. The tool consists of a finite element model, a least squares fitting algorithm and experimental data treatment algorithms. Model data is fit to experimental data by using specific thermo-physical properties as optimization parameters. The new will allow the determination of three thermo-physical properties (thermal conductivity, specific heat and thermal diffusivity) from a single LF measurement. The project will consist of three main stages: 1) adapting the tool for measuring asymmetric specimens - fuel fragments and curved cladding specimen; 2) modifying the INL LF facilities to harvest the full potential of the advanced tool – characterizing laser beam characteristics and spectral emissivity; 3) applying the new methodology to various materials of interest for INL.

The location of this project is at IMCL, FASB, and AL. Chemicals to be used are ethanol and carbon spray paint. The project will generate project specific waste that will be LLW (terry towels).

245: Beyond Nuclear Energy Materials: Utilizing Strong Spin Orbit Coupling and Topology in Actinides – NS&T (C610)

This proposal focuses on fundamental understanding of selected quantum effects in actinide materials, with special attention to phenomena governed by strong spin-orbit interactions. The quantum effects associated with the spin-orbit interactions are directly related to atomic number and are strongest in heavy elements, such as actinides, where relativistic shifting of the energies of the electron energy levels accentuates the spin-orbit coupling effect, making actinides a perfect platform for studying such effects. This project performs systematic studies of selected 5f-electron systems and focus on the topological effects associated with strong spin orbit interactions (including both Dresselhaus and Rashba effects). In order to better understand the interplay of many-body physics and other degrees of freedom, such as topology and strong electronic correlations, this research performs detailed low-temperature, magnetic, transport, thermodynamic, and spectroscopic studies of selected f-electron materials.

The location of this project is at IRC and IMCL. Small amounts of uranium crystals (about 1 mg) and plutonium crystals (about 1 ng) will be used for electrical transport measurements. Small amounts of industrial and LLW will be generated.

<u>FY-2018</u>

154: Accelerating Irradiated Fuel Studies by Advanced Surrogate Samples – MFC (U520)

This work explores an approach to accelerate and reduce the cost of nuclear fuel development, through the fabrication of surrogate samples able to mimic irradiated fuel. The realistic simulated irradiated fuel microstructure is possible by leveraging in house fabrication capabilities, such as spark plasma sintering. The first proof of concept for these surrogates will be attained by producing UO₂ high burn up structure doped with selected sets of fission products and characterized in house to validate microstructure and fission products distribution. This fuel type has been chosen because it provides the best base for comparison with irradiated fuel.

The project is located at FASB and EFF. Polishing solutions and powders will be used to simulate fission product surrogates. The project will generate LLW.

Page 11 of 13

CX Posting No.: DOE-ID-INL-21-030

223: Neutron Diffraction of Irradiated Nuclear Fuel - MFC (U510)

For interrogation of irradiated materials, Neutron diffraction (ND) has significant advantages over x-ray diffraction (XRD) in discriminating the diffracted signal from the gamma radiation emitted by the sample and in providing bulk (as opposed to surface) data. The proposed project performs proof-of-principle experiments and early demonstration of the utility of a first-of-a-kind ND system capable of examining irradiated nuclear fuel and materials. Because neutron beam line facilities suitable for handling highly radioactive materials offer a lower flux relative to other national neutron scattering facilities (e.g., High Flux Isotope Reactor and National Institute of Standards and Technology; NIST), development of ND systems for this area benefits from the use of a polyenergetic neutron beam. Development of this technology will be pursued in conjunction with with ORNL, MIT, Technical University of Munich (TUM), and a new collaboration with NIST. This project will demonstrate the utility of polyenergetic neutron scattering by generating a useful diffraction pattern from an unirradiated material at INL in the first year and of an irradiated fuel specimen in the third year.

The location of this project is at HFEF and RCB. Chemicals to be used will be cleaning agents such as ethanol. Neutron irradiated materials will be used as samples for the experiments to study material structural change. Industrial waste will be generated from this project.

