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Energy Frontier Research Center

Center for Materials Science of Nuclear Fuels

Todd R. Allen

April 2013

Idaho National Laboratory

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Idaho Falls, Idaho 83415

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EXECUTIVE SUMMARY

The mission of the Center for Material Science of Nuclear Fuels (CMSNF) is to develop a first-principles-based understanding of how complex defects affect thermal transport in irradiated nuclear fuel (specifically UO_2), and to develop an experimentally validated multiscale modeling capability for the predictive understanding of the microstructure dynamics and its impact on thermal transport in nuclear fuel. This mission is accomplished by integrating the physics of thermal transport in crystalline solids with microstructure science under irradiation. The center brings together a multi-institutional team of experimentalists (from Idaho National Laboratory, Oak Ridge National Laboratory, Colorado School of Mines, University of Florida, and the University of Wisconsin) and computational materials theorists (from Idaho National Laboratory, University of Florida, and Purdue University). Led by Director Todd Allen, the center is organized around the two closely related research thrust areas: thermal transport and microstructure science under irradiation.

Some key successes since the February 2012 report are highlighted below.

Technical Successes

First of a kind microscopic measurements of thermal transport have shown unexpectedly that highly anharmonic oxygen vibrations and low velocity uranium vibrations transport most of the heat in UO_2. These results have further revealed critical gaps in the basis for current thermal transport simulations and provide a benchmark for testing advances in theory.

The first ab-initio simulations of phonon lifetimes in a strongly correlated material, UO_2, correctly predict the relative importance of the highly anharmonic oxygen vibrations and low velocity uranium vibrations in thermal transport. Comparisons of the microscopic thermal transport simulations with neutron measurements have revealed a surprisingly large impact of phonon dispersion on phonon lifetimes.

A defect disorder model of UO_2 founded on Density Functional Theory results of defect energetics has been extended to investigate local off-stoichiometry near UO_2 surfaces. While bulk UO_2 crystals contain defects and electronic charge carrier densities that solely depend on the oxygen partial pressure and temperature, surfaces were found to significantly modify the defect equilibrium states.

An atom probe technique was used to for the first time to analyze the concentration of Kr in irradiated UO_2. The samples contained a high number density of one to two nanometer gas bubbles. The concentration profile closely matched that obtained by Monte Carlo calculations, indicating that Kr atoms reside in the sample mostly where they stopped at irradiation and that trace amounts of Kr may be soluble in UO_2, contrary to conventional thinking.

The influence of grain boundary on defect production in UO_2 was investigated with molecular dynamics simulations. Near some grain boundaries such as a Σ5 tilt grain boundary, more interstitials than vacancies survived. Such an "abnormal" behavior has never been found in metals, suggesting that the defect/grain boundary interaction in UO_2 is more complex than in simple metals.

Characterization of nanocrystalline ceria has revealed that oxygen vacancies required to accommodate off-stoichiometry tend to segregate along grain boundaries. The influence of grain boundaries decorated with oxygen vacancies is dramatically larger than ideal boundaries and oxygen vacancies themselves pose a smaller impediment to thermal transport when they segregate along grain boundaries.

Personnel Successes

A number of post doctoral fellows and staff members of CMSNF have taken new positions. Of these, the most recent ones include:

- Dr. Marat Khafizov, who was brought into the CMSNF as a post doctoral associate working on spatially resolved thermal transport measurements. In fiscal year (FY) 2011, he transitioned into a full time position at Idaho National Laboratory (INL) and in FY-12, he was promoted from associated scientist to staff scientist. Marat's promotion resulted primarily from his outstanding contribution to the CMSNF in understanding the complex interplay between radiation defects and thermal transport.
- Dr. In-Wook Park, who worked on Magnetron Sputtering deposition of UO_2 films at Colorado School of Mines (CMS), has taken a senior research scientist position at the Korea Institute of Industrial Technology (KITECH).
- Dr. Thomas Hochrainer, who worked on modeling void growth in irradiated materials at Florida State University, has taken a professor position in Mechanical Engineering Department at Bremen University, Germany.
- Dr. Jianliang Lin, CMS, will take a new position at Southwest Research Institute starting after this summer.

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Recipient: Idaho National Laboratory

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ACRONYMS

ATR	Advanced Test Reactor
BTE	Boltzmann Transport Equation
Ce	cerium element
CeO_2	cerium oxide element
CMSNF	Center For Materials Science of Nuclear Fuels
CSM	Colorado School of Mines
dpa	displacement per atom
EDS	Energy dispersive x-ray spectroscopy
EELS	Electron energy loss spectroscopy
EFRC	Energy Frontier Research Center
FY	fiscal year
GSI	Gesellschaft Für Schwerionenforschung (Germany)
HRTEM	high resolution transmission electron microscopy
INL	Idaho National Laboratory
INS	inelastic neutron scattering
IVEM	Intermediate Voltage Electro Microscope
ITU	Institute for Transuranium Elements
KITECH	Korean Institute of Industrial Technology
Kr	Krypton Element
LANL	Los Alamos National Laboratory
MD	Molecular Dynamics
mfp	mean free path
ORNL	Oak Ridge National Laboratory
PI	principal investigator
PNNL	Pacific Northwest National Laboratory
SRIM	Stopping and range of ions in materials
STEM	Scanning tunneling electron microscopy
TEM	Transmission Electron Microscopy

UO_2	uranium dioxide
XAFS	X-ray Absorption Fine Structure Spectroscopy
Xe	xenon element
XRD	X-Ray diffraction

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Energy Frontier Research Center

Center for Materials Science of Nuclear Fuels

1. ACCOMPLISHMENTS AGAINST GOALS AND OBJECTIVES

1.1 Thermal Transport

1.1.1 Neutron Measurement/Simulation

As planned, neutron scattering measurements (at Oak Ridge National Laboratory [ORNL]) and, first-principles lattice dynamics simulation of anharmonicity in single crystal UO_2 (at the University of Florida) have been completed, thus enabling direct comparison between measured and predicted phonon energies and lifetimes at high and low temperatures. Temperature dependent investigations of anharmonicity in UO_2 have been extended to phonon density-of-states measurements at the Spallation Neutron Source. These measurements on polycrystalline UO_2 have been used in connection with neutron phonon lifetime measurements and first-principles density-of-states simulations to study the impact of anharmonicity on vibrational entropy and heat capacity.

Planned investigations of the impact of fission-products on phonon distributions in UO_2 have been initiated. Analysis of phonon density-of-states measurements as a function of temperature on polycrystalline ceria-doped UO_2 has been completed; however, phonon energy and linewidth measurements planned for single crystal ceria-doped and off-stoichiometric UO_2 have been delayed due to lack of crystal availability. Access to large, single-crystal samples is now being addressed directly by a Fuel Cycle Research and Development funded collaboration between Dr. Rory Kennedy of INL and Dr. Eric Burgett of Idaho State University. Large CeO_2 single crystals have been grown successfully as a test of the crystal growth equipment and UO_2 and $UO_{2.1}$ runs are now underway. These crystals will be loaned to CMSNF for phonon energy and linewidth measurements.

In addition to specifically planned activities, the wavevector dependence of the microscopic Grüneisen parameters for individual phonon branches has been extracted from the temperature dependent, neutron scattering measurements on single crystal UO_2. This analysis has made possible a direct comparison of the experimental Grüneisen data with first-principles simulations. Moreover, the direct experimental measurements of phonon lifetimes in UO_2 are presently being used in connection with the microscopic Grüneisen parameter measurements to confront the longstanding, but not critically tested, practice of using Grüneisen parameters as a direct indicator of phonon lifetimes.

1.1.2 Thermal Transport Measurements

As planned, laser-based thermal transport measurements of proton-irradiated samples are well underway. The spatial resolution afforded by these new techniques make it possible to extract the thermal transport properties of thin proton-damaged layers. In ceria, we observed a reduction in conductivity that is consistent with scattering from dislocation loops and point defects. Low-temperature measurements are in progress to isolate these competing effects. In addition, the irradiation regime is being tuned to produce a predominance of dislocation loops for unit mechanism studies. Lastly, initial irradiations of poly-crystalline UO_2 samples have been completed and thermal transport measurements have begun.

As planned, we have continued the investigation of the influence of grain boundaries on thermal transport. The influence of oxygen vacancy segregation has been studied in nanocrystalline ceria films. By combining high-resolution transmission electron microscope (TEM) and energy-loss spectroscopy with laser-based measurements it was found that oxygen vacancies segregating at grain boundaries pose a smaller impediment to thermal transport compared to vacancies that are uniformly distributed. The planned work on isolated grain boundaries in course grained UO_2 has been delayed due to a lack of sample availability. This issue is currently being addressed through a collaboration with Dr. Andrew Nelson of Los Alamos National Laboratory (LANL). Course grained UO_2 samples are being prepared at LANL using an exaggerated grain growth technique and they will be loaned to CMSNF for thermal transport studies.

1.1.3 Monte Carlo Solution of BTE

As planned, a Monte Carlo (MC) scheme has been developed to solve the Boltzmann Transport Equation (BTE) for phonons in UO_2 single crystals. The scheme is able to solve BTE in a transient mode and with space resolution in domains up to a micron. The MC scheme makes use of the classical perturbation theory results for phonon lifetime along with a complex search scheme to determine all phonon-phonon interactions satisfying energy and momentum conservation. The phonon lifetime is determined in terms of the experimental values of Grüneisen parameter and dispersion curves. As such (to the extent the classical perturbation theory is valid), the MC/BTE scheme is considered a first-principles approach for thermal transport. Thermal conductivity of UO_2 simulated by MC compares very well with experimental data.

1.1.4 Molecular Dynamics Simulations

Molecular dynamics simulation was successfully utilized to study the effects of crystal defects on thermal transport in UO_2 from fully atomistic descriptions. In particular, a non-equilibrium molecular dynamics approach was used to study the effect of dislocations on the thermal transport in UO_2 for the first time. Moreover, this is the first such study in any material; hence, it allows researchers to validate approximate theories developed in the past that are widely used in the description of the thermal transport in real materials. Also, as planned, phonon wave-packet dynamics studies of the interface boundary conductance in UO_2 are well underway.

