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Energy Frontier Research Center, Center for Materials Science of Nuclear Fuels

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Idaho National Laboratory
Center for Materials and Science of Nuclear Fuel
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Budget:

FY-09	FY-10	FY-11	FY-12	FY-13	Total
2,000K	2,000K	2,000K	2,000K	2,000K	10,000K

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Energy Frontier Research Center, Center for Materials Science of Nuclear Fuels

1. PARTICIPANTS AND BUDGET SUMMARY

Institutions and their lead investigators participating in the Energy Frontier Research Center, Center for Materials Science for Nuclear Fuel (hereafter referred to as the Center) are:

- Idaho National Laboratory/University of Wisconsin: Professor Todd Allen.
- Colorado School of Mines: Professor John Moore and Research Assistant Professor Jianling Lin
- Florida State University: Professor Anter El-Azab
- Idaho National Laboratory: Dr. David Hurley, Dr. Jian Gan, Dr. Marat Khafizov, Dr. Xianming Bai, and Dr. Jianguo Yu
- Oak Ridge National Laboratory: Dr. Ben Larson and Dr. Judy Pang
- University of Florida: Professor Simon Phillpot and Professor Michele Manuel
- Argonne National Laboratory: Dr. Dieter Wolf

Five-year funding by participating institution is listed and totaled in Table 1-1.

Table 1-1. Summary of 5-year funding by participating institutions.

Lead Institution	FY-09 Funding (K)	FY-10 Funding (K)	FY-11 Funding (K)	FY-12 Funding (K)	FY-13 Funding (K)	Total Funding (5 Years)
Idaho National Laboratory	1,000	700	880	880	880	4,340
Oak Ridge National Laboratory	300	300	300	300	300	1,500
Argonne National Laboratory	0	280	0	0	0	280
University of Wisconsin	150	170	270	270	270	1,130
University of Florida	200	200	200	200	200	1,000
Florida State University	200	200	200	200	200	1,000
Colorado School of Mines	150	150	150	150	150	750
Total Funding	2,000	2,000	2,000	2,000	2,000	10,000

2. CENTER VISION AND MANAGEMENT

2.1 Vision

The Center will develop a first-principles-based understanding of the impact of complex defect structures on thermal transport in irradiated nuclear fuel, specifically UO_2. This will be accomplished by integrating the physics of thermal transport in crystalline solids with microstructure science under irradiation.

The Center will develop an experimentally validated multiscale modeling framework and computational capability for the predictive understanding of the microstructure dynamics and its impact on thermal transport in nuclear fuel under irradiation with application to UO_2.

2.2 Objectives

The Center will enrich the scientific basis of thermal transport in the ceramic materials (UO_2) used as nuclear fuel, based on an understanding of phonon transport through the unique microstructures formed under radiation at high temperature. Although there is significant interaction among the group members across both research areas, the objectives can be broadly classified as thermal transport and microstructure science under irradiation.

The research objective of the thermal transport thrust area is to develop a computational model for thermal transport in irradiated materials with complex defect structures and to conduct lattice dynamics and conductivity measurements targeting the impact of defects on thermal transport.

The research objective of the microstructure science under irradiation thrust area is to develop predictive capabilities for defects and microstructure evolution in irradiated fuels and to conduct irradiation and microstructure characterization experiments to understand defect and microstructure processes in UO_2 and surrogate systems.

The stated objectives are ultimate goals for the Center and are the basis for an ambitious long-term research program. Within this context, the Center is answering a subset of key scientific questions, described in Section 3.3 that will form a foundation for attaining these broader objectives.

2.3 Management Structure

The Center brings together an internationally renowned, multi-institutional team of experimentalists (Idaho National Laboratory, Oak Ridge National Laboratory, Colorado School of Mines, University of Florida, and the University of Wisconsin) and computational materials theorists (Argonne National Laboratory, Idaho National Laboratory, University of Florida, and Florida State University). The Center, led by Director Todd Allen, is organized around the two closely related research thrust areas: thermal transport, and microstructure science under irradiation. Both internal and external advisory structures are used for setting priorities. The Center's management vision is to encourage discovery through collaboration, enhance capability through partnerships, develop staff through educational efforts, and provide support through ties to the best infrastructure. The Center had a major leadership change approximately one year into the project as the original Director, Dr. Dieter Wolf, departed Idaho National Laboratory for Argonne National Laboratory. The current Director, Dr. Todd Allen, who was already on the leadership team, assumed leadership of the Center. This transition had little overall effect on the Center management structure or progress as outlined below. Dr. Wolf remained with the team as a technical contributor through year 2 of the project. His technical role is now assigned to newly hired staff at INL.

As shown in *Figure 2-1*, an internal management structure has been established to guide and integrate each theme and to ensure the integral connectivity of the two themes. Two researchers, one with modeling expertise and the other with experimental expertise, share the responsibility of integrating the intellectual inputs from across the Center for each theme and to assist in ensuring information is shared across themes. An independent integration team, headed by Ben Larson and Todd Allen, was also established to assist in properly integrating the scientific results across the entire team. Anter El-Azab and Todd Allen will coordinate efforts to ensure the Center optimizes the identification of and interaction with external partners. Finally, because of the importance of the educational mission of the Center, a fifth leadership team was established to provide proper focus on the educational mission. Each of the leadership teams is tasked with guaranteeing that integration and validation are ingrained in every aspect of the Center.

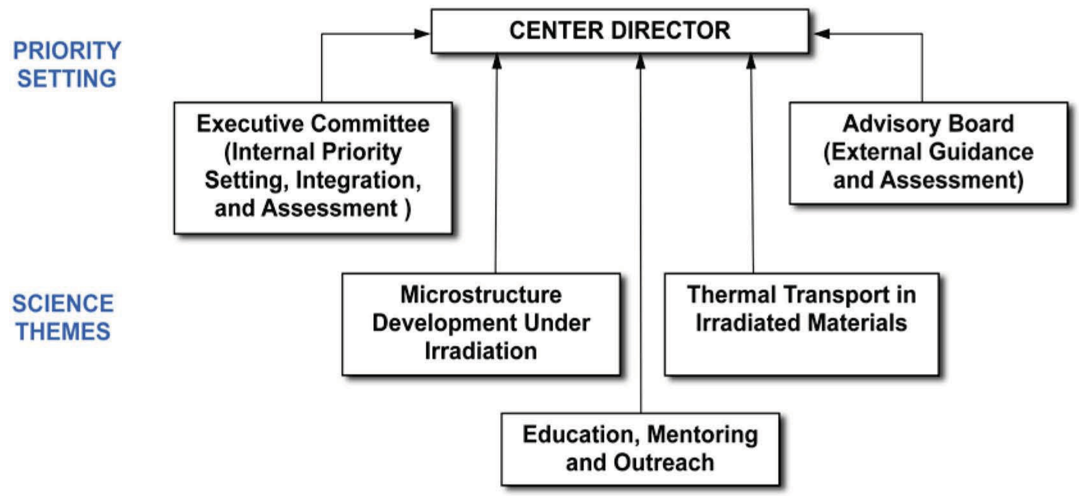


Figure 2-1. Internal management structure of the Center.

2.4 Advisory Committee

The Center's external advisory board conducts a formal assessment and provides an independent assessment on an annual basis. This independent advice from international experts is critical to the success of the Center. The following individuals serve on this committee: Dr. Vincenzo Rondinella (Karlsruhe Institute of Transuranium Elements); Dr. Marius Stan (Argonne National Laboratory); Dr. William Weber (University of Tennessee); Professor Sidney Yip (Massachusetts Institute of Technology); and Dr. Rory Kennedy (Idaho National Laboratory). These experts were chosen because of their modeling and experimental expertise in the areas of fuel performance.

2.5 Decision-making Processes

An executive committee has been established to provide integration, validation, and policy in areas of priority setting, resource allocation, encouragement of high-risk and relevant research, and the means of achieving an integrated Energy Frontier Research Center with synergism among investigators. The executive committee is chaired by Director, Dr. Todd Allen, with Dr. Dave Hurley as experimental lead and Professor Anter El-Azab as computational lead as members.

3. DESCRIPTION OF RESEARCH SUBTASKS/SUBPROJECTS

3.1 Energy Frontier Research Center Research Objectives

Research at the Center is based on the premise that thermal transport in crystalline UO_2 is a phonon-mediated process that is influenced by the scattering mechanisms associated with the defect disorder and microstructural changes caused by irradiation. The Center's research plan has consequently been designed so that the thermal transport investigation drives all the research tasks. The thermal transport problem is tackled in steps matching the levels of complexity of the involved phonon transport process. In this regard, three levels of investigation have been considered. At the most basic level, a reference UO_2 material (high-purity, stoichiometric UO_2 with minimal intrinsic defects, referred to as pure UO_2 from this point forward) is considered and all modeling and experimental tools are used to understand the physics of thermal transport within this material as a function of temperature, from room temperature to ~1,200 K. Next, UO_2 with an impurity representative of a solid fission product (e.g., cerium) or noble gas is considered and the same thermal transport investigations are repeated. At this level, the complexity of irradiation-induced defect clusters or large microstructure features is avoided. Finally, the investigation of thermal transport in an irradiated material is considered.

There is a significant difference between the defect and microstructure state of a material under irradiation and a material that has been irradiated but taken out of the irradiation field. A material under irradiation has a super saturation of intrinsic point defects and microstructure features introduced by irradiation. When irradiation is turned off, the material is left with equilibrium point defects plus the permanent disorder and microstructure that forms during irradiation but has not been annealed out. From a thermal transport point of view, there is also a major difference between the two materials; that is, an in situ thermal transport investigation in a fuel must account for the process of heat deposition in that fuel. The theoretical and experimental tools needed to probe the in situ thermal transport at a fundamental level may not be available at the present time. Based on these considerations, the current 5-year phase of the Center will focus on the ex situ thermal transport in an irradiated fuel, e.g, on the theoretical and experimental understanding of thermal transport in a material that was irradiated in the past.

Within the described context of understanding thermal transport in an irradiated microstructure, the long-term research goals of the Center are to:

- Develop an understanding of the impact of complex defect structures on thermal transport in irradiated oxide fuel from first principles
- Achieve the above for the case of irradiation induced defects in oxide fuel, which will also achieve a first-principles-based understanding of the effects of irradiation on stoichiometry and microstructure in oxide fuel
- By reaching the above two goals through a program of combined theory and experiment, the center will also establish a new research direction that integrates the physics of thermal transport and the physics of defect and microstructure in irradiated oxide fuel.

The Center brings together an internationally renowned, multi-institutional team of (1) experimentalists at Idaho National Laboratory, Oak Ridge National Laboratory, Colorado School of Mines, University of Florida, and University of Wisconsin, and (2) computational materials theorists at Argonne National Laboratory, Idaho National Laboratory, University of Florida, and Florida State University to focus on understanding microstructure science under irradiation and its effects on thermal transport.

The framework of nonlinear dynamics of irradiation-driven materials will lead to an atomistically-informed generalized mesoscale phase-field model for the irradiation-induced microstructure evolution, which will furnish the defect state impacting thermal transport. This approach will capitalize on the team's demonstrated strength in theoretical and computational modeling of materials at all scales. In close synergy with the modeling effort, the experimental team will perform advanced microstructure and thermal-transport studies on ceramic fuel materials using an array of state-of-the-art characterization techniques. They will also use the unique experimental capabilities of U.S. Department of Energy (DOE) user facilities, including the Advanced Test Reactor, Spallation Neutron Source, High Flux Isotope Reactor, and Advanced Photon Source.

3.2 Background

The degradation of thermomechanical behavior results from the cumulative, intricately coupled effects of fission-damage processes, high temperatures, and large thermal gradients. Yet, apart from large empirical databases, a fundamental predictive science basis that connects structure across the relevant length and time scales with fuel behavior and thermal transport does not currently exist. To elucidate the underlying point-defect and microstructural mechanisms controlling the degradation of thermal and mechanical behavior, the Center is developing a predictive computational framework based on the nonlinear dynamical theory of driven material systems and combining multiscale models of defect and microstructure physics with closely correlated experimentation on commensurate length and time scales. This unique combination of theory, computation, and experimentation will ultimately capture the complex interplay between the fission-induced defects and emerging microstructure with preexisting grain structure and their impact on phonon lifetimes, thus enabling the prediction of the impact of microstructure evolution on thermal transport in nuclear fuel. The comprehensive theoretical and computational framework being developed under this program probes the same length- and time-scale domains accessible by the experiments used for its validation. Once validated, this framework will enable the prediction of thermal-transport behavior on both mesoscopic and macroscopic length and time scales, the ultimate goal being time-to-failure and lifetime prediction for the nuclear fuel.

The 2006 basic research needs report, "Basic Research Needs for Advanced Nuclear Energy Systems," noted that one of the grand challenges in developing future advanced nuclear energy systems is "Developing a first-principles multiscale description of material properties in complex materials under extreme conditions." Specifically, the report notes:

> *The current status of microstructure simulation methodology is that models of materials behavior used for design, certification, and licensing of structural and fuel components ignore the microstructure entirely and rely instead on phenomenological description with parameters adjusted to interpolate between available experimental data points. The current interest in nuclear energy materials and the expected availability of massively parallel computing make it feasible to eliminate this disconnect between the microstructure and physical behavior.*
>
> *Modeling of microstructural evolution under irradiation now relies on mean-field approaches (master equations) and rate theory that largely ignore fluctuations and correlations in the spatial and temporal distributions of microstructural elements (Surh et al. 2005). Attempts are being made to replace these approaches with detailed atomistic descriptions using kinetic Monte Carlo methods. So far, however, such attempts are limited to elemental pure metals, soft recoil spectra, small spatial scales, short times, embarrassingly small irradiation doses, and low temperatures. The first challenge is to provide an accurate description of the multiple and complex unit mechanisms of microstructural response. For example, microstructural evolution in irradiated materials results from numerous thermally activated events, for example, dislocation interaction with radiation defects and precipitates or dislocation climb in high-temperature creep. However, much current modeling is performed close to or above the thermal threshold, for example, under unrealistically high*

stress in the molecular dynamics simulations (Bacon et al. 2006). Furthermore, the chemical degrees of freedom (e.g., solute diffusion, segregation) are usually decoupled from the mechanical ones (e.g., dislocation dynamics).

Responding to these challenges, specifically in relation to nuclear fuel, is the focus of the Center. The objectives for the Center listed in Section 3.1 are aimed at meeting these grand challenges, establishing the ultimate direction for the Center, and providing the basis for an ambitious long-term research program. The short-term objectives of the Center are to address a set of key scientific questions that are foundational in meeting these grand objectives, specifically to understand:

- how anharmonicity determines phonon dispersion, phonon lifetimes, and thermal transport as a function of temperature in pure single crystal UO_2,
- how grain boundaries, dislocations, and interfaces, affect thermal transport,
- what types of defect clusters are produced in UO_2 by irradiation and what are the energies and kinetic paths for their formation,
- what is the impact of temperature and local oxygen environment on the stoichiometry of UO_2, and
- how do voids form and grow in irradiated UO_2 and what is the effect of free surfaces on defect migration?

Addressing each question requires the formation of a team of experimental and computational experts from across the country to advance the understanding of each of these key scientific questions. In the initial phases of the Center's studies, in some cases the surrogate CeO_2 was examined while the Center established the ability to examine UO_2 across all the partners.

While a fully validated predictive capability of the thermal-transport behavior is beyond the scope of this initial project, the Center is establishing important scientific foundations for creating that framework. The current research plan for the Center is presented in the next two sections in the form of the set of science questions being pursued. These questions are logically organized to build upon each other in ways that will lead to answering the ultimate question of this center—*what is the impact of irradiation-induced defect disorder and microstructure on thermal transport in UO_2*. The science questions have been grouped into two categories, the first is related to thermal transport investigations and the second focuses on the related defects and microstructure issues. The relationship between the two areas is highlighted as the status of research in both areas is discussed. Each science question is presented in four basic parts. What is the relevant work of others upon which the team is advancing the science? Which team members support addressing the specific science question? What specific tasks are being conducted? What is the question once the specific science question is answered?

3.3 Research Subtasks

3.3.1 Thermal Transport in Irradiated Materials

The ultimate goal of the thermal transport thrust is to develop a fundamental and unified understanding of how anharmonicity, off-stoichiometry, point defects (both those intrinsic to polycrystalline UO_2 fuel, and those arising as fission products), and microstructure impact thermal transport in UO_2 and its surrogate CeO_2. This goal requires the close integration of theory, modeling, and simulation at the atomistic and mesoscopic levels. Atomic-level simulations are used to both mechanistically and quantitatively elucidate the nature of phonon transport. The numerical solution of the Boltzmann transport equation enables the macroscopic simulation of thermal transport through experimentally measured microstructures and defect distributions. The experimental effort involves reactor and spallation-source neutron scattering measurements of phonon dispersion and lifetime as well as laser-based measurements of thermal conductivity. To advance the fundamental science of phonon-mediated heat transport, the emphasis here is placed on designing experiments that correspond in a one-to-one fashion to the modeling and simulation techniques used. The work performed under this thrust is framed by defining fundamental scientific questions that directly address select key elements of our stated ultimate science driver, to understand all elements of microstructure on thermal transport.

3.3.1.1 Science Question 1

What is the impact of anharmonicity on phonon dispersion, phonon lifetimes, and thermal transport as a function of temperature in pure single crystal UO_2?

Background

The dominant determinant of thermal conductivity at elevated temperatures in electrical insulators is phonon-phonon scattering arising from anharmonicity of the atomic interactions. Peierls[1], in the 1920s, developed a fundamental relation of how lattice thermal conductivity depends on anharmonic phonon-phonon scattering by expressing thermal conductivity as a function of phonon lifetimes and velocities through the Boltzmann transport equation. Klemens, whose work made considerable advances in the 1950s,[2] still forms the theoretical backdrop for all experimental and theoretical analyses. However, the prediction of how anharmonicity limits thermal transport is still largely absent from present understanding of thermal transport via phonons. To fully characterize this anharmonicity, it is necessary to determine the full phonon spectrum of UO_2 and characterize the lifetimes of all phonons. To date, no such full characterization has been accomplished for UO_2. The phonon dispersion curves in UO_2 at room temperature were determined by Dolling[3] in 1965, and a few phonon measurements at T >1,600K were made by Clausen[4, 5] in the 1980s. In general, however, phonon lifetime and their wave vector (q) distributions over crystal momentum and phonon branch have not been measured. Indeed, the lack of reliable predictions for phonon lifetimes is a major obstacle in thermal conductivity simulations and limits advancements in theory. A number of recent works attempt to solve the Boltzmann transport equation for phonons to describe thermal transport at the mesoscale. For example, a Monte Carlo method for generating lattice thermal conductivities in the diffusive regime was presented by Peterson[6] who used a linear Debye approximation to the phonon dispersion. Mazumder[7] extended this work by including the dispersion relations for the acoustic phonon branches in silicon and germanium crystals. Lacroix et al.[8] further improved on that by ensuring that the simulation scheme conserves energy, albeit in a statistical sense.

Research Approach and Results

Oak Ridge National Laboratory, University of Florida and Florida State University have made significant progress in using inelastic neutron scattering to measure the phonon dispersion curves and lifetimes, in developing atomic-level lattice dynamics models for the phonon properties, and in developing a mesoscale Monte Carlo solution of the Boltzmann transport equation for phonons.

Inelastic Neutron Scattering Measurements

Although anharmonic interactions are responsible for two very important materials properties—thermal expansion and finite thermal conductivity—anharmonicity has typically not been well characterized. The unique capabilities of the HB3 Triple axis spectrometer at the High Flux Isotope Reactor at Oak Ridge National Laboratory have been used to determine the harmonic and anharmonic phonon properties of UO_2 using an 80 gram crystal provided by WJL Buyers, Chalk River Nuclear Laboratories; and a 40 gm crystal provided by M. Paffett, Los Alamos National Laboratory. Inelastic neutron scattering measurements at ambient temperature and at a typical fuel operating temperature of 1,200 K show that the phonon lifetime in UO_2 has rich wave vector and energy dependencies in that (1) it depends strongly on the phonon wave vector, (2) it does not scale simply with energy within phonon branches, and (3) it does not scale uniformly with temperature. These findings run counter to the assumptions of many early theories of conductivity dating from the 1970s.

By combining the phonon group velocities and lifetimes to get the mean free path, these measurements have made it possible to determine the contribution of individual phonon branches to the overall thermal conductivity at high temperatures (1,200 K). Surprisingly, the transverse acoustic phonons and the high-velocity longitudinal optical phonons were found to transport heat as strongly as the usually dominant longitudinal acoustic phonons. This understanding is contrary to conventional expectations based on the fact that velocities of longitudinal acoustic phonon are approximately twice those of transverse acoustic modes; see *Figure 3-1* (a). This result directly refutes recent first-principles simulations based on quasi-harmonic Grüneisen analysis, which predicted that ~90% of the heat is conducted by the longitudinal acoustic phonons at high temperature.[9]

By summing the measured microscopic heat conductivity over all wave vectors and branches, the experiment provides an estimate of the total heat conductivity, which agrees well with the measured macroscopic conductivity at operating temperature. Most importantly it can already be concluded from the neutron scattering experiments that most of the conductivity loss between 300 and 1,200 K arises from the limitation of lifetime and mean free path by anharmonic processes.

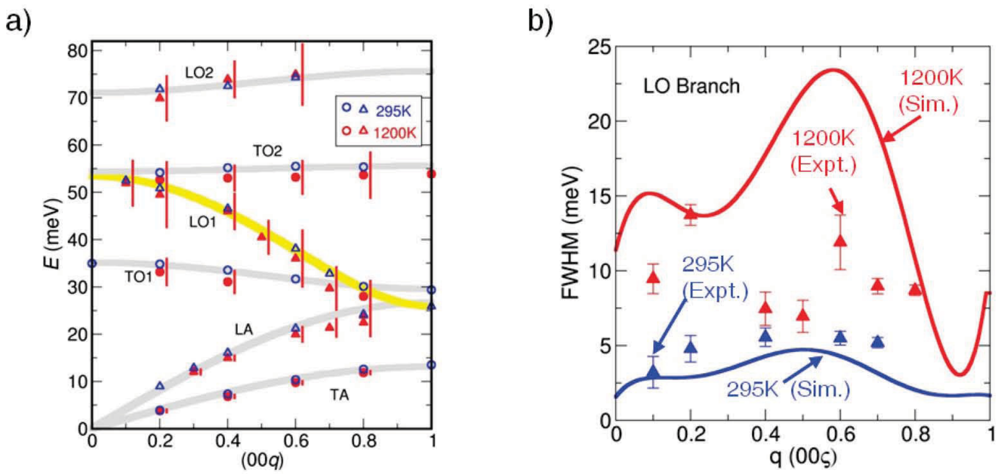


Figure 3-1. (a) Measured dispersion curves for UO_2 at 295 and 1,200 K. Circles (triangles) represent transverse (longitudinal) phonons. Blue (red) symbols denote measurements at 295 K (1,200 K). The red vertical lines are the corresponding measured linewidths at 1200K. The lines through individual phonon branches are guides to the eye and the highlighted line denotes the high-velocity longitudinal optical phonons. (b) Linewidths for longitudinal optical phonons in UO_2, highlighted in yellow in panel a: measurements (blue and red symbols), and simulations (blue and red lines).

Lattice Dynamics Modeling

To understand the measured results in *Figure 3-1* from a theoretical perspective, atomic-level lattice dynamics calculations have been performed for an ideal UO_2 crystal. Within this framework,[10] phonon dispersion, linewidths and overall thermal conductivity as a function of temperature were computed starting from the fundamental interatomic interactions. In particular, the second derivatives of the total energy of the solid with respect to ionic positions yield the phonon frequencies and group velocities as a function of a wave vector. The third derivatives of the interatomic interactions are responsible for the strength of the three-phonon interactions, the dominant phonon-phonon interaction process. The summation over all possible three-phonon processes produces a probability of scattering event for a particular phonon via anharmonic interaxctions and, therefore, determines its lifetime in an ideal crystal. This phonon lifetime can be directly compared with the results of the phonon linewidth measurements performed at Oak Ridge National Laboratory.