244: Development of new experimental capability based on Focused Ion Beam (FIB) micromachining and investigation of thermo-physical properties of nuclear materials at micro and mesoscale – NS&T (C610)

This proposal develops new techniques to study transport and thermal properties of actinide materials and their interaction with material microstructures. Prospects for advanced next-generation reactors demand a solid fundamental understanding of the physical properties of actinide materials and fuels, including transuranic elements. Despite intensive theoretical and experimental efforts, the effect of 5f-electrons (electrons in the 5f orbital characteristic of actinide materials such as uranium, neptunium, plutonium, americium, etc.) transport properties, and their interplay with micro- and meso-scale structures such as grain boundaries, defects, and/or fission products, are still not well understood. The FIB (Focused Ion Beam) instrument enables detailed microstructural characterization (phase identification, grain size/orientation, chemistry, etc.), extraction of single crystal samples, micromanipulation of specimens and other materials, and deposition of conductive materials. The FIB, in conjunction with the newly developed 3 ω -technique, will allow direct measurement of thermal transport properties of nuclear materials at the micro- and meso-scales. By using this technique, this project studies the thermophysical behaviors of various metallic and oxide nuclear materials, pure minor actinides, and the impact of microstructural features on these properties.

The location of this project is at IRC and IMCL. No chemicals or radioactive material will be used. Small amounts of industrial waste will be generated.

204: Nuclear Heated Ultrasonic Calorimeter - NS&T (C620)

This LDRD project creates a sensor in which a wire waveguide is heated by direct nuclear heating in the TREAT reactor. The wire also functions as an ultrasonic thermometer to measure its own temperature and quantify nuclear heating in real time based on calorimetry. Much of this project includes desk work such as modeling, mechanical design, and analytic predictions. The sensor has been fabricated at the HTTL facility in EIL and irradiated in TREAT. The original proposal involved creating this sensor out of uranium bearing alloys, but due to various constraints the sensor that was created and irradiated using non-fuel materials only, thus the measurements were of gamma heating only. Because the sensor did not contain fuel and irradiations in TREAT are brief, it is expected that the sensor can be disposed in the same fashion as all irradiation hardware at TREAT (i.e., as low-level radioactive waste). The physical part of this project is now complete and only desktop work remains.

SECTION C. Environmental Aspects or Potential Sources of Impact:

Air Emissions

Several of these LDRD projects are expected to generate a small amount of air emissions in a variety of constituents. Due to the nature of these LDRD projects, emissions will be minor and covered by existing APAD's for the individual facilities.

At EFF and FASB off-gassing that occurs as a result of heating uranium components is contained within a glovebox that is connected to a radiological facility exhaust system that processes the exhaust through in-line HEPA filters prior to being emitted to the air.

Proposed activities will generate small amounts of air emissions at EIL in the form of CO2 and hydrogen. Exhaust gases containing hydrogen will be diluted with inert gas below 4%H and the mixture will be directly vented to the outside via a laboratory exhaust duct.

Discharging to Surface-, Storm-, or Ground Water

Proposed activities have the potential to discharge chemical to the Idaho Falls Sewer System. No planned discharges are planned to occur out at the site.

Disturbing Cultural or Biological Resources

For projects that occur out at MFC and NSTR, there is the potential to disturb cultural resources that are eligible the National Register of Historic Places or un-surveyed areas.

Generating and Managing Waste

Page 12 of 13

CX Posting No.: DOE-ID-INL-21-030

LDRD projects will generate waste, including office waste, industrial waste (e.g., gloves, non-hazardous hardware, ceramic-type pellets, machining scrap, lab pipettes, wipes, etc.), low-level waste (LLW), mixed LLW (e.g., from irradiated fuel salt and salt-facing components), hazardous waste from chemical solutions and solvents, and transuranic (TRU) waste from certain activities at the INL desert Site. The total estimated sum of the generated TRU waste is about 1550 ml.