1.1.4.1 Microstructure Science Under Irradiation

The microstructure science thrust encompasses theoretical modeling and experimental activities related to UO_2 sample preparation and characterization, irradiation experiments and microstructure examination, and investigation of stoichiometry of UO_2 and surrogate samples. Work on surrogate systems has been phased out over the past year as UO_2 samples and instrumentation that is able to handle radioactive samples have become more available. As summarized below, the team has made progress on all fronts since the midterm review. There has been a minor change in schedule for the microstructure modeling effort; phase field modeling of voids growth in UO_2 has been delayed due to an important discovery in the area of stoichiometry investigation. Basically, we have discovered that, in UO_2, voids must contain oxygen gas and that charged defects segregate around voids as a part of their thermodynamic equilibrium. As such, more attention has been given to this electrochemical aspect of voids in UO_2 because of its implication in understanding post-irradiation data. Because of this schedule change, the microstructure modeling effort has been directed to predicting grain growth in UO_2 instead. Other than this minor change in strategy, our CMSNF team delivered on all planned activities as explained below.

1.1.5 Irradiation and Characterization Experiments

As planned, the team has conducted a large number of irradiation and characterization experiments targeting various aspects of the irradiation and stoichiometric response of UO_2. Some irradiation experiments were conducted to provide samples for thermal transport measurements and others were conducted to understand the defect clustering and microstructure aspects of UO_2 under irradiation. A list of the important investigations that were performed is given below:

- H^+ and He^{2+} ion irradiations for UO_2 were performed to produce samples for the thermal transport measurements. The samples were characterized by X-ray diffraction (XRD) and advanced X-ray absorption spectroscopy (XAFS) to understand irradiation damage formation in atomic scale.

- In situ Kr and Xe irradiation of UO_2 at Intermediate Voltage Electron Microscopy (IVEM) facility at Argonne to study the dislocation and gas bubble formation.
- Atom probe measurement of Kr distribution in irradiated UO_2 was performed to understand the equilibrium distribution of fission gases in irradiated UO_2.
- Swift heavy ion irradiation was performed at GSI Helmholtz Institute in Darmstadt, Germany, on polycrystalline CeO_2 at energy of 1GeV to fluences of 1×10^{12}-1×10^{14} Au ions/cm^2. In conjunction with the experiments, electronic stopping was modeled using a molecular dynamics method.
- The near surface stoichiometry and Xe bubble formation in as-irradiated and high-temperature annealed CeO_2 were characterized by a combination of TEM and XRD techniques.
- Atom probe characterization of near surface stoichiometry in UO_2 and CeO_2. The work was performed to compare with model prediction of local stoichiometry changes near surfaces in controlled thermo-chemical environments.

These experimental studies are backed by an effort to produce thin films UO_2 using magnetron sputtering. After successfully acquiring the license to run the experiments with Uranium, progress has been made by producing columnar-grained UO_2 films of thickness approaching 1 micron and grain diameters on the order of a few hundred nm. The uranium oxide phases that can be formed using magnetron sputtering are found to be sensitive to the experiment parameters such as gas composition and substrate temperature. The regime of formation of UO_2 phase with variable stoichiometry in magnetron sputtering experiments has been identified.

1.1.6 Atomic-Scale Simulation of Defects in UO_2

As planned, progress has been made in the area of atomistic simulation of defects and defect cluster properties in UO_2, as well as the simulation of UO_2 properties relevant to microstructure evolution. This includes:

- Modeling cluster formation and stability and cluster migration by MC and Molecular Dynamics (MD). The results are relevant to microstructure evolution in UO_2 under irradiation.
- Establishing the first cluster dynamics theory for void and dislocation loop nucleation in irradiated UO_2, taking the stoichiometry of the clusters into consideration. This theory is very important for comparison with experiments and in phase-field modeling of defects.
- Atomistic simulation of surface energy of UO_2, for both flat and curved surfaces. The results represent the capillary behavior of UO_2 in microstructure evolution models.
- MD simulation of cascades near grain boundaries in UO_2 to investigate the influence of grain boundary character on defect production and determine the segregation energies of point defects at grain boundaries.

Some of the MD results of cluster formation energies as a function of size are already used in the cluster dynamics model for nucleation of voids in UO_2. The curved-surface energy in UO_2 will also be used in both cluster dynamics and phase field models.

1.1.7 Stoichiometry and Microstructure Evolution in UO_2

As planned, important progress has been made in modeling stoichiometry and microstructure evolution in UO_2 since the midterm review. This progress includes:

- Completing a defect-based thermodynamic model for bulk disorder in UO_2 and generalizing this to investigate local defect disorder near UO_2 surfaces. A significant segregation of charged defects near surfaces was revealed by this model.

- Investigating equilibrium voids in UO_2 as well as the charged defect segregation and local off-stoichiometry around voids. Revealing the regions of charged defect segregation, i.e., stoichiometric changes around voids in UO_2 is very important because of the sensitivity of thermal transport to off-stoichiometry.
- Developing a phase field model for grain growth in porous ceramics and applying the model to both CeO_2 and UO_2; the model predictions showed impressive agreement with experiments in both cases.

The above models are tightly connected with experiments. The stoichiometry model is now being applied to atom probe results of near surface stoichiometry in UO_2, as was originally planned, and the phase field model of grain growth is now being used to design a set of grain growth experiments in UO_2 in a controlled oxygen environment. Attempts are also ongoing to obtain spatially resolved stoichiometry maps around voids in order to validate the equilibrium void model.

2. ACCOMPLISHMENTS FOR THE PERIOD

2.1 Thermal Transport

2.1.1 Neutron Measurements and Simulation of Phonon Transport

The comprehensive neutron scattering measurements of phonon energies and phonon lifetimes performed on UO_2 at high and low temperatures [Pang 1] provide crucial "benchmark" experimental data on anharmonicity in UO_2 that at present do not exist for any other material. As detailed below, these fundamental physics rich microscopic phonon data are providing an entirely new level of thermodynamic and thermal transport information for UO_2 through critical and previously missing tests of groundbreaking first principles simulations of anharmonicity and thermal conductivity.

First principles anharmonicity simulations have been performed for UO_2 representing the first *ab initio* computations of phonon lifetimes and thermal conductivities for a strongly correlated material [Pang1]. The simulations correctly predict the unexpected experimental observation that oxygen vibrations contribute very strongly to the thermal conductivity of UO_2. However, they predict phonon linewidths (inverse lifetimes) more than twice that measured by neutron scattering. Initial probes of this discrepancy suggest, surprisingly, that presently available simulations of phonon energy dispersion using even the most advanced theories for UO_2 are likely to be significant contributing factors.

The temperature dependent phonon energy dispersion measurements have provided the first experimental determination of the microscopic Grüneisen parameters of individual phonons for UO_2. As was found for thermal conductivity of UO_2, the integrated microscopic Grüneisen parameter was in close agreement with macroscopic thermal expansion Grüneisen parameter. Although first principles simulations of the integrated Grüneisen parameter were also in good agreement with the macroscopic value, comparisons of the microscopic values with measurements show significant discrepancies.

An analysis of the energy dependence of the measured phonon lifetime (inverse linewidths) for UO_2 has revealed remarkably that the linewidths rise super-linearly for the uranium dominated acoustic phonons, but remain essentially constant for the oxygen dominated optical modes. This unexpectedly simple energy dependence has in turn made possible the first direct comparison between phonon density of states measurements and quasi-harmonic simulations by convoluting the simulations with the energy dependence of the measured linewidths (Figure 1). The plots demonstrate the importance of including anharmonicity-broadened linewidths in making measurement-theory comparisons and delineate the discrepancies between simulated and measured zone boundary energies (peak positions) and phonon dispersion gradients (intensities).

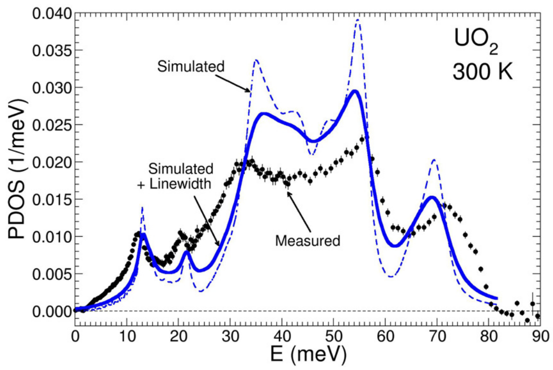

Figure 1. Phonon density of states of UO_2 at 300 K.

Comparisons of phonon density of states measurements on polycrystalline $U(5\%)CeO_2$ with measurements on pure UO_2 have shown that doping UO_2 with 5% ceria as a fission product impurity surrogate only impacts strongly the zone boundary phonons with pure uranium and pure oxygen vibrations, but they represent the two strongest heat carrying phonon branches in UO_2.

MC solution of the BTE for phonons in a UO_2 single crystal showed that the two highest energy phonon branches do not contribute to thermal conductivity due to the low group velocity of these branches. The results of thermal conductivity calculations from the phonon transport details also agree well with the experimental data over the temperature range 300–1000°K. The MC/BTE approach yields critical phonon transport details that can be used to confront the theory of phonon transport with INS experimental data; a detailed calculation of the branch- and wavevector-specific phonon lifetime in terms of the Grüneisen parameter and dispersion data using classical perturbation theory would enable us to understand the difference between the calculated and INS-measured phonon lifetime and understand the role of the Grüneisen parameter in thermal transport. The success in simulating phonon transport in UO_2 will also enable us to study phonon transport in defective UO_2 crystals, which is forthcoming.

Planned Activities

In view of the large role found for oxygen vibrations in UO_2, microscopic phonon physics investigations of the impact of point defects on thermal transport will transition to single crystal neutron scattering measurements for off-stoichiometric $UO_{2.1}$ (i.e., 5% additional oxygen). These experimental measurements will be mirrored by parallel development of MC/BTE-based phonon branch specific simulations of point defect phonon scattering induced changes in linewidths (6-12 months).

Phonon density of states measurements will be performed within the next 6 months on $UO_{2.1}$ using polycrystalline samples to identify phonons of particular interest in time intensive $UO_{2.1}$ single crystal measurements and provide contrast with previously measured $U(5\%\ Ce)O_2$ phonon density-of-states measurements to identify differences between the substitutional cerium and interstitial oxygen defects.

Parallel first principles simulations of the phonon energies, phonon lifetimes, and phonon density of states for $UO_{2.1}$ will be performed for comparison.

We will implement a 3-D discretization scheme of the Brillouin zone for accurate calculation of phonon lifetime in MC/BTE approach.

Simulation of phonon transport in UO_2 with point defects and small defect clusters will be conducted.