The lattice dynamics method requires a reliable interatomic potential to compute derivatives of the total energy of the crystal. Nearly 30 classical potentials are available in the literature for UO_2. Systematic assessments of the quality of these potentials as applied to the thermal transport properties have shown, surprisingly, that only a few of these potentials are capable of satisfactorily describing the phonon frequencies. The calculations of the phonon lifetimes,[11] therefore, use the potential developed by Catlow,[12] which best reproduces the phonon frequencies observed in the experiment.

Comparisons between the inelastic neutron scattering measured and the lattice dynamics calculated phonon linewidths in *Figure 3-1* (b) for the high-velocity LO_1 branch phonons, show strong non-monotonic variations with wave vector in both the measurements and the simulations, especially at high temperature. While the lattice dynamics simulations are in substantial agreement with the measurements for all wave vectors (q) at 295 K, the predicted phonon lifetimes (inverse linewidths) differ by as much as a factor of two from the measurements in the mid-q wave vector region at 1,200 K. In spite of these differences, the calculations are quantitatively consistent with the experiment in that they also show that optical modes make a significant contribution to the thermal conductivity at high temperature. The differences between theory and experiment are most likely the result of the very limited description of the anharmonic interactions by the classical potentials. Accordingly, more robust and reliable calculations based on determining the phonon properties from electronic-structure calculations at the level of density-functional theory are underway.

To provide a more robust description to the interatomic interactions in UO_2, a UO_2 potential is being developed within the framework of Charge Optimized Many Body potentials.[13, 14] Because of the inclusion of dynamical charge optimization, this is a very successful framework that can describe the properties of the complex systems consisting of multiple different systems of different bonding types. This framework will also allow the description of soluble and insoluble fission products. First principles calculations of a range of crystal structures are used for the database, to which parameters of the model are fitted. The development of such potentials requires, as a first step, a good description of the interactions in the metal. Therefore, an interatomic potential for uranium metal has been successfully developed as the first step towards a comprehensive description of the oxide and fission products. The ground state, α-U, is a relatively complex, low-symmetry structure that until now was not captured by any interatomic potential. Mechanical properties of the α-U as predicted by the potential are in excellent agreement with the experimental data. Although somewhat peripheral to the main thrust of the center, this is a significant accomplishment since there are no interatomic descriptions for α-U in the literature.

Boltzmann Transport Equation Modeling

The molecular dynamics and lattice dynamics methods can be used to determine the effects of individual microstructural elements in small volumes of material in which the defect density is significantly higher than in experiment. However, to determine the thermal transport properties of larger materials volumes containing a number of different types of defects at experimentally accessible concentrations, a larger length-scale approach is required. A Monte Carlo scheme for the solution of the Boltzmann transport equation is used to simulate phonon transport in UO_2 at the mesoscale, where ensembles of microstructure features can be included. As a first step, this scheme is tested for a pure single crystal, which provides the opportunity to compare the scheme directly with the atomistic and neutron scattering results above. This information can be used to assign an appropriate scattering time scale to each phonon. This algorithm was first outlined by Wang[15] to study thermal transport in silicon. The search for all phonon triplets that can participate in a three-phonon scattering event is governed by the conservation of energy and crystal momentum equations.

Next Steps

Experimentally, phonon energy and lifetime measurements covering the entire Brillouin zone in single crystal UO_2 will be important for a comprehensive comparison with the new first-principles-based simulations and the development of Monte Carlo schemes. Accordingly, measurements of phonon dispersion and linewidths as a function of temperature are being extended to the Wide Angular Range Chopper Spectrometer (ARCS) and the Fine-resolution Fermi-Chopper Spectrometer (SEQUOIA) time-of-flight beam lines at the Spallation Neutron Source.

The investigations of the impact of anharmonicity on thermal conductivity in UO_2 as a function of temperature will be extended to fundamental investigations of phonon energies and linewidths measurements in cerium doped UO_2 (where cerium is used as a representative fission product) and in off-stoichiometry UO_2 to develop an understanding of the impact of radiation induced defects on thermal conductivity. Of particular interest, in connection with cerium impurities, will be the possibility of resonant phonon modes within the dispersion curves in addition to phonon scattering induced linewidth increases by the mass defects.

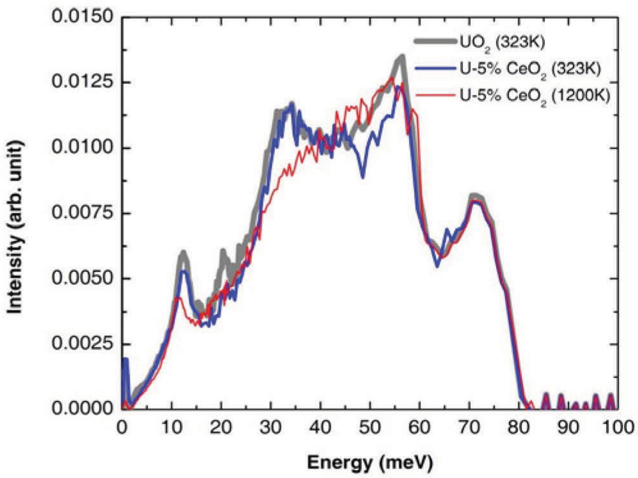


Figure 3-2. Phonon density of states for UO_2 at 323 K and U-5%CeO_2 at 323 K and 1,200K.

Phonon density-of-states measurements in polycrystalline U(5%Ce)O_2 (provided by S. L. Voit of Oak Ridge National Laboratory) have been initiated at the Spallation Neutron Source. Density-of-states measurements do not provide the detailed dispersion or linewidth information afforded by single crystal, triple-axis spectrometer measurements; however, comparisons of the density-of-states spectra for UO_2 and U(5%)CeO_2 show (1) that the phonon energy shifts induced by cerium are small and (2) that qualitative linewidth broadening is present at both 320 and 1,200 K that will be quantifiable using triple-axis and time-of-flight single crystal measurements at the High Flux Isotope Reactor and the Spallation Neutron Source.

Computationally, the coupling of density-functional theory calculations of the phonon properties to Boltzmann transport equation analysis of thermal conductivity will soon be complete, where the higher materials fidelity afforded by the density-functional theory calculations can be expected to provide much better agreement with the experimentally measured phonon properties. In addition, density-functional theory calculations will be extended to include dopants (e.g., cerium as a fission-product representative), including their effects on the phonon spectrum, lifetimes and thermal transport properties. The Monte Carlo scheme for solving the mesoscale Boltzmann transport equation is currently being tested, which will receive input from these simulations and will also come from the density-functional theory calculations. Work on the development of a UO_2 potential will be completed in the near future and its fidelity will be tested against experimental phonon properties.

3.3.1.2 Science Question 2

How does microstructure, specifically grain boundaries, dislocations, and interfaces, affect thermal transport?

Relevant Work by Others

Even at the beginning of life (i.e., before it undergoes any burn up), the structure of a fuel pellet is extremely complex. In particular, the polycrystalline pellet microstructure includes grain boundaries, dislocations and porosity. Moreover, there are a larger number of point defects arising from things such as sintering aids and burnable poisons. During burn up, the microstructure of the pellet continues to develop. For example, the rim region of the fuel pellet develops submicron grains. The thermal resistance posed by grain boundaries in this region is an important contribution to the overall degradation of thermal properties.

In constructing a consistent thermal-conductivity model, it is necessary to characterize the effects of all of the microstructural elements. In particular, it is necessary to be able to characterize the effects of each microstructural element individually, so-called separate effects studies. While there have been preliminary computational studies of the effects of point defects[16] and grain boundaries[17] on thermal transport in UO_2, the effects of dislocations and radiation damage have not been explored. Experimental access to the influence of microstructure has been greatly advanced by the development of spatially resolved thermal transport measurements. These new techniques have the demonstrated potential to isolate the influence of individual microstructure features and are well suited to provide key information for model validation. Among these techniques, laser-based methods have emerged as the leading candidates because of their non-contact nature and well defined optical coupling conditions. Laser excitation can be implemented in the frequency domain using amplitude-modulated, continuous-wave laser heating[18, 19, 20] or in the time domain using pulsed laser heating.[21, 22] Frequency domain measurements are often used to look at thermal transport in the lateral direction. The ability to look in the lateral direction greatly facilitates investigations of microstructure features that are easily identifiable using standard microscopy techniques.[23, 24]

Research Approach and Results

This work, performed by Idaho National Laboratory, Colorado School of Mines, University of Wisconsin, and University of Florida, consists of spatially resolved thermal conductivity measurements, sample fabrication, and molecular dynamics simulation to assess effects of dislocations and interfaces on thermal conductivity.

Isolated Interfaces:

Laser-based modulated thermoreflectance microsocpy is used to gauge the influence of both artifical and naturally occuring grain boundaries. Work on the artifical boundary (bicrystal) enables investigation of a single isolated boundary. This approach is very useful because it corresponds in a one-to-one fashion with molecular dyanamic simuations. Work on naturally occuring grain boundaries considers the collective influence of many boundaries, complementing the Boltzmann transport equation modeling approach.

Because thermal transport across interfaces is sensitively dependent on atomic structure, the initial emphasis is on technique development to isolate the influence of an individual, well characterized interface. In the first research phase, a silicon bicrystal was used as a surrogate material for two important reasons. First, silicon has similar optical properties as UO_2, and the experimental methodolgy for one material can be applied to the other. Second, thermal transport across grain boundaries in silicon has been modeled extensively enabling direct and immediate comparison of experiment and theory. The interface studied was perpendicular to the exposed sample surface as shown in *Figure 3-3*. The thermal wave phase profile was measured as the probe beam was scanned across the bicrystal interface. The intent of this study was to fabricate a highly disordered ($\Sigma 29$ boundary) structure that could be readily compared with existing molecular dynamics simulations. However, high-resolution transmission electron microscopy performed subsequent to our investigation revealed a 4–nm-thick SiO_2 layer at the interface as seen in *Figure 3-3*. Consequently, the physical model of the interface used for both data analysis and thermal transport simulation was altered to reflect the true nature of the interface. The measured Kapitza resistance between the SiO_2 and silicon (2.3×10^{-9} m^2K/W) is smaller than that predicted value using analytical models, suggesting that the transport of vibrational excitations through the interface is more efficient than simple models would predict.

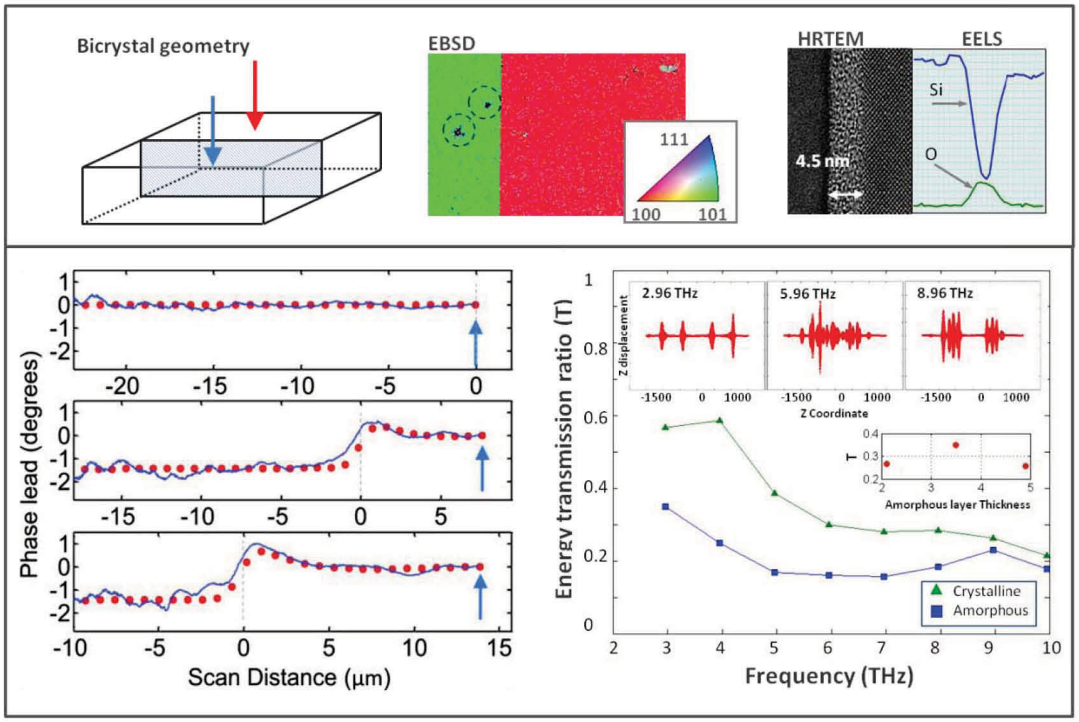


Figure 3-3.Top left: Sample geometry and interface orientation. Top middle: electron backscattered diffraction (EBSD) image used to locate interface. Top right: high-resolution transmission electron microscopy (HRTEM) and electron energy loss spectroscopy (EELS) reveal a thin oxide layer at the interface. Bottom left: The Kapitza resistance is extracted by comparing a continuum model of the interface to experimental results. Bottom right: Energy transmission ratio through the SiO_2 layer (crystalline and amorphous) for the longitudinal acoustic phonon of different energy.

To begin to address this issue, an experimentally convenient model system (Si-SiO_x-Si) has been explored. The interface used for our simulation model, which mimics the interface measured using HRTEM, consists of a thin layer of SiO_2 structure in a micron-long silicon single crystal structure. The interatomic interactions in the silicon and SiO_2 were described by an extended Stillinger-Weber potential. A longitudinal acoustic phonon wave packet (one of the main contributors to phonon transport) is constructed with a narrow distribution of frequency and is sent into the SiO_2 region from the perfect silicon region. The ratio of transmitted energy to reflected energy was analyzed as a function of frequency and SiO_2 layer thickness. Results are shown in the bottom right of *Figure 3-3*, where a decrease in energy transmission with an increase of incident phonon frequency can be seen as expected because the higher frequency corresponds to shorter wavelength that more readily couples to the irregular structure at the interface. While the amorphous layer is more efficient in stopping the energy flow than a purely crystalline interface, the effect is small, particularly at higher frequencies. This result is consistent with the experimental observation that the amorphous layer is not a significant obstacle to thermal transport. Ongoing work will allow the thermal conductivity of this system to be determined from simulation, a result that will then be contrasted with the above experimental result.

Multiple interfaces:

Work has now transition to fluorite-structured materials. Ceria, CeO_2, is a common surrogate material for UO_2 and is convenient for many experiments. The influence of multiple boundaries in ceria thin films was studied. Polycrystalline ceria thin films were fabricated using pulsed-magnetron sputtering at the Colorado School of Mines. Scanning electron microscopy images combined with x-ray diffraction analysis reveal CeO_2 columnar grains having an average diameter of 100 nm. To understand the influence of grain boundaries on thermal transport the phonon mean free path was varied relative to a fixed grain size by performing experiments at cryogenic temperatures. Analyses of the thermal wave profile enable extraction of the temperature dependent conductivity of the ceria film (blue squares in *Figure 3-4*). The large peak in the thermal conductivity with increasing temperature (typical for single crystal and large grained materials) is absent in the data for the ceria film. This observation indicates that thermal transport for the ceria films is limited by phonon scattering at grain boundaries.

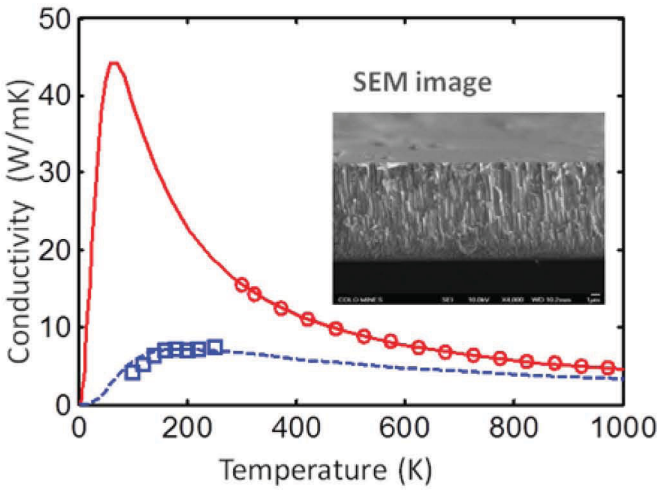


Figure 3-4.Temperature-dependent thermal transport in polycrystalline thin films and sintered pellet with corresponding average grain sizes 100 nm (blue squares) and 5 µm (red circles). Solid lines are model best fits based on Boltzmann transport equation time relaxation (Callaway[25])

Finally, the experimental result was compared with the prediction based on the Boltzmann transport formalism.[25] The strength of phonon-phonon interaction was determined within the relaxation time approximation using high-temperature conductivity data from a sintered ceria sample (red circles in *Figure 3-4*). This sample has a large grain size (~5 µm) and thermal transport is governed by phonon-phonon scattering at moderate to high temperatures.[25] An effective medium approach that directly addresses the fundamental role of the grain boundary was used to account for boundary scattering. This approach calculates the Kapitza resistance at each temperature using a frequency-dependent scattering probability and grain size as fitting parameters. The fitted value for Kapitza resistance is 3.7×10^{-8} m^2K/W, which is considerably larger than values typical of single component materials, indicating that variations in stoichiometry and structure near the grain boundary may play a significant role in scattering phonons.

Dislocations:

Addressing another key aspect of the effects of microstructure, molecular dynamics simulation was used to assess the effects of dislocations on thermal conductivity in the temperature range of 800 to 1,600 K. The results are presented on the *Figure 3-5*. The main graph shows the dependence of the thermal conductivity on the temperature for the different densities. These results are put into the context of classic analysis by Callaway and Klemens. [25, 26, 27] The general trend is in agreement with these analyses, but the dislocations have less of an impact on the thermal conductivity (see insert in the top right corner on the *Figure 3-5*) than predicted. A distinct feature of the Klemens model[26,27] is the temperature independence of the dislocation effect on thermal conductivity. Results of these simulations can also be connected with the continuum fuel performance codes, such as FRAPCON, where thermal conductivity is typically fitted to $k=(A+BT)^{-1}$, with coefficient A, characterizing the temperature independent contribution from elements of the microstructure, including dislocation. By fitting this formula to the data, a linear dependence of coefficient A on the dislocation density is obtained as shown in the bottom left insert of *Figure 3-5*.

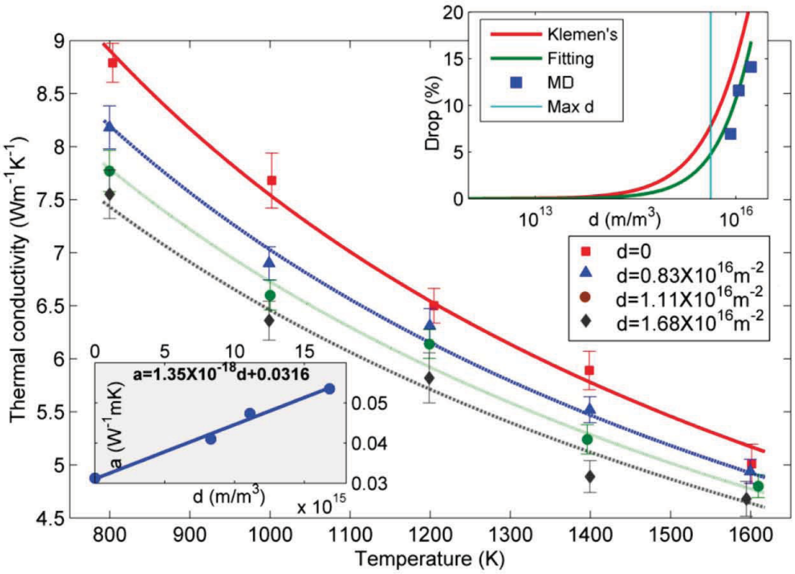


Figure 3-5.Temperature and density of the dislocation dependence of thermal conductivity in UO_2.

Next Steps

Work has started on measuring thermal transport across isolated grain boundaries in a polycrystalline UO_2 sample. The large grain size of this sample enables an experimental methodology similar to one used for the silicon bicrystal describe above. EBSD imaging will be used to isolate high and low-angle grain boundaries for further study. Twin boundaries will be of particular interest because the atomic structure of the interface is well defined. First results from these experimental studies should coincide with the first simulations of the UO_2 grain boundaries. The influence of irradiation is also being addressed by measuring thermal transport in proton irradiated surrogate materials. These measurements put emphasis on extracting the thermal conductivity of the thin irradiation damage layer using modulated thermoreflectance microscopy. Proton irradiation experiments were performed using the tandem ion accelerator at the University of Wisconsin. Initial results on silicon indicate that modulated thermoreflectance microscopy can extract the influence of the proton damage layer if the contribution from anharmonicity is frozen out by conducting experiments at low temperatures.

3.3.2 Microstructure in Irradiated Oxides

Thermal transport is related to the specific microstructural features that form under radiation. To ultimately develop the ability to predict changes in thermal transport in UO_2 in reactor service requires that a fundamental understanding of thermal transport, as described above, be coupled with a fundamental understanding of microstructural development during reactor service. The microstructural development due to the fission product is incredibly complex, driven by the combined effects of radiation damage combined with the introduction of a wide range of fission products into the UO_2 microstructure. The work performed under this thrust is framed by defining fundamental scientific questions that directly address select key elements of our stated ultimate science driver, to understand microstructure development in irradiated oxides. The science questions were chosen to best support the thermal transport studies are described in Section 3.3.1. Thus this subsection summarizes the status of modeling and experimental efforts related to microstructure and defect disorder processes relevant to thermal transport in UO_2 and its surrogate CeO_2 under irradiation.

3.3.2.1 Science Question 1

What types of defect clusters are produced in UO_2 by irradiation and what are the energies and kinetic paths for their formation?

Relevant Work by Others

The number of investigations on various aspects of radiation damage in UO_2 is significant and a complete survey of this work is beyond the scope of this report. However, a few representative investigations relevant to this research are noted: fission product damage[28, 29], electronic stopping damage,[30, 31, 32, 33] and nuclear stopping damage[34] in both UO_2 and CeO_2. Ongoing research involves swift heavy ion molecular dynamics studies[35] and experimental swift heavy xenon ion irradiations.[36] Molecular dynamics simulations are being used to understand displacement cascades and the resulting defects in UO_2.[37, 38] Density functional theory and high-temperature molecular dynamics are being used to understand the stability and formation of cuboctahedral clusters in UO_2.[39, 40, 41] This work examines the directional effects in cascade damage and pathways to the formation of cuboctahedral-type defects and investigates the changes in microstructure and short-range order caused by electronic interactions because of swift heavy ions.

Research Approach and Results

This work, performed by Idaho National Laboratory, Florida State University, University of Florida, and University of Wisconsin, studied statistics of defect production under cascade conditions, temperature accelerated dynamics simulation of pathways to stable defect configurations, electronic and nuclear stopping investigation via ion irradiation, characterization of defects using electron microscopy, and atom probe tomography.