Off-Site Locations: Locations off-site will have the potential to generate industrial waste, office waste, hazardous waste, LLW. No TRU waste will be generated at off-site locations. From LWP-20000, research performed by INL personnel at offsite (non INL) locations must be performed with the same rigor as on-site work. To ensure such rigor is applied, an analysis must occur between the work performer and research line management using Form 420.15, Off-Site Work Request." If it is determined that the work controls are consistent with INL standards, research by the INL performer at the offsite location may be allowed. In the absence of a defined and structured work-control process, INL work-control processes should be applied.

Releasing Contaminants

When chemicals are used, there is the potential the chemicals could be spilled to air, water, or soil.

Using, Reusing, and Conserving Natural Resources

All materials will be reused and recycled where economically practicable. All applicable waste will be diverted from disposal in the landfill where conditions allow. Project description indicates materials will need to be purchased or used that require sourcing materials from the environment. Being conscientious about the types of materials used could reduce the impact to our natural resources Project activities may release known greenhouse gases (GHGs) to the atmosphere and increase INL's energy use.

SECTION D. Determine Recommended Level of Environmental Review, Identify Reference(s), and State Justification: Identify the applicable categorical exclusion from 10 Code of Federal Regulation (CFR) 1021, Appendix B, give the appropriate justification, and the approval date.

For Categorical Exclusions (CXs), the proposed action must not: (1) threaten a violation of applicable statutory, regulatory, or permit requirements for environmental, safety, and health, or similar requirements of Department of Energy (DOE) or Executive Orders; (2) require siting and construction or major expansion of waste storage, disposal, recovery, or treatment or facilities; (3) disturb hazardous substances, pollutants, contaminants, or Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA)-excluded petroleum and natural gas products that pre-exist in the environment such that there would be uncontrolled or unpermitted releases; (4) have the potential to cause significant impacts on environmentally sensitive resources (see 10 CFR 1021). In addition, no extraordinary circumstances related to the proposal exist that would affect the significance of the action. In addition, the action is not "connected" to other action actions (40 CFR 1508.25(a)(1) and is not related to other actions with individually insignificant but cumulatively significant impacts (40 CFR 1608.27(b)(7)).

References:

10 CFR 1021 Appendix B to subpart D, Item B3.6, "Small-scale research and development, laboratory operations, and pilot projects", B1.24 "Property Transfers" and B1.31 "Installation and relocation of machinery and equipment".

Programmatic Spent Nuclear Fuel Management and Idaho National Engineering Laboratory Environmental Restoration and Waste Management Programs Final Environmental Impact Statement and Record of Decision (DOE/EIS-0203, 1995) and supplemental analyses (DOE/EIS-0203-SA-01 and DOE/EIS- 0203-SA-02) and the Amended Record of Decision (1996)

Final Environmental Impact Statement for the Waste Isolation Pilot Plant (DOE/EIS-0026, October 1980) and Final Supplement Environmental Impact Statement for the Waste Isolation Pilot Plant (SEIS-I) (DOE/EIS-0026-FS, January 1990)

Final Waste Management Programmatic Environmental Impact Statement [WM PEIS] (DOE/EIS-0200-F, May 1997) and Waste Isolation Plant Disposal Phase Supplemental EIS (SEIS-II) (DOE/EIS-0026-S-2, September 1997)

Final Site-Wide Environmental Impact Statement for the Continued Operation of the Department of Energy/National Nuclear Security Administration Nevada National Security Site and Off-Site Locations in the State of Nevada (DOE/EIS-0426, December 2014).