2.1.2 Thermal Transport Measurements

More detailed characterization of nanocrystalline ceria has revealed that oxygen vacancies required to accommodate off-stoichiometry tend to segregate along grain boundaries. Characterizing thermal transport in these films required understanding the complex interplay between point defects, dislocations, and grain boundaries. The contribution from the various microstructural features was isolated by analyzing the temperature dependence of the thermal conductivity. It was concluded that the influence of grain boundaries decorated with oxygen vacancies is dramatically larger than ideal boundaries and that oxygen vacancies themselves pose a smaller impediment to thermal transport when they segregate along grain boundaries. The overall effect of vacancy segregation is a net increase in conductivity over a material with a uniform vacancy distribution. This result is consistent with recent thermal transport studies on the high burnup rim region of UO_2 fuels.

We have completed preliminary proton irradiation of polycrystalline ceria. Thermal transport measurements have been performed using a novel laser-based technique that is ideally suited to extract the thermal properties of the thin damage layer. Analysis of our data reveals that thermal transport in the damage layer is limited by dislocations and point defects. In Figure 2, the normalized conductivity of the damage layer versus displacement per atom (dpa) is presented. The inset of Figure 2 shows a typical TEM micrograph of the irradiated region. Also presented is the expected conductivity contribution from point defects and dislocations. Of particular note is the turnaround in the point defect contribution at approximately 0.25 dpa. It is thought that this behavior is caused by a decrease in oxygen vacancy population due to void growth.

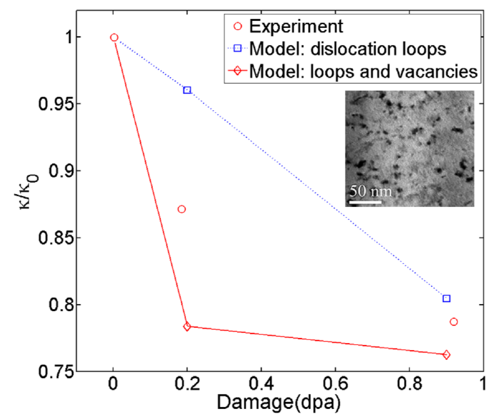

Figure 2. Normalized conductivity vs. dpa for a proton irradiated ceria sample. The TEM micrograph reveals ~10 nanometer loops.

Planned Activities

We will seek to understand both unit mechanisms and cooperative mechanisms in proton irradiated samples. Here we will use annealing temperature as a parameter to change the relevant importance of dislocations, point defects, and voids.

Suggested by our results on surrogate materials, we have begun to investigate a recently developed method to directly measuring the mean free path (mfp) of thermal phonons in UO_2. This approach, first developed outside the CMSNF, essentially involves excluding the contribution of low frequency phonons by modulating the characteristic experimental length scale relative to mean free path. Direct measurement of mfp will enable a one-one comparison between neutron-based linewidth measurements and thermal transport measurements.

2.2 Microstructure Science under Irradiation

2.2.1 Irradiation and Characterization Experiments

IVEM in-situ Kr-irradiations for UO_2 showed that dislocation loops grew quickly at low ion dose and become part of the dislocation network at higher doses through coalescence and coarsening mechanisms. Defect denuded zones were observed at the grain boundaries, indicating that the grain boundaries act as a defect sinks, and the Kr bubble size was found to be mostly dependent on the irradiation temperature.

XRD for the He-irradiated UO_2 showed a significant lattice expansion upon irradiation, which was tentatively addressed to point defects (Frenkel pairs). XAFS indicated a dose-dependent disruption in the U local structure and a rise in multisite oxygen distribution at approximately 1.7 Å bond length. The results give new insight into the atomic level disorder of irradiated UO_2.

Microstructural characterization of the swift heavy ion irradiated CeO_2 (1GeV, 1×10^{12}-1×10^{14} Au ions/cm^2) revealed that ion tracks and dislocations form, and, with increasing fluence, the dislocations grew and formed networks in agreement with modeling.

Xe bubble formation and near surface stoichiometry of Xe-irradiated CeO_2 was examined as a function of post-irradiation annealing. The experimental results showed that oxygen depletion took place within the CeO_2 surface layer allowing a precise identification of the XRD features. Upon annealing, large Xe bubbles preferably formed near surfaces and grain boundaries, indicating the importance of free surfaces on fission gas and defect migration.

ATR neutron irradiation plans were finalized. The experiment (in 2014) consists of neutron irradiations for plain and ion-irradiated (Kr and He) UO_2.

Atom probe techniques were used to analyze the concentration of Kr in irradiated UO_2 for the first time. The samples contained a high number density of 1-2nm gas bubbles. The concentration profile closely matched that obtained from stopping and range of ions in materials (SRIM) code calculations, indicating that Kr atoms resided in the sample mostly where they stopped at irradiation and that trace amounts of Kr may be soluble in UO_2, contrary to conventional thinking. This phenomenon is being further explored using density functional theory calculations. A comparison of the distribution of Kr in UO_2 is shown in Figure 3.

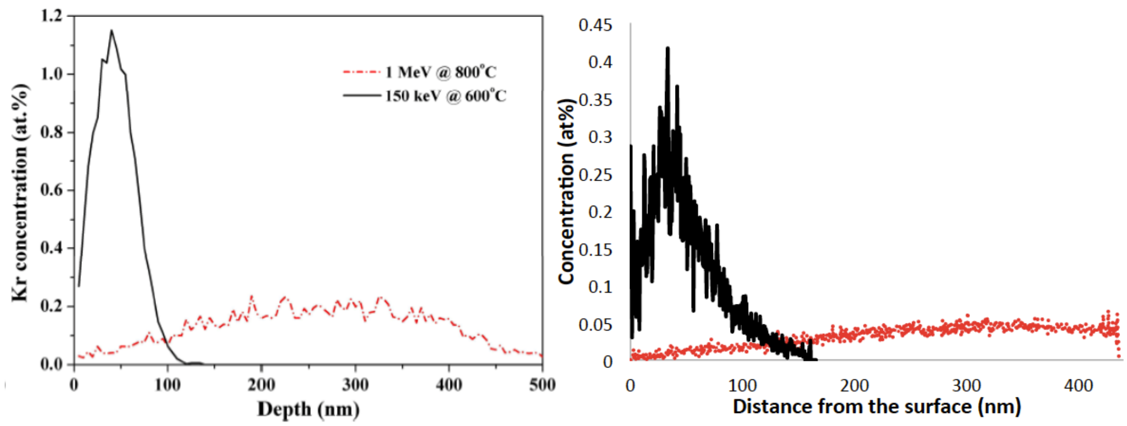

Figure 3. Comparison of the distribution of Kr in UO_2 measured by (a) SRIM code calculations and (b) atom probe Kr concentration measurements corresponding to the (a) panel.

We compared the ionization behavior between UO_2 and its common surrogate material CeO_2. It was observed that the two materials have very different evaporation characteristics which led us to determine that the laser-material interaction of the atom probe accentuated the fundamental differences between UO_2 and CeO_2. It highlighted that the optical properties, electronic structure, and thermodynamic stability differ in the two materials, thus illustrating the difficulty in studying CeO_2 as a replacement for UO_2. This also solidified the need to study UO_2 in order to capture its fundamental behavior.

Planned Activities

The planned activities include He^{2+} and H^+ ion irradiations for UO_2 will be carried out in May 2013 to provide samples with simple microstructures for the thermal conductivity measurements. Grain growth annealing for polycrystalline UO_2 will be also carried out in 2013 to validate the phase field models and to enable the thermal transport measurements over individual grain boundaries. IVEM irradiation will be carried out in June 2013 to study the effect of GB character on the defect evolution in UO_2 under Kr irradiation. ATR sample preparation (including He^{2+} and Kr^+ ion irradiations) will take place in 2013.

Our plans also include a detailed study of the near surface effects in UO_2. Using the atom probe technique is planned. It has already been determined from phase field calculations that the stoichiometry varies as a function of distance from voids and this was also experimentally observed in the atom probe as the stoichiometry varies as the distance from a free surface. Future analysis will experimentally focus on the change in local chemistry near voids and grain boundaries. The importance of this study is to elucidate the fundamental mechanistic roles of high-energy surfaces on the thermal transport properties of fuel.

2.2.2 Atomic-Scale Simulation of Defects in UO_2

The stability of radiation-induced defect clusters was investigated by molecular statics simulations using 9 interatomic potentials. Twelve types of defect clusters were investigated. The results show that significant discrepancies exist between different potentials, particularly for pure oxygen interstitial clusters (Taller 2). Overall, Basak potential predicts more reasonable cluster properties than other potentials (Basak 3).

The surface energies of a flat (110) surface and curved void surfaces of different radii were also evaluated by molecular dynamics. Most interatomic potentials overestimate the surface energy. As expected, the surface of the flat surface is found to be smaller than that of voids.

The complex migration mechanisms of uranium-oxygen interstitial and vacancy clusters were investigated with temperature accelerated dynamics simulations. In terms of migration barriers, the uranium-oxygen interstitial clusters show an opposite trend, as compared to pure oxygen interstitial clusters (Bai 4). For uranium-oxygen vacancy clusters, the migration barrier is dominated by the uranium vacancy diffusion.

The influence of grain boundary on defect production in UO_2 was investigated with molecular dynamics simulations. Near some GBs, such as Σ5 tilt GB, more interstitials than vacancies survived and such an "abnormal" behavior has never been found in simple metals, suggesting that the defect-GB interaction in UO_2 is more complex than in simple metals (Bai 5 and 6).

Planned Activities

Planned activities include further investigations of interaction between point defects and extended defects (GBs, free surfaces, voids, dislocation loops), impurity segregation and diffusion, etc.

2.2.3 Stoichiometry and Microstructure Evolution in UO_2

A defect disorder model of UO_2 founded on density functional theory results of defect energetics has been extended to investigate local off-stoichiometry near UO_2 surfaces. While bulk UO_2 crystals contain defects and electronic charge carrier densities that solely depend on the oxygen partial pressure and temperature, surfaces were found to significantly modify the defect equilibrium states. Analysis of local defect densities near flat surfaces in UO_2 showed that significant defect segregation occurs and that, under fixed thermo-chemical environment, local stoichiometry can change from hyper to hypo as a function of distance from the surface. A further generalization of the theory to void surfaces has led to the discovery that voids in UO_2 must contain oxygen gas. This important finding implies that, as a major component of UO_2, oxygen may have a bigger role to play in the irradiation response of the material than previously believed. It was also found that voids are surrounded by significant defect segregation regions at void sizes in the range few tens to few hundred nanometers. The implications for thermal transport are enormous as the presence of these regions alter the O:U ratio, to which phonon scattering is known to be sensitive. This discovery also implies that the average O:U ratio of irradiated UO_2 crystals containing ensembles of voids will be different from the unirradiated material under the same thermo-chemical conditions. This discovered electrochemical aspect of voids in UO_2 gave us new insight into how to construct microstructure evolution models. A number of chemical characterization experiments are now being designed to validate this prediction.