Primary damage in irradiated UO_2 sets the initial conditions for extended defect formation during subsequent diffusion and evolution of irradiation-induced defects. The cascade damage is also important for modeling production bias in irradiated materials.[42] Although defect production in UO_2 was previously studied with molecular dynamics,[37, 38] only the statistics of defect cluster sizes have been reported—the composition of defect clusters is missing. For instance, a $(UO)_i$ interstitial cluster and a $2O_i$ interstitial cluster have completely different properties, although their sizes are the same. This study used molecular dynamics, based on Basak's potential,[43] to perform cascade simulations to sort out the cascade-induced defect clusters in terms of their compositions. As a starting point, low-energy (2 KeV) cascades at 300 K were investigated. Initial analysis shows that defect clusters of various compositions are created—many of them are not charge-neutral (*Figure 3-6* (a)). The three polymorphs of cuboctahedral clusters, such as $I(O_4)$ in *Figure 3-6* (a), are created directly from collision cascades, indicating that these clusters can form either directly from cascades or kinetically by defect aggregation.[41]

Understanding the migration kinetics of radiation-produced defects is a key to predicting the microstructural evolution and mass transport of nuclear fuels. Although the kinetics of point defects in UO_2 is well explored,[44] the kinetics of defect clusters is not well understood. The O interstitial clusters are of particular interest[45] as they are important for forming various phases in UO_{2+x}.[46, 47] Temperature accelerated dynamics[48] have been used to investigate the long-timescale oxygen defect cluster migration without *a priori* assumptions of the complex diffusion pathways. Surprisingly, the migration barrier has

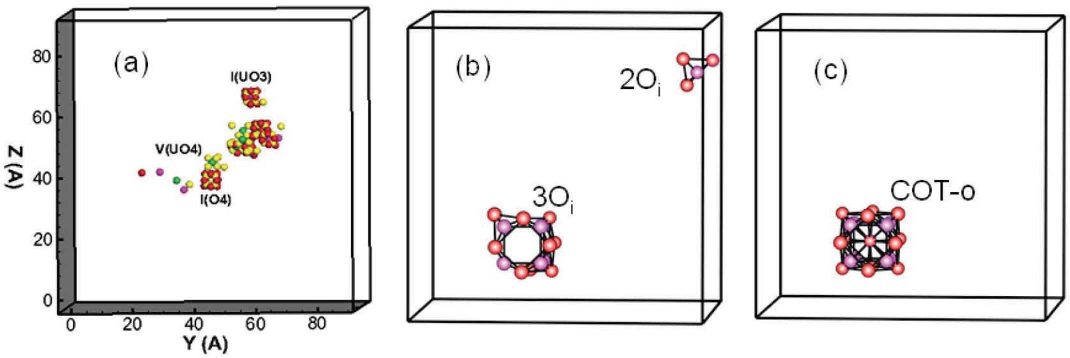
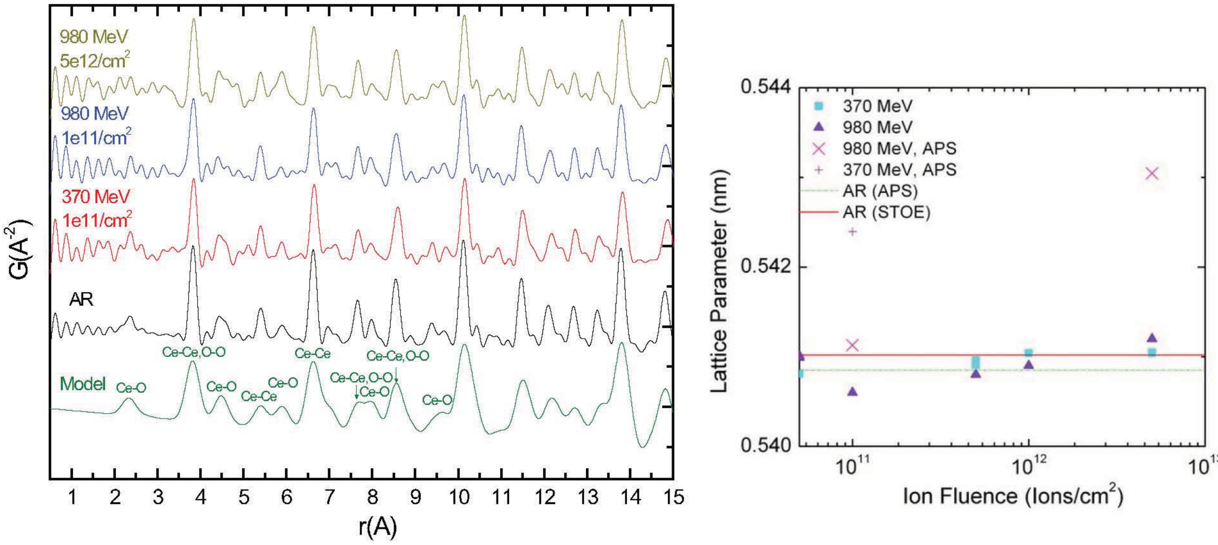


Figure 3-6. (a) Molecular dynamics simulation of defect production from a 2 KeV PKA at 300 K. Sixteen point defects and nine clusters are produced. (b) Temperature-accelerated dynamics simulation of a cuboctahedral (COT-o) cluster formation at 600 K. Initially clusters $2O_i$ and $3O_i$ are placed far from each other. The interstitial clusters displace surrounding atoms to form complex structures consisting of both interstitials (red) and vacancies (purple). The net number of interstitials is two and three in the two clusters respectively. (c) After 0.7 × 10^{-9} s, the $2O_i$ cluster diffuses to the $3O_i$ cluster forming a COT-o cluster, which remains stable after 2.2 × 10^{-2} s.

the following energetic priorities: $2O_i$ (~0.15 eV) <$3O_i$ (~0.25 eV) <$1O_i$ (~1.0 eV) <$4O_i$ (≈ 2.6 eV) <$5O_i$ (≈2.2 eV). These O clusters are the basic building blocks whose migration leads to multiple formation mechanisms of cuboctahedral clusters that were unexplored previously.[41] An example of formation of such clusters by kinetic migration of defect clusters is shown in *Figure 3-6* (b-c).

Swift heavy ion irradiation was performed on surrogate material CeO_2 (a surrogate material for gaining experience before the license for handling UO_2 is issued) at room temperature to understand the contribution of electronic stopping of fission products to overall fuel damage. To investigate fission track damage, gold ions with energies of 300 MeV and 1 GeV were used to irradiate ceria to fluences of 10^{10}-10^{12} ions/cm^2 at room temperature at the GSI Helmholtz Institute in Darmstadt, Germany. The lower-energy, lowest-fluence samples had no significant changes to the crystal structure compared to as-received material. The higher-energy, highest-fluence samples had nanocrystalline features present. These nanocrystals are likely formed during the fission track event, where there is local atomic displacement as the ion passes by, then reconfiguration back into a crystalline form. Investigation of more fluences at both energies to understand the necessary level of damage before nanocrystals begin to form is ongoing. These experimental studies are then contrasted with the computational work performed outside this center[37] that is being shared through an informal communication.

To determine if there is any local disordering in the swift heavy ion irradiated CeO_2, high-energy x-ray scattering was performed for both as-received and irradiated CeO_2 in the Advanced Photon Source at Argonne National Laboratory. X-ray scattering images were recorded and analyzed using image integration, data correction, and a Fourier transform to create a pair distribution function for each sample. Shown in *Figure 3-7* (a) are the pair distribution functions for the as-received 300 MeV Au ion to 1×10^{11} ions/cm^2, 1 GeV gold ion to 1×10^{11} ions/cm^2, and 1 GeV gold ion to 5×10^{12} ions/cm^2. Structure changes were mainly observed in the short range (less than 1 nm) Ce-O peaks, while the long-range order was well maintained for CeO_2 after irradiation.



(a) (b)

Figure 3-7. (a) Pair distribution functions of as-received (AR) and swift heavy ion irradiated ceria at room temperature. (b) Lattice parameters for the samples shown in Figure 7a.

The oxygen sublattices experience more disordering compared to the cerium sublattices. However, the contribution to the short-range disorder caused by the appearance of nanocrystalline features at higher fluence should not be overlooked. *Figure 3-7* (b) shows the lattice constants calculated based on the Advanced Photon Source scattering data compared with the STOE x-ray diffraction data. The results agree that the CeO_2 crystal lattice expands after irradiation, although the measured lattice parameters from the Advanced Photon Source are exaggerated compared to the STOE data. The lattice expansion is most likely due to radiation induced oxygen defects and the formation of Ce^{3+} ions, which are larger compared to the Ce^{4+} ion. Determination of the defect structures by model fitting is ongoing through the refinements of the experimental pair distribution functions. The candidate defect structures will be obtained from the molecular dynamics simulations of displacement cascades. By comparing these models to the experimental pair distribution functions, the short-range changes can be attributed to stoichiometry changes, atomic realignment, or bonding changes as a direct result of the irradiation.

Next Steps

The Center will investigate the types and compositions of defect clusters produced in high-energy cascades using experimental data and modeling, investigating how temperature affects defect cluster production and aggregation. Additional studies combining swift heavy ion irradiation with pair distribution function development and high-resolution TEM will be performed to understand defect formation under radiation. In CY 2012, the first irradiated UO_2 samples will be available for analysis and planning for a test in the Advanced Test Reactor.

3.3.2.2 Science Question 2

What is the impact of temperature and local oxygen environment on the stoichiometry of UO_2?

Relevant Work by Others

A wide range of density functional theory calculations on the defect structure in UO_2[49, 50, 51] and some limited experimental studies on the defect states of stoichiometric UO_2[52, 53] provide the foundation for this novel study of stoichiometric variations. Researchers at Los Alamos National Laboratory are also performing experimental studies on the stoichiometry of CeO_2.[54, 55]

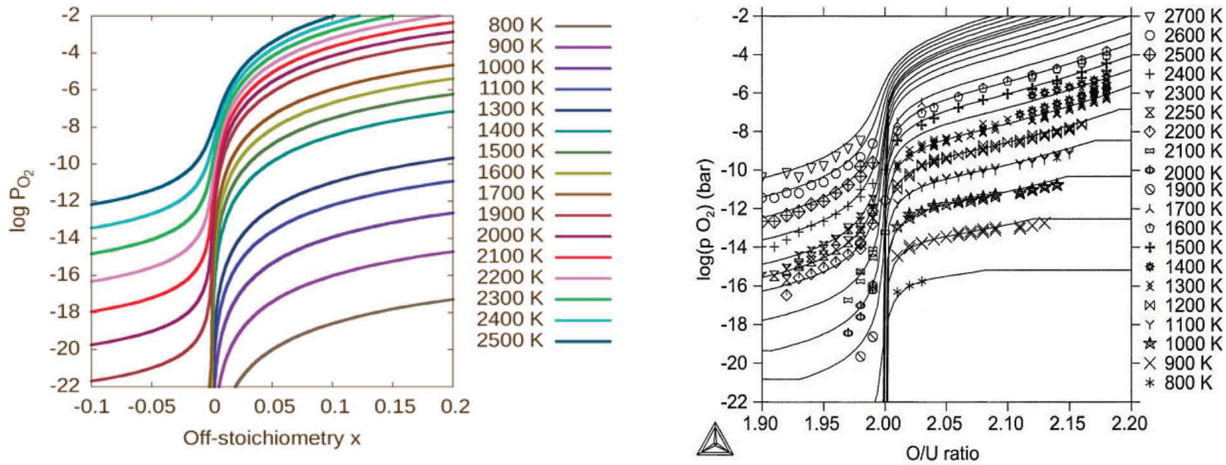
Research Approach and Results

This work, performed by Florida State University, Idaho National Laboratory, Colorado School of Mines, and University of Wisconsin, studied theoretical investigation of equilibrium concentrations of ionic and electronic defects in UO_2, space-time evolution of stoichiometry in UO_2 because of changes in oxygen partial pressure, preparation of thin film samples for stoichiometry measurements at different temperatures, and oxygen pressure with and without irradiation.

Equilibrium thermodynamics of defects in UO_2 have been modeled to determine the concentration of ionic and electronic defects as a function of oxygen pressure and temperature. The model finds all defect concentrations by minimizing the Gibbs free energy under necessary charge equalization constraints. The computed oxygen-pressure/off-stoichiometry diagram is shown in *Figure 3-8* (a). Good agreement with the experimental data shown in *Figure 3-8* (b)[52] is apparent. Some discrepancy between the model predictions and the experiments exists in the range of 800 to 900 K because of the neglect of defect clusters in this model. Nevertheless, the promise of this agreement is not only the reproduction of the observed, but also the demonstration of the reliability of the reported formation energies to calculate the defect levels in UO_2 with variant off-stoichiometry. To obtain the results shown in *Figure 3-8* (a), an estimation of the entropy of formation for each defect was done through comparison with experimental data. The entropy of formation for the uranium vacancies was estimated based on their dominance in the hyper-stoichiometric region and found to be equal to 7.5×10^{-4} eV/K, while, for oxygen vacancies, the hypo-stoichiometric range was used to find a value for their formation entropy and is a small value of 0.2×10^{-4} eV/K. For the oxygen interstitials, the value for the entropy of formation could not be estimated because of their small concentrations throughout the composition range in this model. In a future refinement of the present model, the entropy of formation of such defects will be formally estimated.

Kröger-Vink diagrams, which give the locus of the equilibrium states over the relevant oxygen pressure range, were also produced for the defect concentrations. This was done without the famous Brouwer approximation,[56] which hides all the details about the immediate narrow off-stoichiometric range. It has been found that almost all of the defect types are important in the immediate off-stoichiometry range. The switch from hypo- to hyper-stoichiometry triggers a drastic change in defect concentrations over orders of magnitude and the concentration lines intersect at the intrinsic point. It is, therefore, not safe to assume an individual defect type to be dominant in that range. Moreover, the general solution evades the mistake of assuming a wrong dominant defect type. For example, the dominant defect in most of the hypo-stoichiometry was found to be the neutral oxygen vacancy, contrary to what can be found based on the assumption that the singly charged one is more abundant. In carrying out these calculations, the Fermi level in the crystal bulk of UO_2, which is necessary for the space-charge calculation, was also produced. The density and sign of the surface charge is controlled by the difference between the energy of surface states and the bulk Fermi level. Such mismatch decides whether the substrate atmosphere reaction is oxidation or reduction by dictating the flow of electrons and, consequently, the thickness of the underlying space-charge zone.

Space-charge analysis in disordered oxides yields the initial defect configuration that must be fed to the boundary value problem, describing the space and time resolved kinetics of off-stoichiometry. A full kinetic model of defects was developed and the initial space-charge distributions in UO_2 were analyzed based on a detailed electrochemical model. This treatment of space charge in UO_2 is based on the solution of a static form of the defect diffusion equation coupled with Poisson's equation. Boundary conditions on the surface were prescribed in a similar way to Kliewer's,[57] which was performed for NaCl and did not include electronic-type defects. To account for such defects, the boundary conditions with an arbitrary Fermi level on the surface were supplemented. The space charge's origin is closely related to the extent of



(a) (b)

Figure 3-8. (a) Pressure-off-stoichiometry diagram for different temperature (pressure in units of bar). (b) Thermodynamic model with experimental data for the oxygen partial pressure versus off-stoichiometry for uranium oxide.[52]

chemisorption on the surface and results in the change of some parameters, such as the work function of the solid. Currently, the theory of chemisorption on semiconductors is being applied using density-functional theory calculation results for the chemisorption scenario and the energetic, which has recently been published by Skomurski.[58]

Experimental work at the Colorado School of Mines and University of Wisconsin has focused on using x-ray photoelectron spectroscopy to measure oxygen concentration gradients at sample surfaces following heat treatment. In addition, future work will examine the relative sensitivity of nuclear reaction analysis, wavelength dispersive spectroscopy, and extended x-ray absorption fine structure to measure surface stoichiometry as well as oxygen gradient as a function of depth.

Next steps

The next step is to determine the synergy between off-stoichiometry and microstructure evolution. To tackle this, defect clusters and radiation effects will be included in the models. The last step would be to combine the off-stoichiometry models with the phase-field model of microstructure evolution in UO_2. A key part of this investigation will be the use of density-functional theory calculations to investigate the fundamental question of what mechanisms arise in UO_2 with regard to compensating for off-stoichiometry. It will be necessary to understand if the material will respond by forming electrons and holes or by a change in the charge state of cations, or both. While this issue may not have much impact on static calculations of defects, the kinetics of ionic and electronic-type defects can be different. It will also be important to determine the electron and hole mobility in UO_2.

3.3.2.3 Science Question 3

How do voids form and grow in irradiated UO_2 and what is the effect of free surfaces on defect migration?

Relevant Work by Others

Previous work on void growth in irradiated materials is mostly based on the classical nucleation theory[59, 60] and the rate theory of voids swelling.[61, 62] Only recently, phase-field models have been used as an alternate route that is anticipated to better show the synergistic effects leading to irradiation-induced void formation.[63, 64] Experimental work on fission product defects, specifically relating to xenon and krypton implantation in single crystal CeO_2,[28] has investigated nucleation and growth with increasing damage.

Research Approach and Results

This work, performed by Florida State University, Idaho National Laboratory, and University of Wisconsin, investigated void formation, segregation of U and O vacancies to a surface by molecular statics and migration of O defects near a surface by temperature-accelerated dynamics, ion irradiation in conjunction with noble gas implantation and annealing, and void and bubble formation and distributions.

The strategy is to investigate void nucleation and growth in irradiated UO_2 using a field-theoretic approach in which defect generation, defect diffusion and reactions, nucleation, and growth events are all represented in one model. This model also considers the electrochemical nature of defect interactions in UO_2. The model consists of a set of Cahn-Hilliard equations describing the evolution in space and time of all defect species coupled with Allen-Cahn equation for void nucleation and growth. Because of unresolved questions related to the nature of disorder defects in UO_2 under off-stoichiometry situations, this problem was split into two subproblems: modeling stoichiometry in disordered UO_2 (discussed earlier in this subsection) and the theoretical development of a phase-field model for the coupled chemical, electrostatic, and elastic effects and microstructure evolution under irradiation. To ensure the mathematical consistency of the phase-field model, details of this model are first tested for a single component material. Two pieces of model development have been completed. The first is the development of a thermodynamically consistent phase-field model for void nucleation and growth.[65] The second is the development of its sharp-interface counterpart.[66] The later step was necessary to match the two models and to fix the phase-field model parameters. Asymptotic analysis is now underway to achieve this goal. The sharp interface model has also been extended to UO_2 and preliminary results were obtained.

Modeling void formation in UO_2 requires values for defect energies at the void surface, which is accomplished using molecular dynamics simulations. Basak potential,[43] a fixed-charge potential, was used in the simulations and, for this reason, the (110) surface was chosen as a preliminary investigation because it is charge neutral. The surface energy predicted by this potential is 1.4 J/m^2, which is in good agreement with the experimental values of 1.4~1.5 J/m^2 and theoretical calculation (1.54 J/m^2).[67] The U vacancy formation energy increases as it approaches the surface until at the second U layer where the energy decreases significantly (not shown). The O vacancy formation energy remains constant until at about 5 O layers where the energy fluctuates substantially as shown in *Figure 3-9* (a) (on the following page). Temperature-accelerated dynamics[48] is used to study the migration barriers of an O interstitial and an O vacancy towards and backwards to the surface. Both point defects eventually diffuse to the surface. For the O vacancy, the diffusion barrier is complex as shown in *Figure 3-9* (b). It first decreases to a very small value, then increases to a large value near the surface. The backward barriers are similar to the forward barriers at far distances from the surface. Near the surface, the backward barriers are not detected, possibly because the driving force for attracting defects to the free surface is large. The migration barrier for the O interstitial decreases monotonically as it approaches to the surface (not shown). The surface influence range is about 15 Å and 7 Å for the O interstitial and vacancy, respectively. On the surface, the O vacancy diffusion barrier is about twice as much as in the bulk. The O interstitial causes disorder on the surface. Density-functional theory calculations are underway to validate some of these predictions.

In deriving the sharp interface model for void growth, it was newly discovered that the growth of voids is controlled by an energy barrier for accommodating point defects coming from the matrix. This energy barrier was discovered by insisting on satisfying the second law of thermodynamics in a non-equilibrium diffusion/void growth situation. *Figure 3-9* (c) shows a sample result of the dependence of the void growth rate on this energy barrier. The impact of the value of this important energy barrier on void growth is clear. Similar results were obtained for UO_2 but the barrier values are still under revision. Preliminary molecular dynamics simulations show that it ranges from 0.4 to 0.8 the bulk migration energy for oxygen defects.

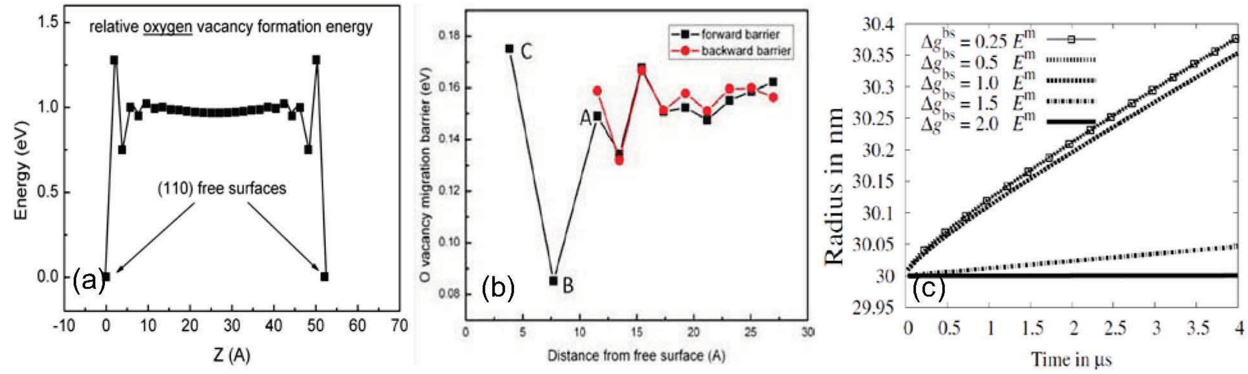


Figure 3-9. (a) Oxygen vacancy formation energy profile as a function of distance from the (110) surfaces. (b) Forward and backward oxygen vacancy migration barriers near a (110) free surface. (c) Effect of surface energy barrier (taken as a fraction of the bulk migration energy) on void growth in a supersaturated vacancy field in copper.[66]

The sharp-interface model for void evolution in UO_2 shows that the local stoichiometry changes associated with defect disorder induced by collision cascades is sensitive to the elastic and electrostatic interactions associated with defects. It is known that defects in UO_2 are charged and the difference in mobility of charged defects leads to nontrivial charge densities in the material. The resulting internal electric field tends to bind the mobile charges to opposite slowly moving defects (or immobile defects such as U interstitials). Elastic interactions also play a similar role in binding defects with elastic opposite relaxation volumes.

Experimental work employs a combination of noble gas implantation, ion irradiation, and annealing to understand defect clusters on the same length scale as predicted in the phase field modeling approach as well as to understand how specific microstructural features like grain boundaries affect bubble formation and growth.

Next Steps

The entire modeling framework is now being advanced to investigate the following issues for irradiated UO_2: the mechanisms of formation of voids and dislocation loops, the synergy between loops and voids, and the effects of microstructure on local stoichiometry. The influence of free surfaces on energetics of impurity atoms will also be investigated. Phase-field model results for voids and loops will be compared with experimental results.