Justification:

The proposed R&D activities are consistent with CX B3.6 "Siting, construction, modification, operation, and decommissioning of facilities for small-scale research and development projects; conventional laboratory operations (such as preparation of chemical standards and sample analysis); small-scale pilot projects (generally less than 2 years) frequently conducted to verify a concept before demonstration actions, provided that construction or modification would be within or contiguous to a previously disturbed area (where active utilities and currently used roads are readily accessible). Not included in this category are demonstration actions, meaning actions that are undertaken at a scale to show whether a technology would be viable on a larger scale and suitable for commercial deployment.",

Page 13 of 13

CX Posting No.: DOE-ID-INL-21-030

B1.31, "Installation or relocation and operation of machinery and equipment (including, but not limited to, laboratory equipment, electronic hardware, manufacturing machinery, maintenance equipment, and health and safety equipment), provided that uses of the installed or relocated items are consistent with the general missions of the receiving structure. Covered actions include modifications to an existing building, within or contiguous to a previously disturbed or developed area, that are necessary for equipment installation and relocation. Such modifications would not appreciably increase the footprint or height of the existing building or have the potential to cause significant changes to the type and magnitude of environmental impacts." and,

B1.24, "Transfer, lease, disposition, or acquisition of interests in personal property (including, but not limited to, equipment and materials) or real property (including, but not limited to, permanent structures and land), provided that under reasonably foreseeable uses (1) there would be no potential for release of substances at a level, or in a form, that could pose a threat to public health or the environment and (2) the covered actions would not have the potential to cause a significant change in impacts from before the transfer, lease, disposition, or acquisition of interests."

After Post-Irradiation Examination (PIE) in the modular hot cell in FCF, irradiated of molten salt systems and PIE remnants will be stored with other similar DOE-owned irradiated materials and experiments at MFC, most likely in the Hot Fuels Examination Facility (HFEF) or the Radioactive Scrap and Waste Facility (RSWF) in accordance with DOE's Programmatic SNF Management and Idaho National Engineering Laboratory Environmental Restoration and Waste Management Programs Final Environmental Impact Statement (FEIS) and ROD (DOE/EIS-0203, 1995) and supplemental analyses (DOE/EIS-0203-SA-01 and DOE/EIS-0203-SA-02) and the Amended Record of Decision (February 1996). Ultimate disposal of the irradiated molten salt systems and PIE remnants will be along with similar DOE-owned irradiated materials and experiments currently at MFC. Categorizing this material as waste is supported under Department of Energy Order (DOE O) 435.1, Att. 1, Item 44, which states "...Test specimens of fissionable material irradiated for research and development purposes only...may be classified as waste and managed in accordance with this Order...".

NEPA coverage for the transportation and disposal of waste to Waste Isolation Pilot Plant (WIPP) are found in the Final Waste Management Programmatic Environmental Impact Statement [WM PEIS] (DOE/EIS-0200-F, May 1997) and Waste Isolation Plant Disposal Phase Supplemental EIS (SEIS-II) (DOE/EIS-0026-S-2, Sept. 1997), respectively. The 1990 ROD also stated that a more detailed analysis of the impacts of processing and handling TRU waste at the generator-storage facilities would be conducted. The Department has analyzed TRU waste management activities in the Final Waste Management Programmatic Environmental Impact Statement (WM PEIS) (DOE /EIS-200-F, May 1997). The WM PEIS analyzes environmental impacts at the potential locations of treatment and storage sites for TRU waste; SEIS-II addresses impacts associated with alternative treatment methods, the disposal of TRU waste at WIPP and alternatives to that disposal, and the transportation to WIPP.

The environmental impacts of transferring LLW from the INL Site to the Nevada National Security Site were analyzed in the 2014 Final Site-Wide Environmental Impact Statement for the Continued Operation of the Department of Energy/National Nuclear Security Administration Nevada National Security Site and Off-Site Locations in the State of Nevada (DOE/EIS-0426) and DOE's Waste Management Programmatic EIS (DOE/EIS-200). The fourth Record of Decision (ROD) (65 FR 10061, February 25, 2000) for DOE's Waste Management Programmatic EIS established the Nevada National Security Site as one of two regional LLW and MLLW disposal sites.

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