Motivated by the need to perform grain growth experiments to obtain coarse grained samples, a grain growth model in porous ceramics was developed to simulate grain growth in UO_2 and CeO_2. An accurate representation of the grain boundary and pore motion kinetics resulted in an impressive agreement with experimental data. The model predicts the growth exponents and growth rate coefficients at different porosity regimes very accurately for both materials. The model shows that the inhomogeneous distribution of pores could lead to abnormal grain growth.

Planned Activities

Planned activities will focus on the solution of the heterogeneous defect disorder model in UO_2 containing ensembles of voids. This will validate our hypothesis regarding the average O:U ratio in irradiated UO_2 and enables the defect-disorder analysis of Kr and Xe irradiated samples. Addition of Kr and Xe to the model will also be pursued to discover the synergy between these defects and intrinsic defect concentration. With regard to the grain growth model, a description of grain boundary and pore kinetics in terms of the point defect kinetics is underway. This will enable us to investigate grain and porosity (voids) evolution under irradiation, with the added feature of capturing the electrochemical effects of voids described in the above bullet into microstructure evolution model. A grain growth experiment for UO_2 in a controlled environment will be conducted to ascertain the growth mechanics and effect of the oxygen environment.

2.3 Education and Outreach

CMSNF continues to develop staff through educational efforts. The team routinely co-loans students and team members from different institutions in order to create greater integration and synergy across research tasks. A key outcome is not only to facilitate creative thinking and scientific exchange among team members, but also to provide educational and training opportunities for students and postdocs. To date, students supported under the project are listed in Tables 1 and 2 below.

Table 1. Students and post docs currently involved in the CMSNF.

Name	Location	PI	Status	Project
Yangzhong Li	University of Florida	Phillpot	Ph.D.	COMB potential for U/UO_2
Aleksandr Chernatynskiy	University of Florida	Phillpot	Ph.D.	Use of BTE methods to determine the thermal conductivity in UO_2
Bowen Deng	University of Florida	Phillpot	Ph.D.	Thermal transport properties of dislocations in UO_2
Billy Valderrama	University of Florida	Manuel	Ph.D.	Microstructural studies of CeO_2/UO_2 using atom probe
Hunter Henderson	University of Florida	Manuel	Ph.D.	Microstructural studies of CeO_2/UO_2 using atom probe
Mahima Gupta	University of Wisconsin	Allen	Ph.D.	Irradiation and associated microstructural changes
Sarah Khalil	University of Wisconsin	Allen	Ph.D.	Modeling microstructural evolution under irradiation
Lingfeng He	University of Wisconsin	Allen	Post-Doc	Microstructural evolution in irradiated CeO_2 and UO_2
Janne Pakarinen	University of Wisconsin	Allen	Visiting	Microstructural evolution in irradiated CeO_2 and UO_2
Karim Ahmed	Purdue	El-Azab	Ph.D.	Phase field modeling of microstructure in UO_2
Abdel-Rahman Hassan	Purdue	El-Azab	Ph.D.	Stoichiometric changes in UO_2 under irradiation
Nan Wang	Purdue	El-Azab	Post-Doc	Parallelization of Monte Carlo Code for Phonon Transport
Zilong Hua	Utah State University	Hurley	Ph.D.	Thermal conductivity analysis using laser
Bo Wang	Colorado School of Mines	Lin	GS	Deposition and characterization of UO_x thin films

Table 2. Individuals that have left the center, either graduating and accepting positions with industry or to further pursue educational opportunities within or outside the CMSNF.

Name	Location	PI	Status	Project
Clarrisa Yablinsky	UW	Allen	Post Doc	Microstructural evolution in irradiated CeO_2 and UO_2
In-Wook Park	CSM	Moore	Post Doc	Synthesis and characterization of CeO_2 and UO_2 crystalline coatings using pulsed de magnetron sputtering • Korea
Thomas Hochrainer	FSU	El-Azab	Post Doc	Defect and microstructure dynamics in irradiated materials
Michael Tonks	INL		Post Doc	Research scientist at INL
Paul Millett	INL		Post Doc	Research scientist at INL
Marat Khafizov	INL		Post Doc	Spatially resolved thermal transport measurements. Now a full-time staff research scientist at INL
Peng Xu	UW	Allen	Post Doc	Westinghouse electric company
Srujan Rokkam	Purdue	El-Azab	Ph.D.	Phase Field Modeling of Void Kinetics in Irradiated Materials
Walter (Ryan) Deskins	Purdue	El-Azab	M.S.	Monte Carlo Solution of BTE for Phonons • Ryan quit school in December 2012 and is working in Orlando Florida with an Insurance company. A new student is replacing him May 2013.
Tony Schulte	UW	Allen	M.S.	Unknown

3. COST STATUS

The approved budget by period and actual plus trended incurred for the CMSNF is shown in Table 3.

Table 3. Approved budget and actual trended for CMSNF.

CMSNF Project[a] (to Date Funding for FY-09 – FY-13)	Prior Year Carryover $K (July 31, 2012)	FY-13 Budget $K (through July 31, 2013)	FY-13 Actuals ($K) (based on trend through July 31, 2013)	Expected Carryover into FY-14 (unspent funds)
Allen Oversight/Admin. Package	153.1	590.5	452.9	137.6
Hurley Package	41.0	261.5	240.2	21.3
Gan Package	12.2	80.0	62.6	17.4
University of Wisconsin	0.0	240.0	240.0	0.0
University of Florida	0.0	200.0	200.0	0.0
Florida State University	0.0	0.0	0.0	0.0
Colorado School of Mines	0.0	150.0	150.0	0.0
Purdue University	0.0	200.0	200.0	0.0
INL Planned (through July 31, 2013)	206.3	1,722.0	1,545.7	176.3
Oak Ridge National Lab (allocated directly to ORNL in support of CMSNF)	102.6	300.0	344.8	57.8
Total	308.9	2,022.3	1,890.5	234.1

4. SCHEDULE STATUS

Activities above are based on the CMSNF roadmap. The CMSNF team developed this roadmap three years ago. It is a living document that is updated at the semiannual project meetings, every 6 months. The roadmap and progress against planned activities is presented to the Advisory Board at its annual meeting. The CMSNF roadmap defines the logical order of implementing the center's research without specifying fixed dates for the completion of various research tasks.

5. CHANGES IN APPROACH

There are no changes in research approach for this reporting period.

6. ACTUAL OR ANTICIPATED PROBLEMS

The Advanced Combustion Synthesis Engineering Laboratory (ACSEL) at the Colorado School of Mines (CSM) received the Colorado State license for depositing UO_2 thin film samples in February 2012. However, the state and CSM radiation officers determined that the originally proposed location for the deposition system (Hill Hall 302) could be used for the UO_2 thin film depositions. This is due to the fact that the main gas intake ports for the entire building are too close to the lab (Hill Hall 302). To solve this problem, ACSEL received the permission from CSM to use a different location (Hill Hall 223) to meet the safety and radiation control requirements. In addition, ACSEL decided to rebuild a new high vacuum deposition system in the new location for UO_2 film depositions. Currently, a new high vacuum deposition system and a glove box are under construction in the new location. It is anticipated that the equipment should be able to produce samples for the CMSNF by the end of June.

7. PERSONNEL CHANGES AND/OR LEAVES

In January of this year, CMSNF Director, Dr. Todd Allen, assumed a full-time position at INL as the Deputy Laboratory Director for Science and Technology. This left the principle investigator (PI) position at the University of Wisconsin vacant. The position was assumed by Dr. Jake Blanchard and Dr. Kumar Sridharan with support from post doctoral, Janne Pakarinen. With Janne's support, the transition to Dr. Blanchard was seamless with no impact to work.

Dr. Jianliang Lin, CSM, will take a new position at SwRi starting after this summer. An official notification of this personnel change will be sent to Dr. John Vetrano and Dr. Linda Horton, as soon as details are finalized.

8. PRODUCTS PRODUCED/TECHNOLOGY TRANSFER

Publications: New publications since last report are listed below. Names in **bold** were fully supported by the EFRC; names in *italics* were partially supported by the EFRC.

1. **Yangzhong Li**, Tzu-Ray Shan, Tao Liang, Susan B. Sinnott, and **Simon R. Phillpot**, "Classical Interatomic Potential for Uranium Metal", *Journal of Physics Condensed Matter,* **24** 235403 (2012) (DOI: 10.1088/0953-8984/24/23/235403**)**.
2. **J. G. Yu**, K. M. Rosso, and S. M. Bruemmer, "Charge and Ion Transport in NiO and Aspects of Ni Oxidation from First Principles." *Journal of Physical Chemistry C,* **116**, 1948–1954 (2012) (DOI: 10.1021/jp208080v).
3. Z. Hua, H. Ban, **M. Khafizov**, R. Schley, R. Kennedy and **D. Hurley**, "Spatially Localized Measurement of Thermal Conductivity Using a Hybrid Photothermal Technique", *Journal of Applied Physics,* **111**, 103505 (2012) (DOI: 10.1063/1.4716474).
4. **Xian-Ming Bai**, Louis J. Vernon, Richard G. Hoagland, Arthur F. Voter, Michael Nastasi, and Blas P. Uberuaga, "The Role of Atomic Structure on Grain Boundary-defect Interactions in Cu," *Physical Review B* 85, 214103 (2012) (DOI: 10.1103/PhysRevB.85.214103).
5. W. Pan, **S. R. Phillpot**, C. Wan, **A. Chernatynskiy** and Z. Qu, "Low Thermal Conductivity Oxides" *MRS Bulletin* 37, 917 (2012).
6. **X.M. Bai, A. El-Azab, J. Yu**, and **T.R. Allen**, "Migration Mechanisms of Oxygen Interstitial Clusters in UO_2", *Journal of Physics Condensed Matter* **25,** 015003 (2013) (DOI: 10.1088/0953-8984/25/1/015003).
7. C. Xing, C, Jensen, Z. Hua, H. Ban **D. H. Hurley**, **M. Khafizov**, R. J. Kennedy, "Parametric Study of the Frequency-Domain Thermoreflectance Technique," *Journal of Applied Physics*, **112**, 103105 (2012) (DOI: 10.1063/1.4761977).
8. **B. Deng, A. Chernatynskiy,** P. Shukla**,** S. B. Sinnott **and S. R. Phillpot,** "Effect of Edge Dislocation on Thermal Transport in UO_2," *Journal of Nuclear Materials*, **434**, 203-209 (2013) (DOI: 10.1016/jnucmat.2012.11.043).
9. **A. Chernatynskiy** and **S. R. Phillpot**, "Phonon-mediated Thermal Transport: Confronting Theory and Microscopic Simulation with Experiment, *Current Opinions in Solid State and Materials Science*." http://dx.doi.org/10.1016/j.cossms.2012.11.001.
10. **X.M. Bai** and B.P. Uberuaga, "On the influence of grain boundaries on radiation damage production in materials: a review of theoretical studies", *JOM (invited review paper), published online*. (DOI: 10.1007/s11837-012-0544-5).
11. **J. W. L. Pang**, W. J. L. Buyers, **A. Chernatynskiy**, M. D. Lumsden, **B. C. Larson and S. R. Phillpot,** "Phonon Lifetime Investigation of Anharmonicity and Thermal Conductivity of UO_2 by Neutron Scattering and Theory," *Physical Review Letters*.(DOI: 10.1103/PhysRevLett.110.157401) http://prl.aps.org/abstract/PRL/v110/i15/e157401.