3.4 References

1. R. Peierls, "The kinetic theory of thermal conduction in crystals," *Annalen Der Physik*, Vol. 3, 1929, p. 1055.
2. P. G. Klemens, Solid State Physics, vol 7, (ed. F. Seitz and D. Turnbull, Academic, New York, 1958) p. 1.
3. G. Dolling, R. A. Cowley, and A. D. B. Woods, "The crystal dynamics of uranium dioxide," *Canadian Journal of Physics*, Vol. 43, 1965, p. 1397.
4. K. Clausen, W. Hayes, M. T. Hutchings, J. E. Macdonald, R. Osborn, and P. Schnabel, "Investigation of Oxygen Disorder, Thermal Parameters, Lattice Vibrations and Elastic Constants Of UO_2 and ThO_2 at Temperatures up to 2,930 K," *Rev. Phys. Appl. (Paris)*, Vol. 19, 1984, p. 719.
5. K. Clausen, W. Hayes, J. E. Macdonald, R. Osborn, and M. T. Hutchings, "Observation of Oxygen Frenkel Disorder in Uranium Dioxide above 2000 K by Use of Neutron-Scattering Techniques," *Physical Review Letters*, Vol. 52, 1984, p. 1238.
6. R. B. Peterson, "Direct Simulation of Phonon-Mediated Heat Transfer in a Debye Crystal," *Journal of Heat Transfer-Transactions of the ASME*, Vol. 116, 1994, p. 815.
7. S. Mazumder, and A. Majumdar, "Monte Carlo Study of Phonon Transport in Solid Thin Films Including Dispersion and Polarization," *Journal of Heat Transfer-Transactions of the ASME*, Vol. 123, 2001, p. 749.
8. D. Lacroix, K. Joulain, and D. Lemonnier, "Monte Carlo Transient Phonon Transport in Silicon and Germanium at Nanoscales," *Physical Review B*, Vol. 72, 2005, p. 064305.
9. Q. Yin, and S. Y. Savrasov, "Origin of Low Thermal Conductivity in Nuclear Fuels," *Physical Review Letters*, Vol. 100, 2008, p. 225504.
10. A. Chernatynskiy, and S. R. Phillpot, "Evaluation of Computational Techniques for Solving the Boltzmann Transport Equation for Lattice Thermal Conductivity Calculations," *Physical Review B*, Vol. 82, 2010, p. 134301
11. A. Chernatynskiy, J. E. Turney, A. J. H. McGaughey, C. H. Amon, and S. R. Phillpot, "Phonon-Mediated Thermal Conductivity in Ionic Solids by Lattice Dynamics-Based Methods," *Journal of the American Ceramic Society*, Vol. 94, 2011, p. 3523.
12. C. R. A. Catlow, "Point Defect and Electronic Properties of Uranium Dioxide," *Proceedings of the Royal Society of London Series a-Mathematical Physical and Engineering Sciences,* Vol. 353, 1977, p. 533.
13. J. Yu, S. B. Sinnott, and S. R. Phillpot, "Charge Optimized Many-body Potential for the Si/SiO_{2} System," *Physical Review B*, Vol. 75, 2007, p. 085311.
14. T.-R. Shan, B. D. Devine, T. W. Kemper, S. B. Sinnott, and S. R. Phillpot, "Charge-optimized Many-body Potential for the Hafnium/Hafnium Oxide System," *Physical Review B*, Vol. 81, 2010, p. 125328.
15. T. Wang, "Sub-micron Thermal Transport in Ultra-Scaled Metal Oxide Semiconductor (MOS) Devices," Ph.D. Thesis, Purdue University 2007.
16. T. Watanabe, S. Srivilliputhur, P. K. Schelling, J. S. Tulenko, S. B. Sinnott and S. R. Phillpot, "Thermal Transport in Off-stoichiometric Uranium Dioxide by Atomic Level Simulation", J. Am. Ceram. Soc. 92, 2009, p. 850.

17. T. Watanabe, S. B. Sinnott, J. S. Tulenko, R. W. Grimes, P. K. Schelling and S. R. Phillpot, "Thermal transport properties of uranium dioxide by molecular dynamics simulation", J. Nucl. Mater. 375, 2008, p. 388.

18. W. B. Jackson, N. M. Amer, A. C. Boccara, and D. Fournier, "Photothermal Deflection Spectroscopy and Detection," *Applied Optics*, Vol. 20, 1981, p. 1333.

19. J. Opsal, A. Rosencwaig, and D. L. Willenborg, "Thermal-wave Detection and Thin-film Thickness Measurements with Laser Beam Deflection," *Applied Optics*, Vol. 22, 1983, p. 3169.

20. J. Hartmann, P. Voigt, and M. Reichling, "Measuring Local Thermal Conductivity in Polycrystalline Diamond with a High Resolution Photothermal Microscope," *Journal of Applied Physics*, Vol. 81, 1997, p. 2966.

21. C. A. Paddock, and G. L. Eesley, "Transient Thermoreflectance from Thin Metal Films," *Journal of Applied Physics*, Vol. 60, 1986, p. 285.

22. D. G. Cahill, "Analysis of Heat Flow in Layered Structures for Time-Domain Thermoreflectance," *Review of Scientific Instruments*, Vol. 75, 2004, p. 5119.

23. F. A. McDonald, G. C. Wetsel, and G. E. Jamieson, "Photothermal Beam-Deflection Imaging of Vertical Interfaces in Solids," *Canadian Journal of Physics*, Vol. 64, 1986, p. 1265.

24. A. M. Mansanares, T. Velinov, Z. Bozoki, D. Fournier, and A. C. Boccara, "Photothermal Microscopy: Thermal Contrast at Grain Interface in Sintered Metallic Materials," *Journal of Applied Physics*, Vol. 75, 1994, p. 3344.

25. J. Callaway, "Model for Lattice Thermal Conductivity at Low Temperatures," *Physical Review*, Vol. 113, 1959, p. 1046.

26. P. G. Klemens, Thermal Conductivity and Lattice Vibration Mode, *Solid State Physics*, edited by F. Seitz, and D. Turnbull, Academic, New York, 1958.

27. P. G. Klemens, "Thermal Resistance Due to Point Defects at High Temperatures," *Physical Review*, Vol. 119, 1960, p. 507.

28. I. Zacharie, S. Lansiart, P. Combette, M. Trotabas, M. Coster, and M. Groos, "Microstructural Analysis and Modelling Of Intergranular Swelling of an Irradiated UO2 Fuel Treated at High Temperature," *Journal of Nuclear Materials*, Vol. 255, 1998, p. 92.

29. B. Ye, M. A. Kirk, W. Chen, A. Oaks, J. Rest, A. Yacout, and J. F. Stubbins, "TEM Investigation of Irradiation Damage in Single Crystal CeO2," *Journal of Nuclear Materials*, Vol. 414, 2011, p. 251.

30. V. V. Rondinella, T. Wiss, H. Matzke, R. Mele, F. Bocci, and P. G. Lucuta, "Radiation Damage and Simulated Fission Product Effects on the Properties of Inert Matrix Materials," *Progress in Nuclear Energy*, Vol. 38, 2001, p. 291.

31. T. Sonoda, M. Kinoshita, N. Ishikawa, M. Sataka, A. Iwase, and K. Yasunaga, "Clarification of High Density Electronic Excitation Effects on the Microstructural Evolution in UO2," *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, Vol. 268, 2010, p. 3277.

32. N. Ishikawa, Y. Chimi, O. Michikami, Y. Ohta, K. Ohhara, M. Lang, and R. Neumann, "Study of Structural Change in CeO2 Irradiated With High-energy Ions by Means of X-ray Diffraction Measurement," *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, Vol. 266, 2008, p. 3033.

33. K. Ohhara, N. Ishikawa, S. Sakai, Y. Matsumoto, O. Michikami, and Y. Ohta, "Oxygen Defects Created in CeO2 Irradiated with 200 MeV Au Ions," *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, Vol. 267, 2009, p. 973.

34. M. Song, W. Weiguo, F. Chu, X. Yang, K. Mitsuishi, K. Furuya, and H. Yasuda, "Structure and Chemical Changes of CeO2 Irradiated with Hydrogen Ions," *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, Vol. 191, 2002, p. 586.

35. R. Devanathan, Ongoing Research MD Studies of Swift Heavy Ion Damage in UO2.

36. M. Lang, and W. J. Weber, Ongoing research- Swift Heavy Xe Ion Damage in UO2.

37. R. Devanathan, J. G. Yu, and W. J. Weber, "Energetic Recoils in UO2 Simulated Using Five Different Potentials," *Journal of Chemical Physics*, Vol. 130, 2009, p. 174502.

38. L. Van Brutzel, J. M. Delaye, D. Ghaleb, and M. Rarivomanantsoa, "Molecular Dynamics Studies of Displacement Cascades in the Uranium Dioxide Matrix," *Philosophical Magazine*, Vol. 83, 2003, p. 4083.

39. H. Y. Geng, Y. Chen, Y. Kaneta, and M. Kinoshita, "Stability Mechanism of Cuboctahedral Clusters in UO_{2+x}: First-principles Calculations," *Physical Review B*, Vol. 77, 2008, p. 180101.

40. D. A. Andersson, J. Lezama, B. P. Uberuaga, C. Deo, and S. D. Conradson, "Cooperativity Among Defect Sites in AO(2+x) and A(4)O(9) (A=U,Np,Pu): Density Functional Calculations," *Physical Review B*, Vol. 79, 2009, p. 024110.

41. D. S. Aidhy, P. C. Millett, T. Desai, D. Wolf, and S. R. Phillpot, "Kinetically Evolving Irradiation-Induced Point Defect Clusters in UO2 by Molecular Dynamics Simulation," *Physical Review B*, 80, 2009, p 104107.

42. B. N. Singh, and A. J. E. Foreman, "Production Bias and Void Swelling in the Transient Regime Under Cascade Damage Conditions," *Philosophical Magazine A*, Vol. 66, 1992, p. 975.

43. C. B. Basak, A. K. Sengupta, and H. S. Kamath, "Classical Molecular Dynamics Simulation of UO2 to Predict Thermophysical Properties," *Journal of Alloys and Compounds*, Vol. 360, 2003, p. 210.

44. K. Govers, S. Lemehov, M. Hou, and M. Verwerft, "Comparison of Interatomic Potentials for UO2. Part I: Static Calculations," *Journal of Nuclear Materials*, Vol. 366, 2007, p. 161.

45. D. A. Andersson, T. Watanabe, C. Deo, and B. P. Uberuaga, "Role of Di-interstitial Clusters in Oxygen Transport in UO_{2+x} from First Principles," *Physical Review B*, Vol. 80, 2009, p. 060101.

46. D. J. M. Bevan, I. E. Grey, and B. T. M. Willis, "The Crystal Structure of β-U4O9−y," *Journal of Solid State Chemistry*, Vol. 61, 1986, p. 1.

47. H. M. He and D. Shoesmith, "Raman Spectroscopic Studies of Defect Structures and Phase Transition in Hyper-Stoichiometric UO(2+x)," *Physical Chemistry Chemical Physics*, Vol. 12, 2010, p. 8108.

48. M. R. Sørensen, and A. F. Voter, "Temperature-Accelerated Dynamics for Simulation of Infrequent Events," *The Journal of Chemical Physics*, Vol. 112, 2000, p. 9599.

49. J.-P. Crocombette, D. Torumba, and A. Chartier, "Charge States of Point Defects in Uranium Oxide Calculated with a Local Hybrid Functional for Correlated Electrons," *Physical Review B*, Vol. 83, Issue 18, 2011, p. 184107.

50. P. Nerikar, T. Watanabe, J. S. Tulenko, S. R. Phillpot, and S. B. Sinnott, "Energetics of Intrinsic Point Defects in Uranium Dioxide from Electronic-Structure Calculations," *Journal of Nuclear Materials*, Vol. 384, 2009, p. 61.

51. J. G. Yu, R. Devanathan, and W. J. Weber, "First-principles Study of Defects and Phase Transition in UO(2)," *Journal of Physics-Condensed Matter*, Vol. 21, 2009, p. 435401.

52. C. Guéneau, M. Baichi, D. Labroche, C. Chatillon, and B. Sundman, "Thermodynamic Assessment of the Uranium–Oxygen System," *Journal of Nuclear Materials*, Vol. 304, 2002, p. 161.

53. S.-H. Kang, J.-H. Lee, H.-I. Yoo, H. Soo Kim, and Y. Woo Lee, "Non-stoichiometry, Electrical Conductivity and Defect Structure of Hyper-stoichiometric UO2+x at 1000°C," *Journal of Nuclear Materials*, Vol. 277, 2000, p. 339.

54. M. Patel, and K. E. Sickafus, Ongoing Stoichiometry Studies of CeO2.

55. M. Patel, and S. Conradson, Ongoing Studies of CeO2 and UO2 Using XANES and EXAFS.

56. J. Maier, *Physical Chemistry of Ionic Materials: Ions and Electrons in Solids*, John Wiley and Sons, Chichester, U.K., 2004.

57. K. L. Kliewer, "Space Charge in Ionic Crystals. II. The Electron Affinity and Impurity Accumulation," *Physical Review*, Vol. 140, 1965, p. A1241.

58. F. N. Skomurski, L. C. Shuller, R. C. Ewing, and U. Becker, "Corrosion of UO2 and ThO2: A Quantum-mechanical Investigation," *Journal of Nuclear Materials*, Vol. 375, 2008, p. 290.

59. R. M. Mayer, and L. M. Brown, "Nucleation and Growth of Voids by Radiation: II. Differential Equations," *Journal of Nuclear Materials*, Vol. 95, 1980, p. 58.

60. K. C. Russell, "Nucleation of Voids in Irradiated Metals," *Acta Metallurgica*, Vol. 19, 1971, p. 753.

61. A. D. Brailsford, and R. Bullough, "The Rate Theory of Swelling Due to Void Growth in Irradiated Metals," *Journal of Nuclear Materials*, Vol. 44, 1972, p. 121.

62. A. D. Brailsford, R. Bullough, and M. R. Hayns, "Point Defect Sink Strengths and Void-Swelling," *Journal of Nuclear Materials*, Vol. 60, 1976, p. 246.

63. P. C. Millett, A. El-Azab, S. Rokkam, M. Tonks, and D. Wolf, "Phase-field Simulation of Irradiated Metals Part I: Void kinetics," *Computational Materials Science*, Vol. 50, 2011, p. 949.

64. S. Rokkam, A. El-Azab, P. Millett, and D. Wolf, "Phase Field Modeling of Void Nucleation and Growth in Irradiated Metals," *Modelling and Simulation in Materials Science and Engineering*, Vol. 17, 2009, p. 064002.

65. S. Rokkam, *Phase Field Modeling of Void Nucleation and Growth in Irradiated Materials*, Ph.D. Thesis, Florida State University, 2011.

66. T. Hochrainer, and A. El-Azab, "Theory of Void Growth in Single Component Systems," to be submitted.

67. P. W. Tasker, "The Surface Properties of Uranium Dioxide," *Surface Science*, Vol. 87, 1979, p. 315.

4. SYNERGISM AND PROGRAMMATIC FOCUS

4.1 Establishing Team Identity

The team of key researchers selected by the Center to focus on understanding thermal transport in irradiated microstructures are located across the country. While this presents a communications challenge, having this caliber of researchers is critical to project success. Team members were selected from the **University of Florida**, **The Florida State University**, **Oak Ridge National Laboratory**, **Argonne National Laboratory,** and **Idaho National Laboratory** because they have the key modeling and experimental skills to advance the knowledge of thermal transport. Team members were selected from **Colorado School of Mines, University of Florida, University of Wisconsin**, and **Idaho National Laboratory** because they have the key modeling and experimental skills to advance the knowledge of microstructural development under radiation. The team leaders were selected because they have the skills to ensure proper coupling between the two major scientific thrusts.

To ensure the team is well aware of other research advances relevant to Center, three methods have been used that go beyond the typical studies of literature and conference attendance. The first is to form informal partnerships with other relevant research institutes to share ongoing results. The second is to invite key researchers to major Center review meetings to present their work. The third is to form an advisory committee with members representing research institutions doing relevant work.

Informal partnerships have been established and review meetings held to interact with researchers from **Idaho State University, University of Illinois, The University of California at Los Angeles**, and **Pacific Northwest National Laboratory**. A meeting is also scheduled in March 2012 to find opportunities to collaborate with staff members from the **Institute for Transuranium Elements (ITU)**—the European Community Center of Excellence in nuclear fuel performance.

The Advisory Committee has representatives from the **European Union Institute for Transuranium Elements in Germany, Argonne National Laboratory, University of Tennessee** (representing the Energy Frontier Research **Center named the Materials Science of Actinides** led by Notre Dame), **Massachusetts Institute of Technology**, and **Idaho National Laboratory** (representing the DOE Nuclear Energy fuels development programs). Finally, every summer the Center co-hosts, an Energy Frontier Research Center summer school jointly planned with the Energy Frontier Research Centers led by **Los Alamos National Laboratory, Oak Ridge National Laboratory,** and **Notre Dame**.

4.2 Research Focus

A roadmap outlining the team's integrated research plan has been produced to capture the long-term plans of the Center and maintain research focus. The specificity of the roadmap is greater for the current year, with future year plans providing a broad outline of the expected research trajectory. The roadmap is a living document, updated each year to reflect progress and adjust to new insights.

The Center has both internal and external mechanisms for assessing performance. Internally, the intertwined contributions of multiple team members to the success of any task naturally lead to an ongoing internal check of the performance of any individual institution. In addition, two senior members of the team assess progress at the semiannual meetings that do not include the advisory board. The external assessment of the Center has two components. The Center's external Advisory Board conducts a formal assessment on a yearly basis. This independent advice from international experts is critical to the success of the Center. The advisory board meets annually with the team of principal investigators. The goal of this meeting is to review progress and make recommendations to the Director and Executive Committee regarding the Center's direction, focus, and operation. The informal mechanism for assessment of external response to the work of the Center will be to track the results of submissions to peer reviewed publications, the number of invited talks, press response, and the student interest in Center-sponsored events.

4.3 Participation and Communication

To ensure a common understanding of the Center's goals and performance, the team meets in person on a semiannual basis, rotating the location of the meeting between the different participating institutions. The team also holds formal monthly internet-base conferences using the *GoToMeeting* software package. These meetings allow discussions among all team members as well as routine research presentations from team members on a rotating basis. In many instances, smaller groups use the *GoToMeeting* functionality to hold discussions between the formal monthly meetings.

The team also routinely co-loans team members from one institution in order to create greater integration and synergy across research tasks, provide additional educational and training opportunities for students and post docs, and to facilitate creative thinking and scientific exchange among team members.

4.4 Synergies

The following examples represent the manner in which the team operates to take maximum advantage of team capabilities, as well as external partnerships:

- *Phonon Dispersion and Lifetime Measurements*. Team members from **Oak Ridge National Laboratory** perform experimental measurements of phonon dispersion and lifetime. These measurements are performed using the neutron scattering facilities available at the Spallation Neutron Source and the High Flux Isotope Reactor—both national scientific user facilities located at Oak Ridge National Laboratory. The sample material was obtained through collaborations with **Atomic Energy of Canada Limited** and **Los Alamos National Laboratory**. The measurements are compared to computational work performed at the University of Florida using Boltzmann transport theory after choosing a best potential following a detailed study of potentials gleaned from over 20 literature sources. In parallel to the **University of Florida** studies are transport studies using a Monte Carlo approach being led by **Florida State University**. Future single crystal samples are anticipated to become available through a partnership with **Idaho State University**.
- *Phonon Scattering Measurements*. Team members at **Idaho National Laboratory** use laser-base techniques to measure the scatter of phonons off of microstructural features such as grain boundaries. Some of the single crystal samples measured come from collaborations with **Atomic Energy Canada Limited**, while team members from the **Colorado School of Mines** produce thin film samples. To determine the effects of irradiation, samples are provided to **Idaho National Laboratory** with irradiated microstructures produced by team members from the **University of Wisconsin**, using both the **University of Wisconsin** ion beam facilities and the heavy ion irradiation facilities at the **GSI Helmholtz Centre for Heavy Ion Research** in Germany. Simulations of the scattering events are performed at the **University of Florida**, providing a direct comparison between measurement and simulation.
- *Microstructural development under Irradiation*. Phase field modeling performed at **Florida State University** is used to predict the microstructural features that develop under irradiation. Partnerships exist with the **Idaho National Laboratory Center for Advanced Modeling and Simulation** and **Argonne National Laboratory** via the SciDAC Program, which develops new formulations and solvers for the phase-field method, an approach that is central to the Center's strategy for modeling microstructure evolution of materials under irradiation. To perform the simulations, input parameters are extracted from the literature but also from first principles calculations performed at **Idaho National Laboratory and Argonne National Laboratory**. Detailed descriptions of the microstructure following controlled irradiation come from the experimental teams at the **University of Florida**, **University of Wisconsin**, **Idaho National Laboratory**, and **Colorado School of Mines**. A portion of the facilities accessed at **Idaho National Laboratory** are through proposals to the Advanced Test Reactor National Scientific User Facility, which has recently added an analytical

transmission electron microscope and an atom probe capable of analyzing radioactive materials. Samples are also analyzed using the synchrotron x-ray facilities at **Argonne National Laboratory's** Advanced Photon Source. Through an informal research partnership, the **University of Illinois** will provide access to data on irradiated microstructures. Irradiated samples are produced using facilities at the **University of Wisconsin's** Intermediate Voltage Electron Microscope, a national scientific user facility at **Argonne National Laboratory**, and at the **GSI Helmholtz Centre for Heavy Ion Research** in Germany. Future projects anticipate using the Advanced Test Reactor at **Idaho National Laboratory**.

5. PUBLICATIONS FROM ENERGY FRONTIER RESEARCH CENTER SUPPORT

5.1 Peer-Reviewed Journals

Solely Supported by this EFRC

1. S. R. Phillpot, A. El-Azab, A. Chernatynskiy, and J. S. Tulenko, "Thermal Conductivity of UO_2 Fuel: Predicting Fuel Performance from Simulation," *J. Metals* (Invited Review—August 2011).
2. M. Khafizov, D. Hurley, "Measurement Of Thermal Transport Using Time-resolved Thermal Wave Microscopy," *Journal of Applied Physics*, Vol. 110, 2011, p. 083525.
3. A. Chernatynskiy, J. E. Turney, A. J. H. McGaughey, C. H. Amon, and S. R. Phillpot, "Phonon-Mediated Thermal Conductivity in Ionic Solids by Lattice-Dynamics-based Methods," *Journal of the American Ceramic Society* (DOI: 10.1111/j.1551-2916.2011.04743.x).
4. D. S. Aidhy, D. Wolf, and A. El-Azab, "Comparison of Defect Clustering in Irradiated CeO_2 and UO_2 from Molecular-Dynamics Simulation," *Scripta Materialia*, July 2011 (DOI: 10.1016/J.scriptamat.2011.07.051).

Partially Supported by this EFRC

5. D. H. Hurley, M. Khafizov, S. Shinde, , "Measurement of Kaptiza Resistance Across a Bicrystal Interface," *Journal of Applied Physics*, Vol. 109, p. 83504 (2011).
6. 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* (accepted).
7. X. M. Bai and B. P. Uberuaga, "Multi-Time Scale Investigation of Radiation Damage near TiO_2 Rutile Grain Boundaries," *Philosophical Magazine* (accepted).

5.2 Book Chapters

1. A. Chernatynskiy, D. R. Clarke, and S. R. Phillpot, "Thermal Transport in Nanostructured Materials," *CRC Handbook of Nanoscience, Engineering and Technology*, 3rd edition (In Press).
2. D. Hurley, J. Sullivan, S. Shinde, Book Chapter, "Interaction of Thermal Phonons with Interfaces," Elsevier, 2012.

5.3 Submitted Manuscripts

1. J. Pang, et al., "Lifetime of a Phonon: Limits to High Temperature Heat Transfer in UO_2 by Neutron Scattering and Theory," *Physics Review Letter* (submitted).

5.4 Conference Presentations/Papers

1. M. Khafizov, D. Hurley, I. Park, J. J. Moore, J. Lin, R. Deskins, A. El-Azab, "Thermal Transport in Ceria Thin Films Having Engineered Microstructure," *Materials Research Society (MRS) Spring 2011 Meeting*, April 25–29, San Francisco, CA.
2. M. Khafizov and D. Hurley, "Measurement of Thermal Transport Using Time-resolved Thermal Wave Microscopy," *Materials Research Society (MRS) Spring 2011 Meeting*, April 25–29, San Francisco, CA.
3. I-W. Park, J. J. Moore, J. Lin, M. M. H. Henderson, A. El-Azab, T. Allen, P. Xu, D. Hurley, and M. Khafizov, "Deposition of Post-annealing of Ceria Fils Deposited by Pulsed Unbalanced Magnetron Sputtering," *International Conference on Metallurgical Coatings and Thin Film, 2011, May 2–6, San Diego, CA.*

4. 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.*

5. X-M. Bai, J. Yu, A. El-Azab, and T. R. Allen, "Temperature Accelerated Dynamics Simulations of Defect Clustering in UO_2," *Materials Research Society (MRS) 2011 Fall Meeting*, Nov 28–Dec 02, Boston, MA.