12. **W.R. Deskins** and **A. El-Azab**, “Monte Carlo Simulation of Phonon Transport in UO_2 Single Crystals,” *Modeling and Simulation in Materials Science and Engineering* (DOI:10.1088/0965-0393/21/2/025013).
13. **I.-W. Park. J. Lin, J. J. Moore, M. Khafizov, D. Hurley, M. V. Manuel and T. Allen**, “Grain Growth and Mechanical Properties of Cerium Oxide Films Deposited on Si(100) Substrates by Pulsed Magnetron Sputtering (PMS),’ *Surface Coatings and Technology* http://dx.doi.org/10.1016/j.surfcoat.2012.11.068.
14. **Jianliang Lin, Hunter Henderson, Michele Manuel, William D Sproul**,"Nanoscale Chemistry and Microstructure of the Films Investigated by TEM and APT", *Applied Surface Science*, (DOI:10.1016/j.apsusc.2013.03.075).
15. **Jianliang Lin**, William D. Sproul, **Bo Wang**, Isaac Dahan, Yixiang Ou, "Anatase and rutile TiO2 films deposited by arc free deep oscillation modulated pulsed power magnetron sputtering", J. Phys. D: Appl. Phys (DOI:10.1088/0022-3727/46/8/084008).

In Press:

16. **L. He**, **C. Yablinsky, M. Gupta, J. Gan**, M. A. Kirk, **T. R. Allen**, “TEM investigation of Kr Bubbles in Polycrystalline CeO_2,” submitted to Nuclear Technology.
17. **Valderrama, B., Henderson, H.B., He, L., Yablinsky, C., Gan, J., Hassan, A.-R., El-Azab, A., Allen, T.R., Manuel, M.V**. “Fission Products in Nuclear Fuel: Comparison of Simulated Distribution with Correlative Characterization Techniques,” Microscopy and Microanalysis (August 4-8, 2013).

8.1.1 Website

The CMSNF website (http:www.inl.gov/efrc) has been significantly improved in FY 2012. The new website provides information on CMSNF’s mission, team members, research approaches, publication list, collaborations and partnerships, education and outreach, and news. The major improvement is in the “Research” section of the web site. To help people who are not CMSNF members better understand the center’s mission, the new website introduces the two thrust areas (microstructural science under irradiation and thermal transport in UO_2) and how they are integrated. The website provides an overview of the five science questions the center is currently addressing. For each science question, detailed explanations of the center’s research approaches are provided. An introduction video of the center’s mission is also provided in the website.

8.1.2 Networks or Collaborations

1. **ITU:** The Institute for Transuranium Elements (ITU) participates in monthly CMSNF conference calls and is working with CMSNF to identify synergy between the research programs. However, they have been limited to participating in the monthly calls and providing some technical support.
2. **Pacific Northwest National Laboratory (PNNL):** Collaborating with Ram Devanathan at PNNL to investigate swift heavy ion damage in CeO_2 and UO_2. Dr. Devanathan will be modeling electronic stopping damage under the same conditions that are being performed experimentally by the University of Wisconsin.
3. **Los Alamos National Laboratory (LANL):** A collaboration between Dr. Andrew Nelson at LANL and CMSNF has been arranged to provide large-grained, non-stoichiometric UO_2 polycrystals on loan for macroscopic and microscopic thermal transport studies.
4. **Idaho State University (ISU):** Access to large, single-crystal samples of UO_2 is now being addressed directly by a collaboration between Dr. Rory Kennedy (INL) and Dr. Eric Burgett (ISU).
5. **University of Michigan:** Dr. El-Azab of Purdue and his student are collaborating with Dr. Hui-Chia Yu of the University of Michigan on the use of smooth boundary method to solve the local stoichiometry fields in UO_2 with a void ensemble.

6. **Boise State University**: Dr. Janne Pakarinen of the University of Wisconsin and Dr. El-Azab of Purdue planned a collaboration with Dr. Darryl Butt of Boise State University to conduct grain growth experiments of UO_2 in controlled oxygen environment and on the modeling of the growth process and effect of oxygen on its kinetics.
7. **National Research Council of Canada (NRC):** Retired principal research officer, Dr. William Buyer, has continued collaborations with Dr. Larson and Dr. Pang on the study of phonon in UO_2 using neutron scattering (see page 35 of report for letter of support)

8.1.3 Technologies/Techniques Developed

8.1.3.1 Enhanced Capability

As a part of the computational modeling of phonon transport in UO_2 single crystals, a robust MC solution scheme for BTE has been developed that extends beyond similar previous works in the literature. A parallel C++ code has been developed based on this MC scheme. This code is now being further enhanced by building in 3-D representations of the first the Brillouin zone of the K-space for accurate representation of phonon-phonon scattering events. Once in a mature stage of development, we intended to make this a standard code for MC simulation of phonon transport in complex crystals that other members of the community can use.

We have developed the first model of grain growth in porous ceramics as part of the microstructure simulation efforts of the center. This model is based on the phase field framework and it combined both grain boundary motion and pore surface migration kinetics. The model has been successfully linked with experiments and it gave us results in very close agreement with experiments for both CeO^2 and UO_2.

Yet, another very important theoretical development that was made under this center is the development of density-functional theory based defect disorder model that predicts the level of various defects and electronic charge carriers in UO_2 under given thermo-chemical conditions (temperature and oxygen pressure). The model can be used to analyze defect levels in UO_2 over a wide range of off-stoichiometry, which is critical for understanding thermal transport. The model has been extended to predict the stoichiometric heterogeneity in UO_2 resulting from microstructure features such as void and bubble ensembles. This model is anticipated to be an important building block of the theory of UO_2 response to thermo-chemical environmental changes and irradiation.

8.1.4 Inventions/Patent

None.

8.1.5 Other Products

8.1.5.1 Conference Presentations/Papers

- I-W. Park, J. J. Moore, J. Lin, D. Hurley, M. Khafizov, A. El-Azab, T. Allen, C. Yablinsky, M. Gupta, J. Gan, M. Manuel, H. Henderson, and B. Valderrama, “Deposition of Microstructure and Mechanical Properties of Mo-doped CeO_2 Films, Prepared by Pulsed Unbalanced Magnetron Sputtering,” *International Conference on Metallurgical Coatings and Thin Film*, April 2012, San Diego, CA.
- Jianliang Lin, Bo Wang, and William D Sproul, “Virtually Arc Free HPPMS Based on Oscillatory Voltage Wave Forms for Insulating Film Depositions,” *TMS 2013 Meeting*, March 3-7, San Antonio, TX, Symposium: Advances in Surface Engineering: Alloyed and Composite Coatings II.
- B. Valderrama, H.B. Henderson, I.W. Park, J. Lin, J. Moore, C. Yablinsky, T.R. Allen, M.V. Manuel, “Atom Probe Tomography of Simulated Fission Product Segregation in CeO2,” *TMS 2012 Meeting*, March 11-15, Orlando, FL, Structural Materials Division (poster).

- Khafizov, M., Hurley, D.H., Gan, J., Gupta, M., Pakarinen, J., Yablinsky, C., He, L., Valderrama, B., Manuel, M.V., "Measurement of Thermal Conductivity in Ion Irradiated Samples," *MRS Spring 2013 Meeting.* San Francisco, CA, April 1-5, 2013.
- J. Yu, X. Bai, A. El-Azab, and T. Allen, "*Parallel KMC Study of Oxygen Clustering Dynamics in* UO_2," Materials Research Society (MRS) 2012 Fall Meeting, December 2012, Symposium TT: Defects and Microstructure Complexity in Materials.
- Anter El-Azab, Multiscale models and experiments for thermal transport in crystalline solids under extreme conditions, 6th International Conference on Multiscale Materials Modeling (MMM-2012), Singapore, October 15-19, 2012 *(Plenary Talk)*
- Anter El-Azab, Continuum Theory of Defects and Materials Response to Irradiation, Symposium on Integrated Computational Modeling of Materials for Nuclear Energy, TMS 2013 Annual Meeting in San Antonio, Texas, March 3-7, 2013 *(Invited Talk)*
- Anter El-Azab, Continuum Theory of Defects and Materials Response to Irradiation, Symposium: Structural Transformations in Solids, International Workshop on Computational Mechanics of Materials, IWCMM XXII, September 24-26, 2012, Baltimore, MD *(Invited Talk)*
- Anter El-Azab, A Continuum Thermodynamic Approach to Radiation Effects in Materials, ANS meeting, Chicago, June 2012, Symposium: Radiation Effects in Ceramic Oxide and Novel LWR Fuels, 2012 TMS Annual Meeting & Exhibition, Orlando, FL, March 11-15, 2012 *(Invited Talk)*
- A.-R. Hassan, Xian-Ming Bai, Anter El-Azab, Thermodynamics and Kinetics of Defect Disorder in UO_2, MRS Fall Meeting/Symposium HH: Advances in Materials for Nuclear Energy, Boston MA, November 25-30, 2012.
- A.-R. Hassan, Jianguo Yu, Anter El-Azab, Microstructure and Defect Disorder in UO_2, TMS 2013 Annual Meeting, San Antonio TX, March 3-7, 2013.
- Karim Ahmed and Anter El-Azab, Computational Modeling of Grain Growth in Porous Uranium Dioxide, TMS 2013 Annual Meeting, San Antonio TX, March 3-7, 2013
- Deskins and El-Azab, Phonon Transport in UO_2 Crystals with Defects, , TMS 2013 Annual Meeting, San Antonio TX, March 3-7, 2013
- Karim Ahmed, Anter El-Azab, Tony Schulte, Spencer Morris, Clarissa Yablinsky, and Todd Allen, Phase Field Modeling of Grain Growth in Ceria and Uranium Dioxide, MRS Fall Meeting/ Symposium TT: Defects and Microstructure Complexity in Materials, Boston MA, November 25-30, 2012
- Ryan Deskins Anter El-Azab, Phonon Thermal Transport in UO_2 Crystals with Defects, MRS Fall Meeting/Symposium TT: Defects and Microstructure Complexity in Materials, Boston MA, November 25-30, 2012
- L. He, M. Gupta, C. Yablinsky, J. Gan, M. A. Kirk, and T. Allen, Microstructural investigation of Kr irradiated UO_2, TMS 2013 Annual Meeting, San Antonio TX, March 3-7, 2013.
- C. Yablinsky, J. Pakarinen, L. He, T. Allen, J. Gan, R. Devanathan, D. Severin, and C. Trautmann, Investigation of Swift Heavy Ion Irradiation Defects in CeO_2, TMS 2013 Annual Meeting, San Antonio TX, March 3-7, 2013.
- Judy Pant, William Buyers, Aleksandr Chernatynskiy, Bennett Larson, and Simon Phillpot, Phonon Lifetime Investigation of Anharmonicity and Thermal Conductivity in UO_2, American Physical Society March Meeting, March 18-22, 2013, Baltimore, MD.