6. J. Yu, X-M. Bai, A. El-Azab, and T. Allen, "Near-surface stoichiometry in UO_2: A DFT study," *Materials Research Society (MRS) 2011 Fall Meeting*, Nov 28–Dec 02, Boston, MA.

7. L. Wang, J. Lee, M. Anitescu, A. El Azab, L. C. McInnes, T. Munson, B. Smith, "A Differential Variational Inequality Approach for the Simulation of Heterogeneous Materials," *2011 SciDAC Conference*, Denver, CO, July 10-14, 2011.

8. C.Yablinsky, P.Xu, A.Schulte, M.Khafizov, D.Hurley, J.Gan, T.Allen, "Effects of Radiation and Annealing on Microstructure and Thermal Transport in CeO_2," Poster- Energy Frontier Research Center: *Energy Summit & Forum, May 2011.*

9. C.A.Yablinsky, P.Xu, A.Schulte, J.Gan, T.R.Allen. "Defect Characterization in Swift Heavy Ion Irradiated CeO_2," Talk- *Spring MRS Meeting, April, 2011.*

10. J. Pang, W. Buyers, A. Chernatynskiy, M. Lumsden, D. Abernathy, B Larson and S. R. Phillpot, "Inelastic Neutron Scattering Measurements and Lattice Dynamics Simulations of Phonon Dispersion and Lifetimes in UO2," Symposium W, Invited Talk - *Fall 2011 MRS Meeting, Boston.*

11. A. El-Azab, T. Hochrainer, A.-R. Hassan and D. Wolf, "Theory of Defects and Microstructure Dynamics in Irradiated Oxides," *Fifth International Conference* on Multiscale Modeling of Materials (MMM-2010), October 4-8, 2010, Freiburg, Germany

12. A. El-Azab, S. Wang, S. Rokkam and D. Wolf, "Stress Effects on Microstructure Evolution in Irradiated Materials," *Fifth International Conference on Multiscale Modeling of Materials (MMM-2010), October 4-8, 2010, Freiburg, Germany*

13. S. Rokkam, A. El-Azab and T. Hochrainer, "Nonequilibrium Thermodynamics of Void Microstructure Evolution and Swelling under Irradiation," *Materials Research Society (MRS) Spring 2011 Meeting, April 25-29, San Francisco*, CA, Symposium RR: Fundamental Science of Defects and Microstructure in Advanced Materials for Energy

14. T. Hochainer, S. Rokkam and A. El-Azab, "On the Void-Surface Reaction Kinetics in Irradiated Materials--The Void Growth Problem Revisited," *Materials Research Society (MRS) Spring 2011 Meeting, April 25-29, San Francisco*, CA, Symposium RR: Fundamental Science of Defects and Microstructure in Advanced Materials for Energy

15. T. Hochainer, A. El-Azab and A.-R. Hassan, "Irradiation-Induced Void Microstructure Evolution in Stoichiometric Oxides," *Materials Research Society (MRS) Spring 2011 Meeting, April 25-29, San Francisco, CA,* Symposium RR: Fundamental Science of Defects and Microstructure in Advanced Materials for Energy

16. S. Rokkam, K. Ahmed and A. El-Azab, "Stress Effects on Void Growth under Irradiation," *Materials Research Society Fall 2011 Meeting, November 28-December 2, 2011, Boston*, MA, Symposium A: Material Challenges in Current and Future Nuclear Technologies

17. A.-R. Hassan, T. Hochrainer, J. Yu, X. Bai, T. Allen, A. El-Azab, "Electrochemistry of Defects in Irradiated UO_2," *Materials Research Society Fall 2011 Meeting, November 28-December 2, 2011, Boston, MA*, Symposium A: Material Challenges in Current and Future Nuclear Technologies

18. T. Hochainer, S. Rokkam and A. El-Azab, "Electrostatic and Elastic Effects in the Theory of Void Growth under Irradiation," *Materials Research Society Fall 2011 Meeting, November 28-December 2, 2011, Boston, MA*, Symposium A: Material Challenges in Current and Future Nuclear Technologies
19. R. Deskins and A. El-Azab, "Monte Carlo Simulation of Phonon Transport in UO_2," *Materials Research Society Fall 2011 Meeting, November 28-December 2, 2011, Boston, MA*, Symposium A: Material Challenges in Current and Future Nuclear Technologies
20. A. El-Azab, "Microstructure Stability in Irradiated Fuels," Materials Modeling and Simulation for Nuclear Fuels workshop, *MMSNF 2011, September 26-28, 2011, Aix en Province, France*
21. S. Rokkam and A. El-Azab, "A Diffuse Interface Model for Void Formation under Non-Equilibrium Irradiation," Proceeding of MRS Symposium RR: Fundamental Science of Defects and Microstructure in Advanced Materials for Energy, *Spring 2011.*
22. L. Wang, J. Lee, M. Anitescu, A. El Azab, L. C. McInnes, T. Munson, B. Smith, *A Differential Variational Inequality Approach for the Simulation of Heterogeneous Materials*, Proceedings of 2011 SciDAC Conference, Denver, CO, July 10-14, 2011.

5.5 Documents in Preparation

1. A. C. Flint and S. R. Phillpot, "Critical Assessment of the UO_2 Classical Potentials for Thermal Conductivity Calculations," (to be submitted to *Journal of Nuclear Materials*).
2. Melendez, Gomez, El-Azab, paper on grain growth in oxides (to be submitted to Acta Mater).
3. B. Deng, A. Chernatynskiy, P. Shukla, S. Sinnott, and S. R. Phillpot, "Effects of Dislocations on the Thermal Conductivity of UO_2," (to be submitted to *Journal of Nuclear Materials*)
4. B. Deng, at al., "Thermal Transport in UO_2: MD Study of the Dislocation Effects," (in preparation).
5. B. Larson, and J. Pang, "Thermal Conductivity of UO_2 Determined from Lattice Dynamics Using Inelastic Neutron Scattering," (in preparation).
6. C. Flint, A. Chernatynskiy and S. R. Phillpot, "Critical Assessment of the UO_2 Classical Potentials for Thermal Conductivity Calculations, (to be submitted to *Journal of Nuclear Materials*).
7. I. -W. Park, J. Lin, J. J. Moore, M. Manuel, A. El-Azab, T. Allen, P. Xu, D. Hurley, and M. Khaflzov, "Deposition and Post Annealing of Ceria Thin Film Produced by Pulsed DC Magnetron Sputtering," *Thin Solid Films*,(in preparation).
8. L. He, C. Yablinsky, M. Gupta, T. Allen, and J. Gan, "Irradiation Damage of CeO2 with Xe and Kr Implantation," TMS 2012 (conference paper).
9. M. Khafizov, I. W. Park, J. Lin J. Moore, and D. Hurley, "Phonon Transport in Polycrystalline Thin Films with Engineered Microstructure," *Physical Review B*, (in preparation)
10. S. Rokkam, and A. El-Azab, "Nonequilibrium Thermodynamics of Void Dynamics in Irradiated Materials," for *Physical Review B*.
11. S. R. Phillpot, A. Chernatynskiy, A. El-Azab and J. S. Tulenko, "Simulation of the Thermal Transport Properties of UO_2: Recent Progress and Current Challenges, to be submitted to the OECD/NEA/NSC/WPMM (Working Party on Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems) report on Multiscale Modeling of Fuel.
12. T. Hochrainer and A. El-Azab, "Theory of Void Growth in Single Component Systems, for *Physical Review E*.

13. X-M. Bai, J. Yu, A. El-Azab, and T.R. Allen, "Temperature Accelerated Dynamics Studies of the Migration Mechanisms of Oxygen Defect Clusters in UO_2", in preparation for *Physical Review B*.
14. Y. Li, T. Shan, T. Liang, S. B. Sinnott, and S. R. Phillpot, "Classic Interatomic Potential for Uranium Metal" (to be submitted to *Physical Review B*).
15. J. Yu, X-M. Bai, A. El-Azab, and T. Allen, "Near-surface stoichiometry in UO_2: A DFT study," (in preparation for *Journal of Physical Chemistry C*).
16. A.-R. Hassan and A. El-Azab, *Equilibrium Defect Disorder in Non-stoichiometric UO_2*, for J. Electrochem. Soc.
17. A.-R. Hassan and A. El-Azab, Dynamics Space Charge in UO_2: Effects of Oxygen Partial Pressure and Temperature, for J. Appl. Phys.

6. BIOGRAPHICAL SKETCHES OF KEY PERSONNEL/SENIOR INVESTIGATORS

Dr. Todd R. Allen

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Prof. Allen is an Associate Professor in the Dept. of Engineering Physics at the University of Wisconsin – Madison since 2003. Prof. Allen's research expertise is in the area of materials related issues in nuclear reactors, specifically radiation damage and corrosion. Dr. Allen is also the Scientific Director for the Advanced Test Reactor National Scientific User Facility at Idaho National Laboratory, a position that he holds in conjunction with his faculty position at the University of Wisconsin.

Education and Training

- Ph.D., University of Michigan, Nuclear Engineering (1997).
- M.S., University of Michigan, Nuclear Engineering (1993).
- M.S., George Washington University, Information Systems Management (1991).
- B.S., Northwestern University, Nuclear Engineering (1984).

Research and Professional Experience

- Associate Professor, Department of Engineering Physics, University of Wisconsin-Madison (2003 to present).
- Research Scientist, Argonne National Laboratory (1997 to 2003).

Relevant Publications

18. T. R. Allen, J. Gan, J. I. Cole, M. K. Miller, J. T. Busby, S. Shutthanandan and S. Thevuthasan, "Radiation Response of a 9 Cr Oxide Dispersion Strengthened ODS to Heavy Ion Irradiation," *J. Nucl. Mater.*, Vol. 375, 2008, p. 26.
19. T. R. Allen and G. S. Was, "Modeling radiation-induced segregation in austenitic Fe-Cr-Ni alloys," *Acta Materialia*, Vol. 46, 1998, pp. 3679–3692.
20. T. R. Allen, J. T. Busby, G. S. Was, and E. A. Kenik, "On the Mechanism of Radiation-Induced Segregation in Austenitic Fe-Cr-Ni Alloys," *Journal of Nuclear Materials*, Vol. 255, 1998, p. 44.
21. T. R. Allen, C. L. Trybus, and J. I. Cole, "The Effects of Low Dose Rate Irradiation and Thermal Aging on Reactor Structural Alloys," *J. Nucl. Mater.*, Vol. 270, 1999, pp. 290–300.
22. L. Tan, T. R. Allen, J. D. Hunn, and J. H. Miller, "EBSD for microstructure and property characterization of the SiC-coating in TRISO fuel particles," *J. Nuc. Mat.*, Vol. 372, 2008, pp. 400–404.
23. T. R. Allen, Y. Chen, L. Tan, X. Ren, and K. Sridharan, "Corrosion of Candidate Materials for Supercritical Water-Cooled Reactors," *12th Environmental Degradation Conference of Materials in Nuclear Power Systems-Water Reactors*, Eds., Todd R. Allen, Peter J. King, and Lawrence Nelson, TMS, 2006, p. 1397.
24. G. S. Was, P. Ampornrat, G. Gupta, S. Teysseyre, E. A. West, T. R. Allen, K. Sridharan, L. Tan, Y. Chen, X. Ren, and C. Pister, "Corrosion and Stress Corrosion Cracking in Supercritical Water," *J. Nucl. Mater.*, Vol. 371, 2007, pp. 176–201.

25. T. R. Allen, J. I. Cole, J. Gan, G. S. Was, R. Dropek, and E. A. Kenik, "Swelling and Radiation-induced Segregation in Austenitic Alloys," *Journal of Nuclear Materials*, Vol. 342, 2005, p. 90.

26. L. Tan, K. Sridharan, and T. R. Allen, "The Effect of Grain Boundary Engineering on The Oxidation Behavior of INCOLOY Alloy 800H in Supercritical Water," *Journal of Nuclear Materials*, Vol. 348, 2006, p. 263.

27. L. Tan, K. Sridharan, and T. R. Allen, "Effect of Thermomechanical Processing on Grain Boundary Character Distribution of a Ni-based Superalloy," *Journal of Nuclear Materials*, Vol. 371, 2007, p. 171.

Collaborators and Co-Editors

Bogdan Alexandreneau, Research Scientist, Argonne National Laboratory; Yiren Chen, Research Scientist, Argonne National Laboratory; Jim Cole, Research Scientist, Idaho National Laboratory; Mike Free, Professor, University of Utah; Jian Gan, Research Scientist, Idaho National Laboratory; Rob Kelley, Professor, University of Virginia; Rudy Koenigs, Research Scientist, ITU; Sindo Kou, Professor, University of Wisconsin; Ed Lahoda, Research Scientist, Westnghouse; Meimei Li, Research Scientist, Argonne National Laboratory; Ning Li, Research Scientist, Los Alamos National Laboratory; Heather MacLean, Research Scientist, Idaho National Laboratory; Mitch Meyer, Research Scientist, Idaho National Laboratory; Dane Morgan, Assistant Professor, University of Wisconsin; Arthur Motta, Professor, Pennsylvania State University; Kumar Sridharan, Research Scientist, University of Wisconsin; Roger Stoller, Research Scientist, Oak Ridge National Laboratory; Izabela Szlufarska, Assistant Professor, University of Wisconsin; Shigaharu Ukai, Hokkaido University; Gary Was, Professor, Nuclear Engineering, University of Michigan; Brian Wirth, Professor, University of California; Shinsuke Yamanaka, Professor, Osaka University; Xinghang Zhang, Assistant Professor, Texas A&M University.

Graduate and Postdoctoral Advisors

Gary Was, University of Michigan

Supervised Graduate Students

Julie Tucker (now at KAPL); Xiaowei Ren (now at Foster Wheeler); Clay Dickerson (now at Argonne); Brandon Miller (now at INL); Hannah Yount (now at KAPL); Kent Wardle (now at Argonne National Laboratory); James Ambrosek (now at Woodward); Alan Kruizenga (now at SNL); McLean Machut (now at AREVA); Alicia Certain, Kevin Field, Tyler, Laura Jamison, Billy Nollet, Tony Schulte, Liang Zhao (now at INPO), Guiqiu Zheng, Tammy Malaney, Jetsenia Toro, Scott Weber (now at SNL), Lucas Wilson, Jacob Jelinek, Mehran Mohammadian, Sean Martin, Dan Ludwig, Sarah Khalil, Alex Mairov, Sam Briggs

Supervised Postdoctoral Scholars

Lizhen Tan (now at Oak Ridge National Laboratory); Yun Chen (now at University of West Virginia); Yong Yang (now at U. Florida), Guoping Cao, Youngki Yang, Peng Xu (now at Westinghouse), Luke Olson (now at SRNL), Vahid Firouzdor, Yina Huang, Clarissa Yablinsky, Beata Tyburska-Pueschel.

Dr. Anter El-Azab

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Education and Training

- Ph.D., Nuclear Engineering, The University of California, Los Angeles, 1994; Major Field: Applied Plasma Physics and Fusion Engineering; Specialty Area: Radiation Effects and Mechanics of Fusion Materials.,
- M.S., Nuclear Engineering, University of Alexandria (1989).
- B.S., , Nuclear Engineering, University of Alexandria (1986).

Research and Professional Experience

- Professor of Computational Materials Science, Department of Scientific Computing, Florida State University (2010).
- Associate Professor of Computational Materials Science, Department of Scientific Computing, The Florida State University (2008 to 2010).
- Faculty Member, Materials Science and Engineering Program, The Florida State University (2008 to Present).
- Associate Professor (joint), School of Computational Science & Mechanical Engineering Department, The Florida State University (2004 to 2008).
- Senior Research Scientist, Fundamental Science Directorate, Pacific Northwest National Laboratory, Richland, WA (1998 to 2004).
- Research Engineer and Lecturer, Mechanical and Aerospace Engineering Department, University of California, Los Angeles (1995 to 1998).

Research Interests

Computational Microstructure Science; Radiation Effects in Nuclear Alloys and Ceramics; Defect Disorder in Oxides; Surface and Interfacial Science; Methods of Multiscale Modeling in Materials.

Some Synergistic Activities

- Chairman: 4th International Conference on Multiscale Modeling of Materials (October 27–31, 2008), Florida State University—the World's Largest Forum on Computational Materials Science.
- Guest Editor: Several special journal issues on defects and microstructure modeling in materials (*Phil. Mag,*; *J. Appl Phys.*; *Modell. Simul. Mater. Sci. & Engng.*; *SIAM J. Multiscale Modeling*).

- Executive Committee: Energy Frontier Research Center for Materials Science of Nuclear Fuel, DOE Basic Energy Sciences (BES).
- Reviewer: Incite Program, DOE (proposals seeking allocation on Leadership Class Computing Facility machines at Argonne National Laboratory and Oak Ridge National Laboratory.

Sample Publications

Dr. Anter El-Azab has published over 100 journal and conference papers, edited volumes, and technical reports.

1. Anter El-Azab (Editor), "Tackling Materials Complexity via Computational Science," *Proceedings of the 4th International Conference on Multiscale Materials Modeling, Florida State University, 2008,* ISBN: 978-0-615-24781-6 (989 pages)
2. S. Rokkam, A. El-Azab, P. Millett, and D. Wolf, "Phase Field Modeling of Void Nucleation and Growth in Irradiated Metals," *Modell. Sim. Mater. Sci. and Engng.*, Vol. 17, No. 064002: pp. 1–18.
3. Paul Millett, Srujan Rokkam, Anter El-Azab, Michael Tonks, and Dieter Wolf, "Void Nucleation and Growth in Irradiated Polycrystalline Metals: A Phase Field Formulation," *Modell. Sim. Mater. Sci. and Engng.*, Vol. 17, 2009, No. 064003: pp. 1–12.
4. Paul Millett, Anter El-Azab, Srujan Rokkam, Michael Tonks, and Dieter Wolf, „Phase Field Simulation of Irradiated Metals, Part I: Void Kinetics," *Computational Materials Science*, Vol. 50, 2011, pp. 949–959.
5. Paul Millett, Anter El-Azab, and Dieter Wolf, "Phase Field Simulation of Irradiated Metals. Part II: Gas Bubble Kinetics." *Computational Materials Science*, Vol. 50, 2011, pp. 960–970.

Collaborators and Co-Editors

Ben Larson, Roger Stoller (Oak Ridge National Laboratory), Brian Wirth (The University of Tennessee), Dieter Wolf, Marius Stan, Mihai Anitescu (Argonne National Laboratory), James Belak (Lawrence Livermore National Laboratory), Mihai Anitescu (Argonne National Laboratory), Simon Phillpot, Susan Sinnott (University of Florida), Paul Millet and Michael Tonks (Idaho National Laboratory), Moe Khaleel (Pacific Northwest National Laboatory), Todd Allen (University of Wisconsin), Max Gunzburger (University of Florida), Russ Caflisch (The University of California, Los Angeles)

Graduate Students and Post-doctoral Scholars Supervised

Post Doctor: Former: Jie Deng (Sandia National Laboratory), Shengyu Wang (Brookhaven National Laboratory), Thomas Hochrainer (Professor, Germany), Srujan Rokkam (Florida State University), Nan Wang (Florida State University)

Current Students: Santosh Dubey (Ph.D.), Shengxu Xia (Ph.D.), Mamdouh Salem(Ph.D.), Ryan Deskins (Ph.D.), Karim Ahmed M.S.), Abdel-Rahman Hassan (M.S.)

Former Students: Jie Deng (Ph.D., Sandia National Laboratory), Srujan Rokkam (Ph.D., Florida State University), Steve Henke (M.S., Florida State University), Jennifer Murray (M.S.), Michael Dyer (M.S., Boeing), Ryan Whitney (M.S.)

Dr. David Hurley

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Materials Science Department
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Education

- Ph.D., Materials Science and Engineering, Johns Hopkins University, (September 1997).
- M.S., Mechanical Engineering, Montana State University (June 1991).
- B.S., Physics, University of North Carolina, Chapel Hill (May 1989).

Research and Professional Experience

- Advisory Scientist, Idaho National Laboratory, Idaho Falls, ID (January 1999 to Present).
- Postdoctoral Fellow, Hokkaido University, Sapporo, Japan (July 1998 to December 1999).
- Postdoctoral Fellow, Johns Hopkins University, Baltimore, Maryland (November 1997 to June 1998).

Research Interests

Ultrafast optical techniques to characterize the electronic, thermal, and elastic properties of thin films and nanostructures. Theoretical and experimental study of linear and nonlinear crystal acoustics. Fundamental interaction of acoustic phonons with individual microstructural features. In situ laser ultrasonic and laser-based thermal wave imaging of material properties in high temperature environments (e.g., fatigue damage, corrosive film growth, development of elastic anisotropy).

Some Synergistic Activities

- Session Organizer, Phonons in Nanomaterials, MRS Fall Symposium (2011).
- Realist, Research and Industrial Collaboration Conference, Boston (2011).
- Session Organizer, Acoustics' 08, Ultrafast Acoustics, Paris, France (2008).
- Session Chair, MRS Spring Meeting, Nanoscale Heat Transport, San Francisco (2007).
- Session Chair, Gordon conference on Photothermal and Photoacoustic Phenomena, Trieste Italy, (July 2005).

Sample Publications

Dr. Hurley has published over 90 journal and conference papers and technical reports.

1. M. Khafizov and D. Hurley, "Measurement of Thermal Transport Using Time-resolved Thermal Wave Microscopy," *Journal of Applied Physics*, Vol. 110, 2011.
2. D. H. Hurley, M. Khafizov, S. Shinde, and Hurley, D. "Measurement of Kaptiza Resistance Across a Bicrystal Interface," *Journal of Applied Physics*, Vol. 109, No. 83504, 2011.
3. D. H. Hurley, S. J. Reese, S. Park, Z. Utegulov, J. R. Kennedy, and K. Telschow, "In situ laser-based resonant ultrasound measurements of microstructure mediated mechanical property evolution," *Journal of Applied Physics*, Vol. 107, No. 063510, 2010.
4. D. H. Hurley, O. B. Wright, O. Matsuda, and S. L. Shinde, "Time Resolved Imaging of Carrier and Thermal Transport in Silicon," *Journal of Applied Physics*, Vol. 106, No. 023521, 2009.

5. Benjamin Clough, David H. Hurley, Pengyu Han, Jun Liao, Rena Huang and X.-C. Zhang, "Detection of Terahertz Pulses Using a Modified Sagnac Interferometer," *Sensing and Imaging*, Vol. 10, 2009, pp. 14–21.
6. D. H. Hurley and M. Fig, "Parametric Study of Thermal Interface Resistance Using Laser-Based Thermal Wave Imaging," *Journal of Applied Physics*, Vol. 104, No. 123703, 2008.
7. D. H. Hurley, R. Lewis, O. B. Wright, and O. Matsuda, "Coherent control of gigahertz surface acoustic and bulk phonons using ultrafast optical pulses," *Applied Physics Letters*, Vol. 93, No. 113101, 2008.

Collaborators

Ben Larson (Oak Ridge National Laboratory); Dieter Wolf (Argonne National Laboratory); Simon Phillpot (University of Florida); Jian Gan, Marat Khafizov, Farhad Farzbod, Dennis Kunerth, and Rory Kennedy (Idaho National Laboratory); Todd Allen and Clarissa Yablinsky (University of Wisconsin); Subash Shinde, John Sullivan, and Edward Piekos (Sandia National Laboratory), Oliver Wright and Osamu Matsuda (Hokkaido University).

Graduate Students and Post-doctoral Scholars Supervised

Farhad Farzbod, Current Idaho National Laboratory postdoctoral fellow; Marat Khafizov, 2010 and 2011 Idaho National Laboratory postdoctoral fellow; Zhandos Utegulov, Current Idaho National Laboratory postdoctoral fellow; Zilong Hua, thesis committee member; Zilong Hua, 2008 Idaho National Laboratory summer student, Utah State University; Benjamin Clough, 2008 Idaho National Laboratory summer student, RPI; Ryan Lewis, 2007-2008 senior project, Whitman College; Ryan Lewis, 2006 Idaho National Laboratory summer student, Whitman College; Chiaki Miyasak, 2004 and 2005 Idaho National Laboratory Postdoctoral Fellow.