8.1.5.2 Semi-annual Meeting

Purdue University hosted the semi-annual meeting in West La Fayette, Indiana on March 12-13, 2013. The focus of the meeting was to evaluate progress to date and to ensure that team members had a clear understanding of the tasks to be completed by the end of the contract, including planned publications.

8.1.5.3 Service

Advisory Boards and Committees

1. Anter El-Azab: Advisory Board Member, 6th International Conference on Multiscale Modeling of Materials (MMM-12), Singapore, October 2012.
2. Anter El-Azab: Advisory Board Member, Cyber-infrastructure for Atomistic Materials Science (CAMS) Center, University of Florida, Gainesville (cams.mse.ufl.edu).
3. Michele Manuel: member of the following TMS committees: Nuclear, Education, Women in Science, and Publications.
4. Judy Pang: Materials Program Advisory Committee (MPAC) Member, Los Alamos Neutron Science Center, 2008–present.
5. Judy Pang: Advanced Test Reactor (ATR) National Scientific User Facility, proposal reviewer, 2011–present.

Conference Symposium Organization

1. Structural and Functional Materials for Fission and Fusion Reactors, 2012 Nuclear Materials Conference (NuMat2012), Osaka, Japan, October 2012. Symposium Chair: Todd Allen (INL).

   Third International Workshop on Structural Materials for Innovative Nuclear Systems (SMINS-3), Idaho Falls, ID, October 2013. Conference Chair: Todd Allen (INL).
2. 2012 Energy Frontiers Research Center (EFRC) Summer School, Knoxville, TN, June 2012. Organizers: Xianming (David) Bai (INL), Michele Manuel (UF), Jian Gan (INL).
3. 2012 The Minerals, Metals and Materials Society (TMS) Radiation Effects in Ceramic Oxide and Novel LWR Fuels Symposium. Organizers: Peng Xu (Formerly UW), Todd Allen (INL), Jian Gan (INL), Bill Weber (UT), Ram Devanathan (PNNL), Anter El-Azab (FSU), Simon Phillpot (UF), Edward Lahoda (Westinghouse), Michele Manuel (UF), Eric Burgett (ISU), Jim Stubbins (UIUC), Ramprashad Prabhakaran (INL).
4. Defects and Microstructural Complexity in Materials Symposium, Materials Research Society (MRS) Fall 2012 Meeting, Boston, Massachusetts. Organizers: Anter El-Azab (Purdue), Fei Gao, Alfrendo Caro, Peter Derlet, Toshimasa Yoshiie.
5. Mesoscale Computational Materials Science of Energy Materials, 2013 The Minerals, Metals and Materials Society (TMS) Annual Meeting, San Antonio, Texas, March 3-7, 2013. Organizers: Pascal Bellon (UIUC), Anter El-Azab (Purdue), L-Q Chen, Alfredo Caro, Ming Tang.
6. Materials and Structural Issues Track, 2013 International Congress on Advances in Nuclear Power Plants (ICAPP2013), Jeju Island, Korea, April 2013. Symposium co-Organizer: Xianming (David) Bai.
7. Microstructure Evolution in Driven Materials, Purdue, April 15-16, 2013. Organizer: Anter El-Azab (Purdue).

8. Organization of the 2014 TMS Radiation Effects in Oxide Ceramics and Novel LWR Fuels Symposium *proposal pending.* Organizers: Xianming (David) Bai (INL), Todd Allen (INL), Blas Uberuaga (LANL), Jianliang Lin (CSM), Michele Manuel (UF), Dragos Staicu (ITE-Germany) San Diego, California

9. Symposium EEE, “Materials behavior under extreme irradiation, stress or temperature" at the 2014 Spring MRS Meeting. Organizers: James R. Morris (ORNL), Jianguo Yu (INL), Andrew Horsfield (Imperial College London, UK), Nan Li (LANL).

9. REFERENCES

1. J. W. L. Pang, W. J. L. Buyers, A. Chernatynskiy, M. D. Lumsden, B. C. Larson and S. R. Phillpot, “Phonon Lifetime Investigation of Thermal Conductivity of UO_2 by Neutron Scattering and Theory,” *Physical Review Letters*. http://prl.aps.org/abstract/PRL/v110/i15/e157401 (http://prl.aps.org/abstract/PRL/v110/i15/e157401).

2. S. A. Taller and X. M. Bai, “Assessment of Structures and Stabilities of Defect Clusters and Surface Energies Predicted by Nine Interatomic Potentials for UO_2,” *Journal of Nuclear Materials* (submitted).

3. C. B. Basak, A. K. Sengupta, and H. S. Kamath, “Classical Molecular Dynamics Simulation of UO_2 to Predict Thermophysical Properties,” *Journal of Alloys and Compounds*, **360**, 210 (2003).

4. X. M. Bai, A. El-Azab, J. Yu, and T. R. Allen, “Migration Mechanisms of Oxygen Interstitial Clusters in UO_2,” *Journal of Physics: Condensed Matter*, 25, 015003 (2013).

5. X. M. Bai and B. P. Uberuaga, “On the Influence of Grain Boundaries on Radiation Damage Production in Materials: a Review of Theoretical Studies,” *JOM,* 65, 360 (2013).

6. X. M. Bai, L. J. Vernon, R. G. Hoagland, A. F. Voter, M. Nastasi, and B. P. Uberuaga, “The Role of Atomic Structure on Grain Boundary—Defect Interactions in Cu,” *Physical Review* B 85, 214103 (2012).

10. CURRENT AND PENDING

Director: Todd Allen

Dr. Allen is fully funded as the Deputy Laboratory Director for Science and Technology at the Idaho National Laboratory. All previous projects at the University of Wisconsin-Madison were transitioned to Dr. Jake Blanchard and Dr. Kumar Sridharan.

DROPPED: (Work transitioned from Todd Allen)

- Research in Support of VHTR Safety Performance, NRC-04-10-173
- Development of Advanced High Uranium Density Fuels for Light Water Reactors
- Freeze-casting as a Novel Manufacturing Process for Fast Reactor Fuels
- Deuterium Retention in Various Tungsten Materials Exposed to High Heat Flux
- Cold Spray Coating Technology for Mitigating High Temperature Corrosion in Coal-fired Power Plants
- Characterization and Engineering of Concrete at Multi-scale and In Situ Monitoring for Improved Resistance to High Temperature and Radiation Change
- Investigation of Molten Bromide-based Salts for Advanced Pyroprocessing Applications
- Effect of Metallic Transmutation Products on the Oxidation, Mechanical, and Electrical Properties of Silicon Carbide
- Technology Development for Advanced Sodium-cooled Fast Reactors
- NEUP General Scientific Infrastructure Support
- An Integrated Approach to Develop Nanostructured High Performance Reactor Cladding Materials
- Accelerated Development of Zr-containing New Generation FM steels for Advanced Nuclear Reactors
- Multilayered Metal/Ceramic Composites for Structural Materials Application
- Material Science Studies for Advanced Nuclear Systems
- Spray Technologies for the Deposition of Advanced Materials for High Performance Reactor Applications
- Fundamental Improvements to Zircaloy Cladding Performance through Application of Self-Healing Coatings

The following PIs had no changes to their current and pending:

- Marat Khafizov, Idaho National Laboratory
- Judy Pang, Oak Ridge National Laboratory

Anter El-Azab
Purdue University

DROPPED:

- Statistical Mechanics Modeling of Mesoscale Deformation of Metals
- Computational Modeling of Mesoscale Deformation of Copper Crystals for Comparison with X-ray Measurements.

ADDITIONS:

Investigator: Anter El-Azab	Other Agencies to which this proposal has been/will be submitted:
Support: Pending	
Project/Proposal Title and grant number, if appropriate: **Computational Mesoscale Materials Design**	
Source of Support: DOE/OFES-BES	
Location of Project: Purdue University	
Total Award Amount:	$2,175K
Total Award Amount to PI's Research:	Total of $270K for the above period
Total Award Period Covered:	3 years
Describe Research Including Synergies and/or Overlaps with EFRC Award: *There is no overlap with EFRC but, if funded, there may be some synergy with EFRC in numerical solution of some phase field models.*	
Person Months Per Year Committed to Project: 0.5 Acad, 0.5 Sumr	1 Pers. Months

Ben Larson
Oak Ridge National Laboratory

Investigator: B.C. Larson (G. M. Stocks, PI) **CHANGE**	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Energy Frontier Research Center for Defect Physics in Structural Materials (ERKCS99)**	
Source of Support: DOE BES	
Location of Project: Oak Ridge National Laboratory	
Annual Award Amount:	$3,325K
Total Award Amount to PI's Research:	$224 K
Total Award Period Covered:	FY 07 - 14
Describe Research including Synergies and Delineate with Respect to the EFRC Award: *Enhance our fundamental understanding of the generation and accumulation of radiation-induced defects and defect clusters in Fe and Fe-alloys. Investigators role involves x-ray diffuse scattering and microbeam x-ray studies; work is distinct from other investigator projects.*	
Person-Months Per Year Committed to Project: Cal	4.8 Pers. Months

David Hurley
Idaho National Laboratory

DROPPED:

- Evaluate the Application of Advanced Measurement Systems to Investigate SIC Nuclear Fuel Cladding.