Dr. Jian Gan

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Education

- Ph.D., Nuclear Engineering, University of Michigan (1999).
- M.S., Nuclear Engineering, University of Michigan (1994).
- M.S., Physics, Central Michigan University (1992).
- B.S., Physics, Fudan University, Shanghai, China (1982).

Employment History

- Idaho National Laboratory, Senior Staff Scientist (2006 to Present).
- Argonne National Laboratory, Staff Scientist (2002 to 2005).
- Pacific Northwest National Laboratory, Postdoctoral Scientist (1999 to 2001).
- Research Assistant, University of Michigan (1992 to 1999).
- Research Assistant, Central Michigan University (1990 to 1992).
- Lecturer, Department of Physics, Fudan University, China (1987 to 1990).

Current Research Interests

Microstructural development in the irradiated fuel and its impact on fuel performance for research and test reactors. Effects of irradiated UO_2 microstructure on thermal conductivity. Characterization of microstructural changes under irradiation using transmission electron microscopy. Correlation between microstructure and material properties. Evaluation and development of advanced alloys and ceramics for radiation tolerant materials for advanced nuclear power systems. Development of diffusion barrier with ceramic coatings for fast reactor and light water reactor fuel claddings.

Selected Recent Publications

1. J. Gan, D. D. Keiser, Jr., B. D. Miller, J. F. Jue, A. B. Robinson, P. Medvedev and D. M. Wachs, "Microstructure of Irradiated U_3Si_2/Al Silicide Dispersion Fuels," *J. of Nucl. Mater.*, Vol. 419, 2011, pp. 97–104.
2. J. Gan, D. D. Keiser, Jr., D. M. Wachs, A. B. Robinson, B. D. Miller, and T. R. Allen, "Transmission Electron Microscopy Characterization of Irradiated U-7Mo/Al-2Si Dispersion Fuel," *J. of Nucl. Mater.*, Vol. 396, 2010, pp. 234–239.
3. J. Gan, D. D. Keiser, D. M. Wachs, B. D. Miller, T. Allen, M. A. Kirk, and J. Rest, "Microstructure of RERTR DU-Alloy Irradiated with Kr Ions up to 100 dpa," *J. of Nucl. Mater.*, Vol. 411. 2011, pp. 174–180.
4. J. Gan, D. D. Keiser, B. D. Miller, M. A. Kirk, J. Rest, T. R. Allen and D. M. Wachs, "Kr Ion Irradiation Study of the Depleted-Uranium Alloys," *J. of Nucl. Mater.*, Vol. 407, 2010, pp. 48-54.
5. J. Gan, Y. Yang, C. A. Dickson, T. R. Allen, "Proton Irradiation Study of GFR Candidate Ceramics," *J. of Nucl. Mater.*, Vol. 389, 2009, pp. 317–325.
6. J. Gan, T. R. Allen, R. C. Birtcher, S. Shutthanandan, and S. Thevuthasan, "Radiation Effects on the Microstructure of a 9Cr ODS Alloy," *J. of Materials*, January 2008, p. 24–28.

7. J. Gan, J. I. Cole, T. R. Allen, S. Shutthandan, and S. Thevuthasan, "Irradiated Microstructure of Alloy 800H," *J. of Nucl. Mater.*, Vol. 351, 2006, pp. 223–227.
8. J. Gan, E. P. Simonen, S. M. Bruemmer, L. Fournier, B. H. Sencer and G. S. Was, "The effect of oversized solute additions on the microstructure of 316SS irradiated with 5 MeV Ni ions or 3.2 MeV protons," *Journal of Nuclear Materials*, Vol. 325, 2004, pp. 94–106.
9. J. Gan, J. I. Cole, T. R. Allen, R. B. Dropek, and G. S. Was, "Effect of Zr on the Irradiated Microstructure and Hardening in 304 Stainless Steel," *Fusion Science and Technology*, Vol. 44, 2003, p. 191.
10. J. Gan, J. S. Vetrano, and M. A. Khaleel, "Microstructure Characterization of Dislocation Wall Structure in Aluminum using Transmission Electron Microscopy," *J. of Engineering Materials and Technology*, Vol. 124, 2002, p. 297.

Advisors, Advisees, and Recent Collaborators

Dr. G. S. Was (University of Michigan), Ph.D. advisor; Dr. S. M. Bruemmer and Dr. J. S. Vetrano (Pacific Northwest National Laboratory), Post-doc advisor. Dr. T. R. Allen (University of Wisconsin), collaborator; Dr. M. A. Kirk (Argonne National Laboratory), collaborator; Dr. J. Bao (University of Houston), collaborator; Dr. G. S. Was (University of Michigan), collaborator; Dr. H. Wang (Texas A&M University), collaborator; Dr. James Stubbins (University of Illinois), collaborator; Dr. Michel Barsoum (Drexel University), collaborator. Dr. S. Shutthanandan and Dr. S. Thevuthasan (Pacific Northwest National Laboratory), collaborator.

Dr. Xianming Bai

Education

- Ph.D., Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA, USA, December 2006.
- M.S., Materials Science and Engineering, Johns Hopkins University, Baltimore, MD, USA, December 2001.
- B.S. & M.S., Materials Science Fudan University, Shanghai, China, July 2000.

Research Experience

- Idaho National Laboratory, Center for Advanced Modeling and Simulation, Idaho Falls, ID (March 2011 to present).
  Staff Scientist:
  - Worked on the Energy Frontier Research Center project funded by DOE Basic Energy Sciences
  - Investigated radiation-induced microstructural evolution in UO_2 via temperature accelerated dynamics, molecular dynamics, and molecular statics methods.
- Los Alamos National Laboratory, Materials Science and Technology Division (MST-8), Los Alamos, NM (December 2008 to present).
  Postdoctoral Research Associate (Mentors: Dr. Blas Uberuaga and Dr. Arthur Voter):
  - Worked on two projects: the Energy Frontier Research Center project funded by DOE Basic Energy Sciences and a "Laboratory Directed Research and Development" project funded by Los Alamos National Laboratory
  - Conducted multitime scale modeling of radiation effects near grain boundaries in metals and oxides via molecular dynamics, temperature accelerated dynamics, and molecular statics methods.
- Northwestern University, Department of Chemical and Biological Engineering, Evanston, IL (June 2007 to November 2008).
  Postdoctoral Fellow (Supervisors: Prof. Randall Q. Snurr and Prof. Leon M. Keer):
  - Worked on a project of modeling particle damping effects funded by US Air Force
  - Performed discrete element method modeling of damping, adhesion, and friction of granular materials.
- Georgia Institute of Technology, School of Materials Science and Engineering, Atlanta, GA (January 2002 to June 2007):
  Graduate Research Assistant (Advisor: Prof. Mo Li):
  - Conducted large-scale molecular dynamics simulations of crystallization and melting in model crystals.
  - Developed parallel molecular dynamics simulation codes with C and MPI.

Selected Journal Publications

1. X. M. Bai and B. P. Uberuaga, "Multi-Time Scale Investigation of Radiation Damage near TiO_2 Rutile Grain Boundaries," Philosophical Magazine (accepted).
2. Z. Di, X. M. Bai, Q. Wei, J. Won, R. G. Hoagland, Y. Wang, A. Misra, B. P. Uberuaga, M. Nastasi, "Tunable helium bubble superlattice ordered by screw dislocation network," *Physical Review B*, Vol. 84, No. 052101, 2011.
3. X. M. Bai, A. F. Voter, R. G. Hoagland, M. Nastasi, and B. P. Uberuaga, "Efficient annealing of radiation damage near grain boundaries via interstitial emission," *Science*, Vol. 327, No. 1631, 2010.

4. X. M. Bai, L. M. Keer, Q. J. Wang, and R. Q. Snurr, "Investigation of particle damping mechanisms via particle dynamics simulations," *Granular Matter*, Vol. 11, No. 417, 2009.
5. X. M. Bai and M. Li, "Comparing crystal-melt interfacial free energies through homogenous nucleation rates," *Journal of Physics: Condensed Matter*, Vol. 20, No. 375103, 2008.
6. X. M. Bai and M. Li, "Ring-diffusion mediated homogeneous melting in the superheating regime," *Physical Review B*, Vol. 77, NO. 134109, 2008.
7. X. M. Bai and M. Li, "Nucleation and melting from nanovoids," *Nano Letters*, Vol. 6, No. 2284, 2006.
8. X. M. Bai and M. Li, "Calculation of solid-liquid interfacial free energy: a classical nucleation theory based approach," *Journal of Chemical Physics*, Vol. 124, No. 124707, 2006.
9. X. M. Bai and M. Li, "Differences between solid superheating and liquid supercooling," *Journal of Chemical Physics*, Vol. 123, No. 151102, 2005.
10. X. M. Bai and M. Li, "Nature and extent of melting in superheated solids: Liquid-solid coexistence model," *Physical Review B*, Vol. 72, No. 052108, 2005.

Media Highlights

1. Radiation effects near grain boundaries, X. M. Bai et al., *Science*, 327, 1631, (2010): *The New York Times; DOE Pulse* (U.S. Department of Energy); *Materials Today* (Elsevier), *American Scientist, Los Alamos National Laboratory News Release*
2. Melting of superheated crystals X. M. Bai and M. Li, *Physical Review B*, 77, 134109 (2008): *Physical Review Focus* (American Physical Society), *Georgia Tech News Release*

Collaborators from other institutions (in alphabetical order)

Kerry Allahar (Boise State University), David Andersson (LANL), Jon Baldwin (LANL), Xiaoying Bao (Genral Electric), Lyudmyla Barannyk (University of Idaho), Nicole Benedek (Cornell), Valery Borovikov (LANL), Darryl Butt (Boise State University), Indrajit Charit (University of Idaho), Samrat Choudhury (LANL), Steve Conradson (LANL), Zengfeng Di (Shanghai Institute of Microsystem and Information Technology), David Dubbeldam (University of Amsterdam), Megan Frary (Boise State University), Richard Hoagland (LANL), Leon Keer (Northwestern University), Mo Li (Georgia Tech), Amit Misra (LANL), Michael Nastasi (LANL), Gloria Oxford (NIST), Alexander Panchenko (Washington State University), Danny Perez (LANL), Batric Pesic (University of Idaho),Davy Pillet (France, unknown), Gabriel Potirniche (University of Idaho), Karl Rink (University of Idaho), Binoy Shah (GE), Susan Sinnott (University of Florida), Randall Snurr (Northwestern University), Xian-Zhu Tang (LANL), Blas Uberuaga (LANL), Arthur Voter (LANL), Qian (Jane) Wang (Northwestern University), Yongqiang Wang (LANL), Qiangmin Wei (LANL), Jonghan Won (LANL), Ahmet Ozgur Yazaydin (University of Surrey, UK), Bilge Yildiz (Massachusetts Institute of Technology)

Graduate and Postdoctoral Advisors

Blas Uberuaga (LANL), Arthur Voter (LANL), Randall Snurr (Northwestern Univ.), Leon Keer (Northwestern Univ.), Mo Li (Georgia Tech).

Dr. Jiangou Yu

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Professional Interests

Dr. Jianguo Yu is a research staff scientist at the Center for Materials Science of Nuclear Fuel and Advanced Modeling & Simulation, Idaho National Laboratory. He has an extensive experience with first-principles calculations and computer simulations for basic radiation defects and their mobility in uranium oxide (UO_2). In particular, he has substantially computational expertise in simulation methodology development and modeling of materials, including mesoscale modeling, modular dymanics, kinetic Monte Carlo, and *ab initio* calculations. He also has extensive experience in thin film growth simulations, and developed parallel algorithms and the charge optimized many-body potentials. He has also been developing simulation methodologies to study defect properties, and mechanical and thermal behaviors of nuclear fuels and cladding materials under extremely operant conditions.

Education

- Ph.D., Physics (2003), University of Toledo, Toledo, Ohio, USA
- M. Sc., Physics (1996), Institute of High Energy Physics, Chinese Academy of Sciences, Beijing, China
- B.Sc., Physics (1989), Hubei Normal College, Hubei, China

Professional Experience

- Scientist, Idaho National Laboratory, Idaho Falls, Idaho, USA (2011 to Present).
- Postdoctoral Fellow, Pacific Northwest National Laboratory, Richland, Washington, USA (2007 to 2011).
  Supervisor: Ram Devanathan and Kevin M. Rosso, Pacific Northwest National Laboratory, William J. Weber, University of Tennessee.
- Postdoctoral Research Associate, University of Florida, Gainesville, Florida, USA (2004 to 2007).
  Supervisor: Susan Sinnott and Simon Phillpot, University of Florida.
- Postdoctoral Research Associate, Ohio State University, Columbus, Ohio, USA (2003 to 2004).
  Supervisor: Ju Li, Massachusetts Institute of Technology.
- Research Assistant, University of Toledo, Toledo, Ohio, USA (1998 to 2003).
  Advisor: Jacques G. Amar, University of Toledo.
- Research Assistant & Scientist, Institute of High Energy Physics, Beijing, Chinese Academy of Sciences, China (1993 to 1998).

Sample Publications

1. J. Yu, K. M. Rosso, J. G. Zhang, and J. Liu, "Ab initio study of lithium transition metal fluorophosphate cathodes for rechargeable batteries," *Journal of Materials Chemistry*, Vol. 21, No. 32, 2011, pp. 12054–12058.
2. J. Yu, R. Devanathan and W. J. Weber, "Structure properties and phase transformation of UO_2 in the GGA+U formalism," *Journal of Physics: Condensed Matter*, Vol. 21, No. 435401, 2009.
3. J. Yu, R. Devanathan and W. J. Weber, "Unified interatomic potential for zircon, zirconia and silica systems," *Journal of Materials Chemistry*, Vol. 19, No. 3923, 2009.

4. J. Yu, S. Sinnott and S. Phillpot, "Optimized Many-Body Potential for fcc metals," *Philosophical Magazine Letters*, Vol. 89, 2009, p. 136.
5. J. Yu, S. Sinnott and S. Phillpot, "Charge Optimized Many-Body (COMB) Potential for the Silicon-Silica System," *Physical Review B*, Vol. 75, No. 085311, 2007.
6. J. Yu, A. Bogicevic, and J. G. Amar "First Principles Calculations of Steering Effects in Epitaxial Growth," *Physical Review B*, Vol. 69, 113406 (2004).
7. J. Yu and J. G. Amar, "Short-range Attraction, Surface Currents, and Mound Formation in Metal (111) Epitaxial," *Physical Review B*, Vol. 69, No. 045426, 2004.
8. J. Yu and J. G. Amar, "Effects of Short-Range Attraction in Metal Epitaxial Growth," *Physical Review Letters*, Vol. 89, No. 286103, 2002.
9. J. Yu and J. G. Amar, "Dynamical Scaling Behavior in Two-Dimensional Ballistic Deposition with Shadowing," *Physical Review E*, Vol. 66, No. 021603 (2002).
10. J. Yu and J. G. Amar, "Scaling Behavior of the Surface in Ballistic Deposition," *Physical Review E*, Vol. 65, No. 060601, (Rapid Communications), 2002.

Collaborators from Other Institutions

- R. Devanathan, Pacific Northwest National Laboratory; W. J. Weber, University of Tennessee; K. M. Rosso, Pacific Northwest National Laboratory; J. G. Zhang, Pacific Northwest National Laboratory; J. Liu, Pacific Northwest National Laboratory.

Dr. Jianliang Lin

Professional Preparation

- Ph.D., Metallurgical and Materials Engineering, Colorado School of Mines, USA (2007).
- M.Sc., Metallurgy and Materials Engineering, Central South University (CSU), China (1999).
- B.Sc., Metallurgy and Materials Engineering, Central South University (CSU), China, (1996).

Academic Experience

- Research Assistant Professor, Metallurgical and Materials Engineering Department, Colorado School of Mines (2009 to present).
- Associate Director, Advanced Coatings and Surface Engineering Laboratory (ACSEL) , Colorado School of Mines (2010 to present).
- Research Associate, Department of Metallurgical and Materials Engineering, Colorado School of Mines, (2007 to 2009).
- Research faculty, State Key Laboratory for Powder Metallurgy, Central South University of Technology, China (1999 to 2002).

Publications

Fourty-four peer-reviewed international journal papers, 20 peer-reviewed conference proceedings.

Six Publications Most Closely Related to the Proposed Project

1. J. Lin, B. Mishra, J. J. Moore, X. H. Zhang, W. D. Sproul, "CrN/AlN superlattice coatings synthesized by pulsed closed field unbalanced magnetron sputtering with different CrN layer thicknesses," *Thin Solid Films*, Vol. 517, 2009, pp. 5798–5804. (http://dx.doi.org/10.1016/j.tsf.2009.02.136)
2. J. Lin, J. J. Moore, J. Wang, W. D. Sproul, "High temperature oxidation behavior of CrN/AlN superlattice coatings," *Thin Solid Films*, Vol. 519, 2011, pp. 2402–2408. (http://dx.doi.org/10.1016/j.tsf.2010.11.042)
3. J. Lin, J. J. Moore, B. Mishra, M. Pinkas, W. D. Sproul, "Nano-structured CrN/AlN multilayer coatings synthesized by pulsed closed field unbalanced magnetron sputtering," *Surf. Coat. Technol.*, Vol. 204, 2009, pp. 936–940. (http://dx.doi.org/10.1016/j.surfcoat.2009.04.013)
4. J. Lin, J. J. Moore, B. Mishra, M. Pinks, W. D. Sproul, and J. A. Rees, "Effect of Asynchronous Pulsing Parameters on the Structure and Properties of CrAlN Films Deposited by Pulsed Closed Field Unbalanced Magnetron Sputtering (P-CFUBMS)," *Surface and Coatings Technology*, Vol. 202, 2008,: pp. 1418–1436. (http://dx.doi.org/10.1016/j.surfcoat.2007.06.068)
5. J. Lin, J. J. Moore, W. D. Sproul, B. Mishra, Z. Wu, "The structure and properties of chromium nitride coatings deposited using dc, pulsed dc and modulated pulse power magnetron sputtering," *Surface and Coatings Technology*, Vol. 204, 2010, pp. 2230–2239. (http://dx.doi.org/10.1016/j.surfcoat.2009.12.013).
6. J. Lin, J. J. Moore, W. D. Sproul, B. Mishra, J. A. Rees, Z. Wu, R. Chistyakov, and B. Abraham, "Ion energy and mass distributions of the plasma during modulated pulse power magnetron sputtering," *Surface and Coatings Technology*, Vol. 203, 2009, pp. 3676–3685. (http://dx.doi.org/10.1016/j.surfcoat.2009.05.048).

Six Other Publications

1. J. Lin, J. J Moore, B. Mishra, M. Pinkas, W. D Sproul, "Structure, Mechanical and Tribological Properties of TiBCN Nanocomposite Coatings," *Acta Mater.* Vol. 58, 2009, pp. 1554–1564. (http://dx.doi.org/10.1016/j.actamat.2009.10.063)
2. J. Lin, B. Mishra, J. J. Moore, and W. D. Sproul, "Microstructure, mechanical and tribological properties of $Cr_{1-x}Al_xN$ films deposited by pulsed-closed field unbalanced magnetron sputtering (P-CFUBMS)," *Surface and Coatings Technology*. Vol. 201, 2006, pp. 4329–4334. (http://dx.doi.org/10.1016/j.surfcoat.2006.08.090)
3. J. Lin, B. Mishra, J. J. Moore, and W. D. Sproul, "A study of the oxidation behavior of CrN and CrAlN thin films in air using DSC and TGA analyses," *Surface and Coatings Technology*, Vol. 202, 2008, p. 3272. (http://dx.doi.org/10.1016/j.surfcoat.2007.11.037)
4. J. Lin, Z. L. Wu, X. H. Zhang, B. Mishra, J. J Moore, W. D. Sproul, "A Comparitive Study of CrNx coatings Synthesized by DC and Pulsed Magnetron Sputtering," *Thin Solid Films*, Vol. 517, 2009, pp. 1887–1894. (http://dx.doi.org/10.1016/j.tsf.2008.09.093)
5. J. Lin, B. Mishra, J. J. Moore, X. H. Zhang, W. D. Sproul, "CrN/AlN superlattice coatings synthesized by pulsed closed field unbalanced magnetron sputtering with different CrN layer thicknesses," *Thin Solid Films*, Vol. 517, 2009, pp. 5798–5804. (http://dx.doi.org/10.1016/j.tsf.2009.02.136)
6. J. Lin, J. J. Moore, W. D. Sproul, S. L. Lee, and J. Wang, "Effect of negative substrate bias on the structure and properties of Ta coatings deposited using modulated pulse power magnetron sputtering," *IEEE Transactions on plasma science, Special Issue on HIPIMS and High Power Glow Discharges*,Vol. 38, 2010, p. 3071. (http://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=5567170&tag=1)

Synergistic Activities and Contributions

- Contribution to the development of curricular book "Nanostructure and Nanocomposite Thin Films," in "Introduction to Nanoscience and Nanotechnology- Fundamentals of Nanotechnology," CRC Press, FL, USA ISBN-978-1-4200-4779-0, 2008.
- Contribution to the development of curricular book "Applications of Thin Films," *Introduction to Nanoscience and Nanotechnology - Fundamentals of Nanotechnology*, CRC Press, FL, USA ISBN-978-1-4200-4779-0, 2008.
- Helped and organized the annual international HPPMS/MPP workshop in Colorado School of Mines for 2009 and 2010.
- Member of American Vacuum Society; Committee Member of North American Die Casting Association; Member of The Society of Vacuum Coaters.
- Symposium Chair of Section B3 for the 39th International Conference on Metallurgical Coatings & Thin Films (2012), San Diego, USA.

Collaborators and Other Affiliations

Collaborators within last 48 months. William D. Sproul (Reactive Sputtering, LLC), Sastry Cheruvu (Soutwest Research Inhistitute), Frank Kustas (Engineering Coatings, Inc.), Sabrina L Lee (Army), Bassam Abraham and Roman Chistyakov (Zpulser).

Thesis Advisors. John J Moore and Brajendra Mishra (Colorado School of Mines).

Graduate students (over last 2 years). Sterling Myers, Masood Hashemi, Ningyi Zhang, and Bo Wang (all of Advanced Combustion Synthesis) Engineering Laboratory , Colorado School of Mines)

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Education and Training

- Postdoctoral Fellow Argonne National Laboratory (1987–1989).
- Postdoctoral Fellow, Xerox Corporation (1985–1987).
- Ph.D., University of Florida Physics (1985).
- B.A., Physics, Oxford University (United Kingdom) (1980).

Appointments

- Director, Nuclear Engineering Program, University of Florida (2011–present).
- Chair, Department of Materials Science and Engineering, University of Florida (2010–present).
- Professor, Department of Materials Science and Engineering, University of Florida (2003–present).
- Group Leader, Materials Science Division, Argonne National Laboratory (2002–2003).
- Physicist, Materials Science Division, Argonne National Laboratory (1995–2003).
- Assistant Physicist, Materials Science Division, Argonne National Laboratory (1989–1995).

Most Relevant Publications (Total 190+ with 7600+ citations)

1. S. R. Phillpot and S. B. Sinnott, "Simulating Multifunctional Structures," *Science* 325, 1634-1635 (2009).
2. T. Watanabe, S. B. Sinnott, J. S. Tulenko, R. W. Grimes, P. K. Schelling, and S. R. Phillpot, "Thermal Transport Properties of Uranium Dioxide by Molecular Dynamics Simulation," *Journal of Nuclear Materials* 375, 388-396 (2008)
3. D. S. Aidhy, P. C. Millett, T. Desai, D. Wolf, and S. R. Phillpot, "Point-Defect Clustering in UO_2 by Molecular-Dynamics Simulations," *Physical Review B* 80, 104107 (2009).
4. T.-R. Shan, T. K. Kemper, S. B. Sinnott, and S. R. Phillpot, "Empirical Charge Optimized Many Body Potential for Hafnium and Hafnium Oxide Systems," *Physical Review B* 81 125328 (2010).
5. D. A. Vega, T. Watanabe, S. B. Sinnott, S. R. Phillpot, and J. S. Tulenko, "Towards an Atomistically Informed Fuel Performance Code: Thermal Properties using FRAPCON and Molecular Dynamics Simulation," Nuclear Technology 165, 308-312 (2009)

Other Significant Publications

1. A. Chernatynskiy, R. W. Grimes, M. A. Zurbuchen, D. R. Clarke and S. R. Phillpot, "Thermal Properties of the Ruddlesden-Popper Phases of the Sr-Ti-O system," Applied Physics Letters 95, 161906 (2009).
2. H. Xu, D. W. Lee, J. He, S. B. Sinnott, V. Gopalan, V. Dierolf and S. R. Phillpot, "Stability of Intrinsic Defects and Defect Clusters in $LiNbO_3$ from Density Functional Theory Calculations," *Physical Review B* 78, 174103 (2008).

3. D. P. Aidhy, J. C. Nino, S. B. Sinnott, E. D. Wachsman and S. R. Phillpot, "Vacancy-Ordered Structure of Cubic Bismuth Oxide from Simulation and Crystallographic Analysis," *Journal of the American Ceramic Society* 91, 2349-2356 (2008).
4. S. B. Sinnott and A. Asthagiri, "Atomic-Level Simulation of Ferroelectricity in Oxides: Current Status and Opportunities," S. R. Phillpot, *Annual Review of Materials Research* 37 239-270 (2007).
5. D.–H. Kim, M. V. Manuel, F. Ebrahimi and S. R. Phillpot, "Deformation Processes in [11-20]-textured Nanocrystalline Mg by Molecular-Dynamics Simulation," *Acta Materialia* 58, 6217–6229 (2010).

Synergistic Activities

- Honors and Awards:
  - Fellowships: American Association for the Advancement of Science (2011), American Physical Society (2008); Institute of Materials, Minerals and Mining (2006), Institute of Physics (2006)
  - University of Florida Research Foundation Professorship (2010-2013)
  - Department of Materials Science and Engineering, University of Florida, Faculty Excellence Award (2009, 2008, 2007)
  - No. 56 on the list on the Thomson-Reuters list of the World's Top 100 most influential materials scientists, 2000-2010
- Editorships:
  - *Journal of Applied Physics:* Associate Editor (1993-present)
  - *Science:* Member of Board of Reviewing Editors (2009-present)
  - *Annual Review of Materials Research*: Editorial Board (2010-present)

Collaborators (outside UF)

David Cahill (Illinois), Long-Qing Chen (Penn State), David Clarke (Harvard), Beth Dickey (Penn State), Volkmar Dierolf (Lehigh), Anter El-Azab (FSU), Mike Finnis (Imperial College London), Venkat Gopalan (Penn State), Robin Grimes (Imperial College London), Hanchen Huang (U. Conn.) Pawel Keblinski (RPI), Alan McGaughey (CMU), Patrick Schelling (UCF), Darrell Schlom (Cornell), Srini Srivilliputhur (UNT), Chris Stanek (LANL), Blas Uberuaga (LANL), Dieter Wolf (ANL),Vesselin Yamakov (NIA), Mark Zurbuchen (UCLA).

Graduate and Postdoctoral Advisors

Doctoral: Pradeep Kumar (U. Florida)
Postdoc: Michael Rice (Xerox, deceased), Dieter Wolf (ANL)

Thesis Advisor and Postgraduate-Scholars Sponsored

Former postdoctoral associates. Past: Marcelo Sepliarsky (U. Rosario, Argentina), Patrick Schelling (UCF), Alan McGaughey (CMU), Inkook Jang (Samsung), Jianguo Yu (INL), Boris Ni (UNC Charlotte).

Current postdoctoral associates. Tao Liang, Aleksandr Chernatynskiy, Dundar Yilmaz.

Former graduate students. Taku Watanabe (Ph.D. Georgia Tech); Dilpuneet Aidhy (Ph. D., IBM Bangalore), Peter Barry (Ph.D., Gabriel Lipmann Institute), Rakesh Behera (Ph.D., Georgia Tech), Haixuan Xu (Ph.D., Oak Ridge) Donghwa Lee (Ph.D., Livermore), Priyank Shukla (Ph.D., Georgia Tech), Kun-Ta Tsai (M.S., Industry), Jasmine Davenport (Ph.D., US government), Dong Hyun Kim (Ph.D., Ames Lab).

Current graduate students. Yangzhong Li, Bowen Deng, Mark Noordhoek, Jackelyn Martinez, Anuj Goyal, Zizhe Lu, Tsu-Wu Chiang, Katherine Harris.

Dr. Ben Larson

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Education and Training

- Ph.D., University of Missouri, Columbia Physics, (1970).
- M.S., Physics, University of North Dakota (1965).
- B.A., Physics, Concordia College (1963).

Research and Professional Experiences

- Corporate Fellow, Materials Science and Technology Division, Oak Ridge National Laboratory (2006–present).
- Group Leader, Condensed Matter Sciences Division, Oak Ridge National Laboratory (2001–2006).
- Section Head, Solid State Division, Oak Ridge National Laboratory (1990–2006).
- Group Leader, Solid State Division, Oak Ridge National Laboratory (1973–2001).
- Guest Scientist, KFA–Jülich, Germany (1974–1975).
- Research Staff, Solid State Division, Oak Ridge National Laboratory (1969–1973).

Selected Publications

1. G. E. Ice, C.R. Hubbard, B.C. Larson, J.W.L. Pang, J.D. Budai, S. Spooner, S.C. Vogel, R.B. Rogge, J.H. Fox and R.L. Donaberger, "High-Performance Kirkpatrick-Baez Supermirrors for Neutron Milli- and Micro-beams," *Mat. Sci. and Eng.* A 437(1) 120-125 (2006).
2. L. E. Levine, P. Geantil, B. C. Larson, J. Z. Tischler, M. E. Kassner, W. J. Liu, M R. Stoudt, and F. Tavazza, "Disordered Long-Range Internal Stresses in Deformed Copper and The Mechanisms Underlying Plastic Deformation," *Acta Mater.* 59, 5803 (2011).
3. B. C. Larson, W. Ku, J. Z. Tischler, et al. "Nonresonant Inelastic X-Ray Scattering And Energy-Resolved Wannier Function Investigation of *d-d* Excitations in NiO and CoO," *Phys. Rev. Lett. 99, 026401* (2007).
4. B. C. Larson, J. Z. Tischler, A. E.-Azab, and W. Liu, "Dislocation Tensor Characterization of Deformation Using 3D X- Ray Microscopy," *Journal of Engineering Materials and Technology* 130, 021024-1 (2008).
5. L. E. Levine, B. C. Larson, W. Yang, M. E. Kassner, J. Z. Tischler, M. A. Delos-Reyes, R. J. Fields, and W. Liu, "X-Ray Microbeam Measurements of Individual Dislocation Cell Elastic Strains in Deformed Single-Crystal Copper," *Nature Materials* 5, 619 (2006).
6. B. C. Larson, Wenge Yang, G. E. Ice, J. D. Budai, and J. Z. Tischler, "Three-dimensional X-ray Structural Microscopy with Submicrometre Resolution," *Nature*, 415, 887 (2002).
7. B. C. Larson, A. El-Azab, W. Yang, J. Z. Tischler, W. Liu, and G. E. Ice, "Experimental Characterization of The Mesoscale Dislocation Density Tensor," *Philosophical Magazine A* 87, 1327 (2007).

8. J. Z. Tischler, G. Eres, B. C. Larson, C. M. Rouleau, P. Zschack, and D. H. Lowndes, "Nonequilibrium Interlayer Transport in Pulsed-Laser Deposition," *Phys. Rev. Lett.* 96, 226104 (2006).
9. G. E. Ice, C. R. Hubbard, B. C. Larson, J. W. L. Pang, J. D. Budai, S. Spooner, and S. C. Vogel, "Kirkpatrick-Baez Microfocusing Optics for Thermal Neutrons," *Nuc. Inst. Meth.* A 539, 312-320 (2004).
10. B. C. Larson and B. Lengeler, "High-Resolution Three-Dimensional X-Ray Microscopy," *MRS Bulletin* 29, 152 (2004).
11. W. Yang, B. C. Larson, G. M. Pharr, G. E. Ice, J. D. Budai, J. Z. Tischler, and W. J. Liu, "Deformation Microstructure Under Microindents in Single-Crystal Cu Using Three-Dimensional X-Ray Structural Microscopy," *Journal of Materials Research* 19, 66 (2004).
12. G. E. Ice, B. C. Larson, W. Yang, J. D. Budai, J. Z. Tischler, J. W. L. Pang, R. I. Barabash, and W. Liu, "Polychromatic X-Ray Microdiffraction Studies of Mesoscale Structure and Dynamics," *J. Synch. Radiat.* 12, 155 (2005).

Synergistic Activities

- Fellow, American Physical Society.
- Member, Cornell High Energy Synchrotron Source Policy & Advisory Board (2000–Present).
- Member, ChemMatCARS Scientific Advisory Committee (2011).
- Guest Editor, *MRS Bulletin*, Theme Article "High Resolution X-Ray Microscopy," (March 2004).
- Co-Organizer, Plasticity-2006 mini-symp. on "3D Plasticity Meas. and Sim.," (Halifax 2006).
- Member, Advanced Photon Source Proposal Evaluation Panel (2002–2005).

Collaborators and Co-editors

A. El-Azab (Florida State/Purdue), A. Bertram (Magdeburg University), G. Chen (Ohio Univ.), O. Eryilmaz (ANL), R. Fields (NIST), K. Finkelstein (Cornell), P. Geantil (USC), I. Gurtubay (Basque University), M. Kassner (ONR), W. Ku (BNL), L. Levine (NIST), J. Narayan (NCSU), G. Pharr (UT-Knoxville), O. Restrepo (Ohio State Univ.), J. Routbort (ANL), D. Singh (ANL), M. R. Stoudt (NIST), F. Tevassa, (NIST), W. Yang (Carnegie Institution of Washington),P. Zschack (Advanced Photon Source).

Graduate and Postdoctoral Advisors and Advisees

Graduate Advisor: Prof. C. W. Tompson (University of Missouri, Columbia); Wenge Yang (1999-2002), Carnegie Institution of Washington; Wenjun Liu (2000-2003), Advanced Photon Source, ANL.

Dr. Judy W. L. Pang

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Education and Training

- Ph.D., Physics, University of Toronto, Canada (1998).
- M.S., Physics, University of Toronto, Canada (1995).
- B.A., Physics, Queen's University, Canada (1994).

Research and Professional Experiences

- Staff scientist, Materials Science and Technology Division, Oak Ridge National Laboratory (2006–present).
- Staff scientist, Metals and Ceramics Division, Oak Ridge National Laboratory (2001–2006)
- Post Doctoral Fellow, University of Manchester, UK (1999–2001)

Selected Publications

1. J. W. L. Pang, G. E. Ice, and W. Liu, "The role of crystal orientation and surface proximity in the self-similar behavior of deformed Cu single crystals," *Mat. Sci. Eng. A*, in press.
2. G. E. Ice, and J. W. L. Pang, "Tutorial on x-ray MicroLaue Diffraction," *Materials Characterization*, 60, 1191 (2009).
3. T. Ohashi, R. Barabash, J. W. L. Pang, G. E. Ice, O. M. Barabash, "X-ray microdiffraction and strain gradient crystal plasticity studies of geometrically necessary dislocations near a Ni bicrystal grain boundary," *International Journal of Plasticity*, 25(5), 920 (2009).
4. J. W. L. Pang, R. B. Rogge, and R. L. Donaberger, "Effects of grain size on intergranular strain evolution in Ni," *Mater. Sci. Eng.* A-Struct. Mater. Prop. Microstruct. Process., 437, 21 (2006).
5. G. E. Ice, J. W. L. Pang, R. I. Barabash, and Y. Puzyrev, "Characterization of three-dimensional crystallographic distributions using polychromatic X-ray microdiffraction," *Scr. Mater.*, 55, 57 (2006).
6. R. I. Barabash, G. E. Ice, and J. W. L. Pang, "Gradients of geometrically necessary dislocations from white beam microdiffraction," *Mater. Sci. Eng. A*, 400, 125 (2005)
7. M. Preuss, J. W. L. Pang, P. J. Withers, and G. J. Baxter, "Inertia welding nickel-based superalloy: Part II. Residual stress characterization," *Metall. Mater. Trans. A-Phys. Metall. Mater. Sci.*, 33, 3227 (2002).
8. J. W. L. Pang, T. M. Holden, J. S. Wright, and T. E. Mason, "The generation of intergranular strains in 309H stainless steel under uniaxial loading," *Acta Mater.*, 48, 1131 (2000).
9. J. W. L. Pang, T. M. Holden, P. A. Turner, and T. E. Mason, "Intergranular stresses in Zircaloy-2 with rod texture," *Acta Mater.*, 47, 373 (1999).
10. J. W. L. Pang, T. M. Holden, and T. E. Mason, "In situ generation of intergranular strains in an A17050 alloy," *Acta Mater.*, 46, 1503 (1998).
11. J. W. L. Pang, T. M. Holden, and T. E. Mason, "The development of intergranular strains in a high-strength steel," J. Strain Anal. Eng. De., 33, 373 (1998).

Synergistic Activities

- Member, American Physical Society (Advanced Photon Source).
- Member, The Materials, Metals and Minerals Society (TMS).

Collaborators and Co-editors

J. Budai (Oak Ridge National Laboratory), G. E. Ice (Oak Ridge National Laboratory), J. Z. Tischler (Oak Ridge National Laboratory), E. A. Payzant (Oak Ridge National Laboratory), C. R. Hubbard (Oak Ridge National Laboratory), Y. Gao (University of Tennessee), Peter Liaw (University of Tennessee), Hahn Choo (University of Tennessee), D. Penumadu (University of Tennessee), R. Barabash (University of Tennessee), S. R. Agnew (Univeristy of Virginia), D. W. Brown, (LANL), C. N. Tome (LANL), B. N. Clausen (LANL), W. Liu (Advanced Photon Source), W. J. L. Buyers, (Chalk River Lab)

Graduate and Postdoctoral Advisors and Advisee

Graduate Advisor: Prof. T. E. Mason (University of Toronto), Dr. T.M. Holden (Chalk River Lab), Elena Garlea (2003–2008) (University of Tennessee).

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Education and Training

- Postdoctoral Fellow, General Motors Technical Center (2007 and 2008)
- Ph.D., Materials Science and Engineering, Northwestern University (2007)
- B.S., Materials Science and Engineering, University of Florida (2002)

Research and Professional Experience

Assistant Professor, Department of Materials Science and Engineering, University of Florida (2008–present).

Selected Awards and Honors

- National Science Foundation CAREER Award (2009)
- TMS Young Leaders Award (2009)
- ASA/Harriett G. Jenkins Award (2002–2007)
- National Academies Ford Foundation Award (2002-2007)

Selected Publications

1. H. S. Brar, J. Wong, and M. V. Manuel, "Investigation of the Mechanical and Degradation Properties of Mg-Sr and Mg-Zn-Sr Alloys as Potential Biodegradable Implant Materials." *Journal of the Mechanical Behavior of Biomedical Materials, In Press.*
2. D.-H. Kim, M. V. Manuel, F. Ebrahimi, J. S. Tulenko, and S. R. Phillopt, "Grain-Boundary Activated Pyramidal Dislocations in Nano-Textured Mg by Molecular Dynamics Simulations." *Materials Science and Engineering A.* Vol. 528, 2011, pp. 5411–5420.
3. M. V. Manuel and N. Hort, "Magnesium: An Essential Nutrient for a Good Biomaterial." *Journal of Metals.* Vol. 63, 2011, p. 95.
4. H. S. Brar, B. G. Keselowsky, M. Sarntinoranont, M. V. Manuel, "Design Considerations for Developing Biodegradable Magnesium Implants." *Journal of Metals.* Vol. 63 No. 4, 2011, pp. 96–100.
5. D.-H. Kim, M. V. Manuel, F. Ebrahimi, J. S. Tulenko, and S. R. Phillopt, "Deformation Processes in $[11\bar{2}0]$-textured Nanocrystalline Mg by Molecular-Dynamics Simulation." *Acta Materialia.,* Vol. 58, 2010, pp. 6217–6229.
6. H. S. Brar, P. O. Manu, M. Sarntinoranont, I. P. Martin, M. V. Manuel, "Magnesium as a Biodegradeable and Bioabsorbable Material for Medical Implants." *Journal of Metals.*, Vol. 61 No. 9, 2009, pp. 31–34.
7. J. E. Daniels, M. V. Manuel, C. W. Brink, and J. L. Jones, "Phase Transformation of Constrained $BaTiO_3$ Particles in a Sn Matrix." *Scripta Materialia.*, Vol. 61 No. 4, 2009, pg. 391–394.
8. M. V. Manuel, "Principles of Self-Healing in Metals and Alloys: An Introduction." *Self-Healing Materials: Fundamentals, Design Strategies and Applications*, ed. S. Ghosh, Wiley, 2008.

9. M. V. Manuel, A. F. McKenna, G. B. Olson, "Hierarchical Model for Coaching Technical Teams." *International Journal of Engineering Education*, Vol. 24, No. 2, 2008, pp. 260–265.

10. J. G. Polihronov, T. Dubroca, M. Manuel, and R. E. Hummel, "Porosity and Density of Spark Processed Silicon" *Materials Science & Engineering B*, Vol. 107, 2004, pp. 124–133.

Synergistic Activities

Service: Member of the Minerals, Metals and Materials Society (TMS), Materials Research Society (MRS), American Society for Metals (ASM), Alpha Sigma Mu Materials Honor Society, American Society for Engineering Education (ASEE), National Society of Black Engineers (NSBE), and the Society for Women Engineers (SWE). Member of the International Advisory Committee for the 2008 MRS International Materials Research Conference and Scientific Advisory Committee for the 2nd and 3rd International Conference on Self-Healing Materials.

Courses Taught

- Mechanical Behavior of Materials.
- Materials Design (Graduate and undergraduate specialty course).
- Materials Selection and Failure Analysis (Undergraduate capstone design course).
- Materials Thermodynamics (Graduate core course).

Collaborators and Other Affiliations

Collaborators and Co-editors: J.E. Daniels (European Synchrotron Radiation Facility), N. Hort (Magnesium Innovation Center), (A.F. McKenna (Arizona State Univ.), M. Platt (Georgia Tech), H. Seifert (Karlsruhe Institute of Technology), H.C. Shaw (NASA Goddard Space Flight Center)

Graduate Advisor and Postdoctoral Sponsor: Gregory B. Olson (Northwestern University) and Anil Sachdev (General Motors Technical Center)

Graduate Advisees: Ida Berglund, Ryan Hooper, Cynthia Papesch, Glenn Bean, Billy Valderrama, Zachary Bryan, Hunter Henderson, Charles Fisher, Fatmata Barrie, Derek Hsu, Harpreet Brar (all University of Florida affiliations). Total number of Ph.D students advised as major advisor is 11.

Dr. Marat Khafizov

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Education

- Ph.D., Physics, University of Rochester, Rochester, New York (2007).
- M.A., Physics, University of Rochester, Rochester, New York (2003).
- B.S., Physics, Middle East Technical University, Ankara, Turkey (2001).

Research Experience

- Associate Research Scientist, Idaho National Laboratory, Idaho Falls, ID (2011 to present).
- Postdoctoral Research Associatem, Department of Chemistry, University of Rochester, Rochester, New York (2007 to 2010).
- Research Assistant, Laboratory for Laser Energetics, University of Rochester, Rochester, New York (2002 to 2007).

Publications

1. M. Khafizov and D. H.Hurley, "Measurement of thermal transport using thermal wave microscopy," *J. Appl. Physics* 110, 083525 (2011).
2. M. Asle Zaeem, H. El Kadiri, M.F. Horstemeyer, M. Khafizov, Z. Utegulov, "Effects of internal stresses and intermediate phases on the coarsening of coherent precipitates: A phase-field study," *Current Applied Physics*, in press (2011).
3. D. H.Hurley, M. Khafizov, S. L. Shinde, "Measurement of the Kapitza resistance across a bicrystal interface," *J. of Appl. Physics* **109**,083504 (2011).
4. S. Wang, M. Khafizov, X. Tu, M. Zheng, T. D. Krauss, "Multiple Exciton Generation in Single-walled Carbon Nanotubes," *Nano Lett.* **20**, 2381 (2010).
5. D. Pan, G. P. Pepe, V. Pagliarulo, C. De Lisio, L. Parlato, M. Khafizov, I. Komissarov, and Roman Sobolewski, "Nano-layered ferromagnet/superconductor heterostructures: nonequilibrium quasiparticle dynamics and photodetector applications," *Phys. Rev. B.* **78**, 174503 (2008).
6. Y. Xu, M. Khafizov, L. Satrapinsky, P. Kús, A. Plecenik, and Roman Sobolewski, "Time-Resolved Photoexcitation of the Superconducting Two-Gap State in MgB_2 Thin Films" *Physical Review Letters,* **91**, 197004, (2003).

Seminar Talks

- Idaho National Laboratory, Idaho Falls, ID, September, 2009.
- Massachusetts Institute of Technology, Cambridge, MA, August 2008.
- University of Michigan, Ann Arbor, MI, July 2007.
- University of Illinois at Urbana Champaign, IL, May 2007.
- CBC Seminar, University of California, Irvine, CA, April 2007.

Professional Activities

- Membership in professional organizations: MRS (2009 to present), Advanced Photon Source.
- Reviewer for Journal of Applied Physics, Physical Review Letters.

Collaborations

Prof. Heng Ban (Utah State University), Prof. Haitham el Kadiri (Mississippi State University), Prof. Kenan Gundogdu (North Carolina State University), Prof. Giampiero Pepe (University of Naples Federico II, Italy), Dr. Subash Shinde, (Sandia NL), Prof. Izabela Szlufarska (University of Wisconsin), Prof. Zhandos Utegulov (Nazarbayev University, Kazakhstan), Dr. Ming Zhang (Nat. Inst. Stand. Tech.).