ADDITIONS:

Investigator: David Hurley	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: L**aser-based Characterization Technique Development**	
Source of Support: Nuclear Energy, Advanced Fuel Cycle Initiative	
Location of Project: Idaho National Laboratory	
Total Award Amount:	$756K
Total Award Amount to PI's Research:	$756K
Total Award Period Covered:	FY 12
Describe Research Including Synergies and/or Overlaps with EFRC Award: *Develop laser-based instruments to measure the mechanical and thermal properties of highly radioactive nuclear materials.*	
Person-Months Per Year Committed to Project: Cal	8 Pers. Months
Investigator: David Hurley	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **SiC Feasibility Gap Analysis**	
Source of Support: Nuclear Energy, Light Water Reactor Sustainability	
Location of Project: Idaho National Laboratory	
Total Award Amount:	$250K
Total Award Amount to PI's Research:	$50K
Award Period Covered:	FY13
Describe Research Including Synergies and/or Overlaps with EFRC Award: *None*	
Person-Months Per Year Committed to Project: Cal	1.5 Pers. Months

David Hurley
Idaho National Laboratory (continued)

Investigator: David Hurley	Other Agencies to which this proposal has been/will be submitted: NA
Support: Pending	
Project/Proposal Title and grant number, if appropriate: **In situ Monitoring of Deformation across Length Scales using Laser Ultrasonics**	
Source of Support: DOE NE (NEET-3)	
Location of Project: INL	
Total Award Amount:	$315k/yr
Total Award Amount to PI's Research:	$315 k
Total Award Period Covered:	FY 14 - 17
Describe Research Including Synergies and/or Overlaps with EFRC Award: *Use laser ultrasonics to monitor deformation in a high temperature creep fatigue environment.*	
Person-Months Per Year Committed to Project: Cal	1 Pers. Months

Simon Phillpot
University of Florida

DROPPED:

- Rapid Discovery of Tribological Material with Improved Performance using Materials Informatics.

Investigator: Simon Phillpot ADDITION	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Molecular Dynamics Simulations of Local Structure in a BaTiO3-based Ferroelectrics**	
Source of Support: NIST	
Location of Project: University of Florida	
Annual Award Amount:	$50,000
Annual Award Amount to PI's Research:	$200,000
Total Award Period:	07/01/12 to 06/30/14
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *None*	
Person-Months Per Year Committed to Project:	0 Pers. Months
Investigator: Simon Phillpot ADDITION	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **NRC Fellowship Program**	
Location of Project: University of Florida	
Annual Award Amount:	$399,999
Annual Award Amount to PI's Research:	
Total Award Period:	08/01/08 to 07/31/13
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *Current NRC student fellowship program with no relationship to this EFRC*	
Person-Months Per Year Committed to Project:	0 Pers. Months
Investigator: Simon Phillpot ADDITION	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **UF NRC-10 Faculty Development**	
Source of Support:	US NRC
Location of Project:	University of Florida
Annual Award Amount:	$450,000
Annual Award Amount to PI's Research:	
Total Award Period:	05/01/10 to 04/30/13
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *NRC faculty development program with no relationship to this EFRC*	
Person-Months Per Year Committed to Project: Specify: Cal., Acad., or Sumr:	0 Pers. Months

Simon Phillpot
University of Florida (continued)

Investigator: Simon Phillpot ADDITION	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Engineered Zircaloy Cladding Modifications for Improved Accident Tolerance of LWRs**	
Source of Support: DOE-NE	
Location of Project: *University of Illinois (Prime), University of Florida*	
Annual Award Amount:	$3,500,000
Annual Award Amount to PI's Research:	$250,000
Total Award Period:	01/01/13 to 12/31/15
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *No relationship to this EFRC*	
Person-Months Per Year Committed to Project: Cal	0 Pers. Months
Investigator: Simon Phillpot CHANGE	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Consortium for the Advanced Simulation of Light Water Reactors (CASL)**	
Source of Support: DOE	
Location of Project: ORNL (Prime), University of Florida	
Annual Award Amount:	$125,000,000
Annual Award Amount to PI's Research:	$200,000
Total Award Period:	10/01/10 to 09/30/13
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *No relationship to this EFRC*	
Person-Months Per Year Committed to Project: Cal	0 Pers. Months

Xianming (David) Bai
Idaho National Laboratory

DROPPED:

- Multilayered Metal/Ceramic Composites for Structural Materials Application
- Cladding Performance through Application of Self-healing Coatings.

ADDITIONS:

Investigator: Xianming Bai (Jian Gan)	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support):	C
Project/Proposal Title and grant number, if appropriate: **Micro/Nano Scale AFM-based Thermal Conductivity Measurement and Atomistic Modeling for Oxide Fuel: the effects of grain boundary, fission gas and radiation damage**	
Source of Support: INL - LDRD	
Location of Project: Idaho National Laboratory	
Annual Award Amount:	$219 K
Annual Award Amount to PI's Research:	$28 K
Total Award Period:	10/2012 – 09/2015
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *Use atomistic modeling methods to study how GB character affects the thermal transport in CeO2. The knowledge and methods developed in this work are complementary to EFRC.*	
Person-Months Per Year Committed to Project: Cal	1 Pers. Months
Investigator: Xianming Bai	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **In situ Micro-raman Spectroscopy and Modeling of Breakaway Oxidation of Zircaloy Cladding**	
Source of Support: INL - LDRD	
Location of Project: Idaho National Laboratory	
Annual Award Amount:	$91K
Annual Award Amount to PI's Research:	$8K
Total Award Period:	10/2012 – 09/2013
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *The PI was transferred to Xianming Bai in FY13 due to the leave of the previous PI. Help INL to manage this project in which the main work is conducted at Mississippi State University. No overlap with EFRC.*	
Person-Months Per Year Committed to Project: Cal	0.3 Pers. Months

James (Jake) Blanchard
University of Wisconsin-Madison

ADDITIONS:

Investigator: James Blanchard	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **NEUP Scholarships and Fellowships**	
Source of Support:	DOE
Location of Project:	UW
Annual Award Amount:	$40,000
Annual Award Amount to PI's Research:	$ 0
Total Award Period:	2009-2017
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *No research*	
Person-Months Per Year Committed to Project:	0 Pers. Months
Investigator: James Blanchard	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Fusion Advanced Design Studies**	
Source of Support:	DOE
Location of Project:	UW
Annual Award Amount:	$245,000
Annual Award Amount to PI's Research:	$50,000
Total Award Period:	1998-2015
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *Mechanical design for fusion devices. No relation to EFRC research*	
Person-Months Per Year Committed to Project: Sum	1 Pers. Months
Investigator: James Blanchard	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **IRP on Fuel Aging in Storage and Transportation**	
Source of Support:	DOE
Location of Project:	UW/Texas A&M
Total Award Period:	2011-2014
Annual Award Amount:	$287,000 (UW)
Annual Award Amount to PI's Research:	$10k
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *Sensor development for dry cask storage. No connection to EFRC research.*	
Person-Months Per Year Committed to Project: Sumr	0.3 Pers. Months

James (Jake) Blanchard
University of Wisconsin-Madison (continued)

Investigator: James Blanchard	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Development of Advanced High Uranium Density Fuels for LWRs**	
Source of Support: DOE	
Location of Project: UW	
Annual Award Amount:	$250,000
Annual Award Amount to PI's Research:	$0
Total Award Period:	2011-2015
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *Study irradiation stability of composite fuels at intermediate and high temperatures.*	
Person-Months Per Year Committed to Project: Specify: Cal., Acad., or Sumr:	0 Pers. Months

Jian Gan
Idaho National Laboratory

DROPPED:

- Fiber Optical Sensor for In-pile Temperature Monitoring
- Coating and Liner Development for Fuel/Cladding Chemical Interaction (FCCI) Mitigation.

CHANGES:

Investigator: Jian Gan (Dennis Keiser; Dan Wachs) CHANGE	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Reduced Enrichment for Research and Test Reactors (RERTR) Fuel Development Program**	
Source of Support:	DOE/NNSA
Location of Project:	Idaho National Laboratory
Total Award Amount:	$~18M/year
Total Award Amount to PI's Research:	$250K
Total Award Period Covered:	FY2013
Describe Research Including Synergies and/or Overlaps with EFRC Award: *My RERTR work mainly focus on TEM characterization of irradiated U-Mo based nuclear fuels for research and test reactors. It also includes the ion irradiation study of depleted uranium alloys. There is no overlap with EFRC CMSNF work. The synergy is on the irradiated microstructure in nuclear fuel due to fission.*	
Person-Months Per Year Committed to Project: Specify: Cal., Acad., or Sumr:	6 Pers. Months; Cal.
Investigator: Jian Gan CHANGE	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **ATF alloy and Thin-wall cladding weld R&D**	
Source of Support: DOE/NE	
Location of Project: Idaho National Laboratory	
Total Award Amount:	$600K
Total Award Amount to PI's Research:	$600K
Total Award Period Covered:	FY 2013
Describe Research Including Synergies and/or Overlaps with EFRC Award: *This research project is to develop weld technique for Fe-based thin-wall cladding for accident tolerant fuel for LWR. There is no overlap with EFRC CMSNF work.*	
Person-Months Per Year Committed to Project: Cal	3 Pers. Months

Jian Gan
Idaho National Laboratory (continued)

Investigator: Jian Gan CHANGE	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Nano/micro scale AFM-based thermal conductivity measurement and Modeling for Oxide fuel**	
Source of Support: DOE/NE/LDRD	
Location of Project: Idaho National Lab	
Total Award Amount:	$ 750K
Total Award Amount to PI's Research:	$60K/yr
Total Award Period Covered:	FY 13 - 15
Describe Research Including Synergies and/or Overlaps with EFRC Award: *This project is to develop the nano/micro scale AFM-based thermal conductivity measurement for CeO_2 (a surrogate for UO_2). It is fundamentally relevant to this EFRC work but takes different approach.*	
Person-Months Per Year Committed to Project: Specify: Cal., Acad., or Sumr:	1 Pers. Months; Cal.
Investigator: Jian Gan (James Stubbins; Michell Barsoum) CHANGE	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Advanced Test Reactor – National Scientific User Facility (ATR-NSUF) project with University of Illinois, and The Drexel University)**	
Source of Support: DOE	
Location of Project: Idaho National Laboratory	
Total Award Amount:	N/A
Total Award Amount to PI's Research:	$25K
Total Award Period Covered:	FY 2013
Describe Research Including Synergies and/or Overlaps with EFRC Award: *This project is to conduct post-irradiation examination on TEM characterization of irradiated metals and ceramics. There is no overlap with EFRC work.*	
Person-Months Per Year Committed to Project: Cal	0.5 Pers. Months

Jianliang Lin
Colorado School of Mines

DROPPED:

- Evaluation of Metal Target for Producing Conductive Films Used in Device Applications
- Coating Trials and Characterization for ACSEL Industrial Collaborators
- Modulated Pulsed Power Magnetron Sputtering of Multifunctional Tribological Coatings for Non-ferrous Structural Alloys
- Super Dense and Thick W-based Coating Systems Deposited by the Novel Modulated Pulsed Power Magnetron Sputtering Techniques for Fusion Applications
- Establishing Links Between the Plasma Properties, Reactive Species Behavior and Process Stability During Arc Free Deep Oscillation High-power Pulsed Magnetron Sputtering
- Hydride Microspheres Glasses Particles in Solid Moderator Reactor Concept RD&D (MS-RC1).

ADDITIONS:

Investigator: Jianliang Lin	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Lubricant Free Die Coatings**	
Source of Support:: Defense Logistics Agency	
Location of Project: Colorado School of Mines	
Total Award Amount:	$300K/5 years
Annual Award Amount to PI's Research:	$60k
Total Award Period:	5/30/12 – 5/30/17
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *Nano-composite multilayer coating systems for the high pressure die casting dies There are no synergies and/or overlaps with this proposal.*	
Person-Months Per Year Committed to Project: Cal	3 Pers. Months
Investigator: Jianliang Lin	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Investigation of the thermal diffusion behavior in Cu-refractory metal thin films**	
Source of Support: H.C.Starck	
Location of Project: Colorado School of Mines	
Total Award Amount:	$270K/3 years
Annual Award Amount to PI's Research:	$90k
Total Award Period:	7/1/12 – 6/30/15
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: None	
Person-Months Per Year Committed to Project: Sum	3 Pers. Months

Michele Manuel
University of Florida

DROPPED:

- High-temperature Thermal Analyzer and EBSD System in a FIB for Studying Advanced Fuels, Aged Fuel in Dry Storage, and Core Structural Materials
- NSF EFRI: BioFlex Ingestible Electronic Capsules for Monitoring and Diagnostics
- Integrated Computational Materials Science and Engineering and Structural Materials
- Synthesis of Prototype Magnesium Alloys
- Novel Materials Design and Characterization for Validation and Verification of Advanced Computational Models
- Magnetic Field Processing: Enabling Customized Lightweight Nano Composites and Cast Materials for Transportation and Energy Transmission Applications
- Advanced Materials Design and Processing Development.

ADDITIONS:

Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Self-Repair and Damage Mitigation of Metallic Structures**	
Source of Support: NASA	
Location of Project: University of Florida	
Annual Award Amount:	$200,000
Annual Award Amount to PI's Research:	$200,000
Total Award Period:	09/15/12-09/14/15
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *The central goal of this study is to design a self-healing composite material that can repair itself in response to structural damage. There are no synergies with the EFRC award.*	
Person-Months Per Year Committed to Project: Sum	1.0 Pers. Months
Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Thermo-mechanical Evaluation of Self-healing Metallic Structures for Aerospace Vehicles Utilizing Memory Alloys**	
Source of Support: NASA	
Location of Project: University of Florida	
Annual Award Amount:	$65,000
Annual Award Amount to PI's Research:	$65,000
Total Award Period:	08/01/12-09/17/13
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *The objective of this research project is to use liquid-assisted healing of reinforced metal matrix composites for structural applications. Of particular interest is the understanding of the fatigue behavior of advanced shape memory alloy reinforced composites. There are no synergies with the EFRC award.*	
Person-Months Per Year Committed to Project: Sum	0.75 Pers. Months

Michele Manuel
University of Florida (continued)

Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Crack Closure and Intrinsic Toughening Mechanisms for Shape Memory Embedded Composites**	
Source of Support: NASA	
Location of Project: University of Florida	
Annual Award Amount:	$24,998
Annual Award Amount to PI's Research:	$24,998
Total Award Period:	10/15/12-10/14/13
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *This project seeks to understand the role of phase transformation in shape memory alloy composites on intrinsic and extrinsic toughening mechanisms. There are no synergies with the EFRC award*.	
Person-Months Per Year Committed to Project: Pers. Months; Specify: Cal., Acad., or Sumr:	0.0 Pers. Months
Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support: Pending	
Project/Proposal Title and grant number, if appropriate: **Joining of Aluminum MMCs to Aluminum Alloys**	
Source of Support: DSC Materials	
Location of Project: University of Florida	
Annual Award Amount:	$36,979
Annual Award Amount to PI's Research:	$36,979
Total Award Period:	06/01/13-02/28/14
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *The proposed work involves the mechanical and microstructural characterization of joined dispersion strengthened aluminum (Al) alloys with conventional Al alloys. DSC Materials will produce a 2 piece piston design using their proprietary DSC A356 Al alloy to a standard Al based piston alloy for pin bosses and skirt. Joining technologies could include friction welding, electron beam welding and diffusion bonding or brazing. There are no synergies with the EFRC award.*	
Person-Months Per Year Committed to Project: Sum	0.5 Pers. Months

Michele Manuel
University of Florida (continued)

Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support: Pending	
Project/Proposal Title and grant number, if appropriate: **Sub-Micron Ceramic Particulate Reinforced Materials**	
Source of Support: DSC Materials	
Location of Project: University of Florida	
Annual Award Amount:	$36,979
Annual Award Amount to PI's Research:	$36,979
Total Award Period:	06/01/13-02/28/14
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *The proposed work involves the mechanical and microstructural characterization of DSC™ AZ91 magnesium (Mg) alloy produced by DSC Materials. These materials are optimized and design to display excellent mechanical properties at room and elevated temperatures, while being machineable. There are no synergies with the EFRC award.*	
Person-Months Per Year Committed to Project: Sum	0.5 Pers. Months

Jianguo Yu
Idaho National Laboratory

ADDITIONS:

Investigator: Jiangou Yu	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Modeling Guided Development of Nanostructured High Energy Electrode Materials for Li-Ion Batteries**	
Source of Support: INL LDRD	
Location of Project: Idaho National Laboratory	
Annual Award Amount:	$313.9 K
Annual Award Amount to PI's Research:	$80K
Total Award Period:	02/2012-09/2014
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *No direct overlap.*	
Person-Months Per Year Committed to Project: Cal	3 Pers. Months
Investigator: Jiangou Yu	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Fickian and Thermal Diffusion in Nuclear Materials From Linear Response Theory and Multiscale Calculations**	
Source of Support: INL LDRD	
Location of Project: Idaho National Laboratory	
Annual Award Amount:	$55K
Annual Award Amount to PI's Research:	$5K
Total Award Period:	10/01/2012-07/31/2013
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: N*o direct overlap.*	
Person-Months Per Year Committed to Project: Cal	.2 Pers. Months
Investigator: Jiangou Yu	Other Agencies to which this proposal has been/will be submitted:
Support : Pending	
Project/Proposal Title and grant number, if appropriate: **Microstructural and Microchemical Evolution of Interfaces in Nanostructured Materials**	
Source of Support: BES DOE	
Location of Project: Idaho National Laboratory	
Annual Award Amount:	$500K
Annual Award Amount to PI's Research:	$500K
Total Award Period:	10/01/2013-09/30/2018
Describe Research Including Synergies and Delineate with Respect to the EFRC Award: *No direct overlap. The first-principles based multiscale methods developed in this project may benefit the Energy Frontier Research Center.*	
Person-Months Per Year Committed to Project: Cal	7 Pers. Months

LETTER OF SUPPORT

National Research Council Canada
Conseil national de recherches Canada

Canadian Neutron Beam Centre
Le centre canadien de faisceaux de neutrons

NRC · CNRC

Stn. 18 Building 459
Chalk River Laboratories
Chalk River
Ontario
K0J 1J0

April 14, 2013

To: Dr. Todd R. Allen, Director,
Center for Materials Science of Nuclear Fuel
Idaho Nuclear Laboratory
2525 Fremont Avenue
Idaho Falls, ID 83415

From: Dr. William J.L. Buyers, O.C., D.Sc. (Hon.), F.R.S.C., F.Inst.P.

Letter of Support for EFRC Research into Thermal Conductivity of UO_2

As a retired Principal Research Officer of the National Research Council of Canada (NRC), I am currently affiliated with the NRC Canadian Neutron Beam Centre, located at Chalk River Laboratories, where I am a Guest Scientist. I contribute my knowledge and know-how to an NRC program of experimental and theoretical research on the basic properties of materials. This research has no intended military or commercial applications.

To support NRC's research program in the basic properties of materials, I regularly travel to perform research in other countries. Such activity is an open collaboration between researchers, addressing the scientific goals of NRC as well as the institutions I visit, with no commercial implications. I am independently and fully funded by a pension from the Government of Canada. I receive no salary from any organization or laboratory in the United States.

The project on thermal conductivity of oxide fuels is of considerable interest to my personal research program. It is also of interest to NRC since the first measurements of phonon energies in uranium dioxide were carried out with neutron inelastic scattering at Chalk River Laboratories as early as 1965. Despite this pioneering start, the transport of heat has never been measured in a microscopic way for each phonon, the quantum of lattice vibration. Development of this new quantum method is what I and my Oak Ridge collaborators have brought to the achievement of the EFRC goal. The EFRC mission requires specific knowledge of the technology of extracting the phonon lifetime from very high resolution neutron scattering measurements. I have

Canada

considerable experience dating from the sixties in experimental phonon methods to determine anharmonic phonon collisions.

I have loaned a high-quality, massive single crystal of depleted uranium dioxide to my Oak Ridge collaborators for the work of the EFRC. In this way we were able to make an early start to a key part of the EFRC program focused on how thermal transport is limited by anharmonic phonon collisions. Definitive results, now published in the high impact journal Physical Review Letters, have enabled a direct comparison with ambitious but untested theoretical approaches. Our findings have revealed important weaknesses in current theory, and have pointed the way in which the theory should be improved. Our results provide the first comprehensive benchmark against which future theories maybe tested.

The EFRC program on thermal conductivity was not only needed for a thorough understanding of energy production with its broad benefits, but also presented a challenge requiring development of a new method. The research is of personal interest to me, and I have excellent collaborators to work with at MST, HFIR and SNS at ORNL. I have travelled to Oak Ridge National Laboratory several times since the EFRC began in order to participate in experiments at the HFIR and the SNS. I intend to continue my active participation as required.

I require no salary or fee, but expect to receive appropriate recognition of my scientific contribution in disseminated documents.

W. J. L. Buyers

William J.L. Buyers, O.C., D.Sc. (Hon), F.R.S.C., F.Inst.P.