Graduate and Postdoctoral Advisors

Prof. Roman Sobolewski, (graduate, University of Rochester), Prof. Todd Krauss, (postdoc, University of Rochester)

7. CURRENT AND PENDING SUPPORT

Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Void Swelling Characterization of Austenitic Stainless Steels Irradiated in the BOR-60 Reactor, 6F-00035**	
Source of Support: Argonne National Laboratory Location of Project: University of Wisconsin	
Total Award Amount: $437,540	Total Award Period Covered: 01/01/06 – 9/31/11
Total Award Amount to PI's Research: $437,540	
Describe Synergies and/or overlaps with This Proposal/Award: This project is in the same general technical area of radiation effects.	
Person-Months Per Year Committed to Project: No time commitment; Specify: Cal., Acad., or Sumr:	
Investigator: K. Sridharan **Co-Investigator: T. Allen**	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Liquid Salts as Media for Process Heat Transfer from VHTR: Forced Convective Channel Flow, DE-FC07-07ID14826**	
Source of Support: Department of Energy- Location of Project: University of Wisconsin	
Total Award Amount: $575,590	Total Award Period Covered: 06/01/07 – 01/31/12
Total Award Amount to PI's Research: $575,590	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: No time commitment; Specify: Cal., Acad., or Sumr:	
Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **INL Employee Leasing**	
Source of Support: Idaho National Laboratory Location of Project: Idaho	
Total Award Amount: $274,230	Total Award Period Covered: 04/01/10 – 03/31/12
Total Award Amount to PI's Research: $274,230	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 6 Pers. Months; Specify: Cal., Acad., or Sumr: Cal	

Investigator: I. Szlufarska **Co-Investigator: T. Allen**	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Radiation Effects in Nanocrystalline Ceramics: Multi-Scale Model and Experiment, DE-FG02-08ER46493**	
Source of Support: Department of Energy-Idaho Location of Project: University of Wisconsin	
Total Award Amount: $ 1,322,648	Total Award Period Covered: 06/15/08 – 06/14/14
Total Award Amount to PI's Research: $1,322,648	
Describe Synergies and/or overlaps with This Proposal/Award: This project is in the same general technical area of radiation effects.	
Person-Months Per Year Committed to Project: 0.25 Pers. Months; Specify: Cal., Acad., or Sumr: Acad	
Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Studies in Support of the Deep Burn Concept, 4000086941**	
Source of Support: Department of Energy, UT-Battelle, LLC Location of Project: University of Wisconsin	
Total Award Amount: $210,000	Total Award Period Covered: 11/17/09 – 12/31/11
Total Award Amount to PI's Research: $210,000	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.1 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	
Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Sodium Compatibility of Advanced Fast Reactor Materials, 4000077248**	
Source of Support: Department of Energy, UT-Battelle, LLC Location of Project: University of Wisconsin	
Total Award Amount: $395,000	Total Award Period Covered: 01/16/09 – 06/30/12
Total Award Amount to PI's Research: $395,000	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: No time commitment; Specify: Cal., Acad., or Sumr:	
Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Ion Beam Analysis, 00074713**	
Source of Support: Department of Energy, Battelle Energy Alliance LLC Location of Project: University of Wisconsin	
Total Award Amount: $175,696	Total Award Period Covered: 04/18/08 – 09/30/12
Total Award Amount to PI's Research: $175,696	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.1 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: W. Crone **Co-Investigator: T. Allen**	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Assessment of Embrittlement of VHTR Structural Alloys in Impure Helium Environments, 00088925**	
Source of Support: Department of Energy, Battelle Energy Alliance LLC Location of Project: University of Wisconsin	
Total Award Amount: $489,707	Total Award Period Covered: 10/01/09 – 09/30/12
Total Award Amount to PI's Research: $489,707	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.25 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	
Investigator: D. Morgan **Co-Investigator: T. Allen**	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Ab Initio Enhanced Calphad Modeling of Actinide Rich Nuclear Fuels, 00088978**	
Source of Support: Department of Energy, Battelle Energy Alliance, LLC Location of Project: University of Wisconsin	
Total Award Amount: $486,338	Total Award Period Covered: 10/01/09 – 09/30/12
Total Award Amount to PI's Research: $486,338	
Describe Synergies and/or overlaps with This Proposal/Award: This project is in the same general technical area of nuclear fuel.	
Person-Months Per Year Committed to Project: 0.25 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	
Investigator: K. Sridharan **Co-Investigator: T. Allen**	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Development of Diffusion Barrier Coatings and Deposition Technologies for Mitigating Fuel Cladding Chemical Interactions (FCCI), 00088881**	
Source of Support: Department of Energy, Battelle Energy Alliance LLC Location of Project: University of Wisconsin	
Total Award Amount: $ 441,584	Total Award Period Covered: 10/01/09 – 09/30/12
Total Award Amount to PI's Research: $441,584	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.15 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	
Investigator: K. Sridharan **Co-Investigator: T. Allen**	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Thermal Properties of LiCl-KCl Molten Salt for Nuclear Waste Separation, 00088757**	
Source of Support: Department of Energy, Battelle Energy Alliance LLC Location of Project: University of Wisconsin	
Total Award Amount: $478,584	Total Award Period Covered: 10/01/09 – 09/30/12
Total Award Amount to PI's Research: $478,584	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.15 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: I. Szlufarska **Co-Investigator: T. Allen**	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Modeling Fission Product Sorption in Graphite Structures, 00089350**	
Source of Support: Department of Energy, Battelle Energy Alliance, LLC Location of Project: University of Wisconsin	
Total Award Amount: $479,473	Total Award Period Covered: 10/01/09 – 09/30/12
Total Award Amount to PI's Research: $479,473	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.25 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	
Investigator: M. Anderson **Co-Investigator: T. Allen**	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Materials, Turbomachinery, and Heat Exchangers for Supercritical CO2 Systems, 00088775**	
Source of Support: Department of Energy, Battelle Energy Alliance LLC Location of Project: University of Wisconsin	
Total Award Amount: $ 533,354	Total Award Period Covered: 10/01/09 – 09/30/12
Total Award Amount to PI's Research: $533,354	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: No time commitment; Specify: Cal., Acad., or Sumr:	
Investigator: M. Anderson **Co-Investigator: T. Allen**	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Liquid Salt Heat Exchanger Technology for VHTR-Based Applications, 00088234**	
Source of Support: Department of Energy, Battelle Energy Alliance LLC Location of Project: University of Wisconsin	
Total Award Amount: $495,958	Total Award Period Covered: 10/01/09 – 09/30/12
Total Award Amount to PI's Research: $495,958	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: No time commitment; Specify: Cal., Acad., or Sumr:	
Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Energy Frontier Research Center Support, Center for Materials Science of Nuclear Fuel, 00091644**	
Source of Support: Department of Energy, Battelle Energy Alliance, LLC Location of Project: University of Wisconsin	
Total Award Amount: $1,045,000	Total Award Period Covered: 09/28/09 – 09/30/14
Total Award Amount to PI's Research: $1,045,000	
Describe Synergies and/or overlaps with This Proposal/Award: NA	
Person-Months Per Year Committed to Project: No time commitment; Specify: Cal., Acad., or Sumr:	

Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Bulk Nanostructured Austenitic Stainless Steels with Enhanced Radiation Tolerance, A8741**	
Source of Support: Texas A&M University, DOE/Battelle Energy Alliance Location of Project: University of Wisconsin	
Total Award Amount: $210,000 to UW	Total Award Period Covered: 10/01/09 – 09/30/12
Total Award Amount to PI's Research: $210,000	
Describe Synergies and/or overlaps with This Proposal/Award: This project is in the same general technical area of radiation effects.	
Person-Months Per Year Committed to Project: 0.25 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: K. Sridharan **Co-Investigator: T. Allen**	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Corrosion in Supercritical Carbon Dioxide: Materials, Environmental Purity, Surface Treatments, and Flow Issues, 00102081**	
Source of Support: Department of Energy, Battelle Energy Alliance LLC Location of Project: University of Wisconsin	
Total Award Amount: $651,447	Total Award Period Covered: 07/28/10 – 07/28/13
Total Award Amount to PI's Research: $651,447	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.1 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: K. Sridharan **Co-Investigator: T. Allen**	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Study of Interfacial Interactions using Thin Film Surface Modification: Radiation and Oxidation Effects in Materials, 00102092**	
Source of Support: Department of Energy, Battelle Energy Alliance, LLC Location of Project: University of Wisconsin	
Total Award Amount: $538,032	Total Award Period Covered: 07/14/10 – 07/30/13
Total Award Amount to PI's Research: $538,032	
Describe Synergies and/or overlaps with This Proposal/Award: This project is in the same general technical area of radiation effects.	
Person-Months Per Year Committed to Project: 0.1 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Pulsed Magnetic Welding for Advanced Core and Cladding Steels, 00102267**	
Source of Support: Department of Energy, Battelle Energy Alliance LLC Location of Project: University of Wisconsin	
Total Award Amount: $525,206	Total Award Period Covered: 07/28/10 – 07/28/13
Total Award Amount to PI's Research: $525,206	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.10 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Freeze-Casting as a Novel Manufacturing Process for Fast Reactor Fuels, 239291-3668**	
Source of Support: Drexel University, DOE/Battelle Energy Alliance Location of Project: University of Wisconsin	
Total Award Amount: $1,149,327 to Drexel Univ Total Award Period Covered: 09/14/10 – 09/30/13	
Total Award Amount to PI's Research: $229,898	
Describe Synergies and/or overlaps with This Proposal/Award: This project is in the same general technical area of nuclear fuel.	
Person-Months Per Year Committed to Project: 0.25 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Critical Experiments to Understand the Radiation Response of Materials for Fast Reactor Cladding and Duct Application, 3001678748**	
Source of Support: University of Michigan, DOE/Battelle Energy Alliance Location of Project: University of Wisconsin	
Total Award Amount: $1,181,379 to Univ of Michigan Total Award Period Covered: 09/01/10 – 07/31/13	
Total Award Amount to PI's Research: $542,944	
Describe Synergies and/or overlaps with This Proposal/Award: This project is in the same general technical area of radiation effects.	
Person-Months Per Year Committed to Project: 0.25 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: Dane Morgan **Co-Investigator: T. Allen**	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Understanding the Irradiation Behavior of Zirconium Carbide, 4228-UWM-BINL-0975**	
Source of Support: Pennsylvania State University, DOE/Battelle Energy Alliance Location of Project: University of Wisconsin	
Total Award Amount: $870,613 to Penn State University Total Award Period Covered: 07/14/10 – 07/31/13	
Total Award Amount to PI's Research: $486,348	
Describe Synergies and/or overlaps with This Proposal/Award: This project is in the same general technical area of radiation effects.	
Person-Months Per Year Committed to Project: 0.1 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Determining the Factor of Improvement in Resistance of Stress Corrosion Crack Initiation of Alloy 690 over Alloy 600, EP-P37815/C16969**	
Source of Support: Electric Power Research Institute Location of Project: University of Wisconsin	
Total Award Amount: $300,000	Total Award Period Covered: 04/01/10 – 03/31/14
Total Award Amount to PI's Research: $300,000	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.1 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	
Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Transmission Electron Microscopy Examination of Irradiated Stainless Steel Hex Blocks**	
Source of Support: Nuclear Fuel Industries, Ltd. Location of Project: University of Wisconsin	
Total Award Amount: $30,628	Total Award Period Covered: 08/01/10 – 07/31/12
Total Award Amount to PI's Research: $30,628	
Describe Synergies and/or overlaps with This Proposal/Award: This project is in the same general technical area of radiation effects.	
Person-Months Per Year Committed to Project: No time commitment; Specify: Cal., Acad., or Sumr:	
Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **General Scientific Infrastructure Support, DE-NE0000321**	
Source of Support: Department of Energy-Idaho Location of Project: University of Wisconsin	
Total Award Amount: $246,173	Total Award Period Covered: 09/01/10 – 11/30/11
Total Award Amount to PI's Research: $246,173	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: No time commitment; Specify: Cal., Acad., or Sumr:	
Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Irradiation Creep of Graphite, 00105072**	
Source of Support: Department of Energy, Battelle Energy Alliance LLC Location of Project: University of Wisconsin	
Total Award Amount: $61,912	Total Award Period Covered: 10/1/10 – 1/01/12
Total Award Amount to PI's Research: $61,912	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: No time commitment; Specify: Cal., Acad., or Sumr:	

Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Research in Support of VHTR Safety Performance, NRC-04-10-173**	
Source of Support: Nuclear Regulatory Commission Location of Project: University of Wisconsin	
Total Award Amount: $300,000	Total Award Period Covered: 10/1/10 – 9/30/13
Total Award Amount to PI's Research: $300,000	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.25 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Diffusion of Silver through SiC to Determine Mechanisms of Fuel Performance in TRISO Fuel, 00107188**	
Source of Support: Department of Energy-Idaho Location of Project: University of Wisconsin	
Total Award Amount: $25,000	Total Award Period Covered: 10/29/10 – 10/31/11
Total Award Amount to PI's Research: $25,000	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: No time commitment; Specify: Cal., Acad., or Sumr:	

Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Mitigating Corrosion of 5xxx Series Al-Mg Alloys in Marine Environments: Grain Boundary Engineering and Cold Spray Approaches, N00014-11-1-0326**	
Source of Support: Office of Naval Research Location of Project: University of Wisconsin	
Total Award Amount: $293,253	Total Award Period Covered: 01/01/11 – 12/31/13
Total Award Amount to PI's Research: $293,253	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.25 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Diffusion of Silver in Silicon Carbide, 00116597**	
Source of Support: Department of Energy, Battelle Energy Alliance, LLC Location of Project: University of Wisconsin	
Total Award Amount: $50,000	Total Award Period Covered: 07/13/11 – 05/31/12
Total Award Amount to PI's Research: $50,000	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: No time Commitment ; Specify: Cal., Acad., or Sumr:	

Investigator: D. Morgan **Co-Investigator: T. Allen**	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Collaborative Research: Determination of Ni-Fe-Cr Species Dependent Transport Through Control of Temperature, Irradiation, and Grain Size, DMR-1105640**	
Source of Support: National Science Foundation Location of Project: University of Wisconsin	
Total Award Amount: $370,000	Total Award Period Covered: 09/01/11 – 08/31/14
Total Award Amount to PI's Research: $370,000	
Describe Synergies and/or overlaps with This Proposal/Award: This project is in the same general technical area of radiation effects.	
Person-Months Per Year Committed to Project: 0.1 Pers. Months; Specify: Cal., Acad., or Sumr:	

Investigator: I. Szlufarska **Co-Investigator: T. Allen**	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Ag Transport through Non-Irradiated and Irradiated SiC, 00118099**	
Source of Support: Department of Energy, Battelle Energy Alliance, LLC Location of Project: University of Wisconsin	
Total Award Amount: $1,055,456	Total Award Period Covered: 08/22/11 – 9/30/14
Total Award Amount to PI's Research: $1,055,456	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.1 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Surface Treatments to Improve Wear Resistance of Agricultural Equipment**	
Source of Support: University of Wisconsin Graduate School Location of Project: University of Wisconsin	
Total Award Amount: $49,260	Total Proposed Period Covered: 07/01/11 – 06/30
Total Award Amount to PI's Research: $49,260	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: No time commitment; Specify: Cal., Acad., or Sumr:	

Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Award in Process	
Project/Proposal Title and grant number, if appropriate: **Development of Advanced High Uranium Density Fuels for Light Water Reactors**	
Source of Support: Department of Energy, Battelle Energy Alliance, LLC Location of Project: University of Wisconsin	
Total Award Amount: $900,000	Total Award Period Covered: 10/01/11 – 09/30
Total Award Amount to PI's Research: $900,000	
Describe Synergies and/or overlaps with This Proposal/Award: This project is in the same general technical area of nuclear fuel.	
Person-Months Per Year Committed to Project: 0.1 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Pending/Award in Process	
Project/Proposal Title and grant number, if appropriate: **High-Temperature Salt-Cooled Reactor for Power and Process Heat**	
Source of Support: Massachusetts Institute of Technology, DOE/Battelle Energy Alliance Location of Project: University of Wisconsin	
Total Award Amount: $7,500,000 to Massachusetts Institute of Technology Total Proposed Period Covered: 10/01/11 – 09/30/14	
Total Award Amount to PI's Research: $900,000	
Describe Synergies and/or overlaps with This Proposal/Award: This project is in the same general technical area of radiation effects.	
Person-Months Per Year Committed to Project: 0.1 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: K. Sridharan **Co-Investigator: T. Allen**	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Pending/Award in Process	
Project/Proposal Title and grant number, if appropriate: **Fuel Aging in Storage and Transportation (FAST): Accelerated Characterization and Performance Assessment of the Used Nuclear Fuel Storage System**	
Source of Support: Texas A&M University, DOE/Battelle Energy Alliance Location of Project: University of Wisconsin	
Total Award Amount: $4,500,000 to Texas A&M Total Proposed Period Covered: 10/01/11 – 09/30/14	
Total Award Amount to PI's Research: $710,000	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.1 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Pending/Award in Process	
Project/Proposal Title and grant number, if appropriate: **Advanced Nuclear Technology Development Infrastructure**	
Source of Support: Department of Energy, Battelle Energy Alliance, LLC Location of Project: Wisconsin	
Total Award Amount: $292,756	Total Proposed Period Covered: 10/01/11 – 09/30/12
Total Award Amount to PI's Research: $292,756	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: No time commitment; Specify: Cal., Acad., or Sumr:	

Investigator: T. Allen	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Pending	
Project/Proposal Title and grant number, if appropriate: **Cavitation Mechanisms in Amorphous Materials**	
Source of Support: Department of Energy, Battelle Energy Alliance, LLC Location of Project: Wisconsin	
Total Award Amount: $292,384	Total Proposed Period Covered: 01/01/12 – 12/31/14
Total Award Amount to PI's Research: $292,384	
Describe Synergies and/or overlaps with This Proposal/Award: This project is in the same general technical area of radiation effects.	
Person-Months Per Year Committed to Project: **0.1** Pers. Months; Specify: Cal., Acad., or Sumr:	
Investigator: Anter El-Azab	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Statistical Mechanics Modeling of Mesoscale Deformation of Metals**	
Source of Support: DOE Basic Energy Sciences/MSED Location of Project: Florida State University	
Total Award Amount: $325,252 Total Award Period Covered: 06/01/2008-02/29/2012	
Total Award Amount to PI's Research: $325,252	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.5 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	
Investigator: Anter El-Azab	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title And Grant Number, If Appropriate: **Computational Modeling of Mesoscale Deformation of Copper Crystals for Comparison with X-Ray Measurements**	
Source of Support: Oak Ridge National Lab Location of Project: Florida State University	
Total Award Amount: $ 105K Total Award Period Covered: 1/1/2010-5/31/2012	
Total Award Amount to PI's Research: $ 105K	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: __0__ Pers. Months; Specify: Cal., Acad., or Sumr:	
Investigator: Anter El-Azab	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Structure and Morphological Stability of Oxide Thin Film Systems Produced by Pulsed-laser Deposition**	
Source of Support: Oak Ridge National Lab Location of Project: Florida State University	
Total Award Amount: $52,571	Total Award Period Covered: 7/26/2010-12/15/2011
Total Award Amount to PI's Research: $52,571	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0 Pers. Months; Specify: Cal., Acad., or Sumr:	

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: **Energy Frontier Research Center, CMSN—Computational Microstructure Science**	
Source of Support: DOE Location of Project: Florida State University	
Total Award Amount: $960K	Total Award Period Covered: 3 years
Total Award Amount to PI's Research: estimated $35k per year for 3 years	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0 Pers. Months; Specify: Cal., Acad., or Sumr:	

Investigator: Anter El-Azab	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Uncertainty Analysis of Mesoscale Models of Radiation Effects in Materials**	
Source of Support: Idaho National Laboratory Location of Project: Florida State University	
Total Award Amount: $164.8K	Total Award Period Covered: 7/1/2011-9/30/2012
Total Award Amount to PI's Research: estimated $164.8k for the above period	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.5 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: David Hurley	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, Center for Materials Science of Nuclear Fuels**	
Source of Support: DOE Basic Energy Sciences Location of Project: Idaho National Laboratory	
Total Award Amount: $2M Total Award Period Covered: 08/01/2009-09/2012	
Total Award Amount to PI's Research: $300K	
Describe Synergies and/or overlaps with This Proposal/Award: Oversee phonon transport studies conducted at INL, Advanced Photon Source (at Argonne National Lab), University of Florida, and Florida State University	
Person-Months Per Year Committed to Project: 2 Pers. Months; Specify: Cal., Acad., or Sumr: Cal	

Investigator: David Hurley	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Laser-based Characterization Technique Development**	
Source of Support: Nuclear Energy, Advanced Fuel Cycle Initiative Location of Project: Idaho National Laboratory	
Total Award Amount: $865K Total Award Period Covered: FY12	
Total Award Amount to PI's Research: $865K	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 8 Pers. Months; Specify: Cal., Acad., or Sumr: Cal	

Investigator: David Hurley	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Non Destructive Thermal Analysis and In Situ Investigation of Creep Mechanism of Graphite using Phase-sensitive THz Imaging and Nonlinear Resonant Ultrasonic Spectroscopy**	
Source of Support: Nuclear Energy, Nuclear Energy University Programs (NEUP) Location of Project: Idaho National Laboratory	
Total Award Amount: $150K Total Award Period Covered: FY12	
Total Award Amount to PI's Research: $30K	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 0.5 Pers. Months; Specify: Cal., Acad., or Sumr: Cal	

Investigator: David Hurley	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Evaluate the Application of Advanced Measurement Systems to Investigate SiC Nuclear Fuel Cladding**	
Source of Support: Nuclear Energy, Light Water Reactor Sustainability Location of Project: Idaho National Laboratory	
Total Award Amount: $300K Award Period Covered: FY12	
Total Award Amount to PI's Research: $300K	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 1.5 Pers. Months; Specify: Cal., Acad., or Sumr: Cal	

Investigator: B. C. Larson	Other Agencies to which this proposal has been/will be submitted:
Support (XCurrent, Pending, Submission Planned in Future or Transfer of Support):	
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 Nat. Lab.	
Total Award Amount: $ 3.8 M/yr Total Award Period Covered: FY 07-14	
Total Award Amount to PI's Research: $244 K	
Describe Synergies and/or overlaps with This Proposal/Award: Enhance our fundamental understanding of defects, defect interactions, and defect dynamics that determine the performance of structural alloys in extreme radiation environments. Investigators role involves time-resolved and microbeam x-ray studies; work is distinct from other investigator projects.	
Person-Months Per Year Committed to Project: _4.8_ Pers. Months; Specify: XCal., Acad., or Sumr:	

Investigator: B. C. Larson	Other Agencies to which this proposal has been/will be submitted:
Support (XCurrent, Pending, Submission Planned in Future or Transfer of Support):	
Project/Proposal Title and grant number, if appropriate: **Center for Materials Science of Nuclear Fuel Energy Frontier Research Center (ERKCM58). This project is part of the INL Energy Frontier Research Center by this name, but direct funded to Oak Ridge National Laboratory under ERKCM58)**	
Source of Support: DOE BES Location of Project: Idaho National Laboratory	
Total Award Amount: $ 2 M/yr Total Award Period Covered: FY 07-14	
Total Award Amount to PI's Research: $ 92 K	
Describe Synergies and/or overlaps with This Proposal/Award: Develop predictive computational models, validated by experiments, for the thermal and mechanical behavior of analogues to nuclear fuel. Investigator's role involves inelastic neutron scattering and interaction with theory. Distinct from other investigator projects.	
Person-Months Per Year Committed to Project: _1.8_ Pers. Months; Specify: XCal., Acad., or Sumr:	

Investigator: B. C. Larson	Other Agencies to which this proposal has been/will be submitted:
Support X(Current, Pending, Submission Planned in Future or Transfer of Support):	
Project/Proposal Title and grant number, if appropriate: **Epitaxial Complex Oxides: Growth Mechanisms and Cooperative Phenomena (ERKCS80)**	
Source of Support: DOE BES Location of Project: Oak Ridge National Laboratory	
Total Award Amount: $ 1200 K Total Award Period Covered: FY 10-12	
Total Award Amount to PI's Research: $ 31 K	
Describe Synergies and/or overlaps with This Proposal/Award: Fundamental investigations of nonequilibrium pulsed-laser deposition growth using in-situ time-resolved synchrotron x-ray diffraction at the Advanced Photon Source. Investigator's role is in situ x-ray scattering and is distinct from investigators work in other projects.	
Person-Months Per Year Committed to Project: 0.6_ Pers. Months; Specify: XCal., Acad., or Sumr:	

Investigator: Simon Phillpot	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, Center for Material Science of Nuclear Fuels**	
Source of Support: DOE Basic Energy Sciences Location of Project: University of Florida	
Total Award Amount: $1,000K Award Period Covered: 10/8/2009 – 9/30/2014	
Total Award Amount to PI's Research: $1,000K	
Describe Synergies and/or overlaps with This Proposal/Award:	
Person-Months Per Year Committed to Project: 1.5 Pers. Months; Specify: Cal., Acad., or Sumr: Acad.	

Investigator: Simon Phillpot	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Computational Study of Fission Product Clustering in Nuclear Fuels**	
Source of Support: Los Alamos National Laboratory Location of Project: University of Florida	
Total Award Amount: $119,625 Award Period Covered: 04/02/10-10/01/12	
Total Award Amount to PI's Research: $	
Describe Synergies and/or overlaps with This Proposal/Award:	
Person-Months Per Year Committed to Project: .21 Pers. Months; Specify: Cal., Acad., or Sumr: Acad.	

Investigator: Simon Phillpot	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Rapid Discovery of Tribological Material with Improved Performance using Materials Informatics**	
Source of Support: ONR Location of Project: University of Florida	
Total Award Amount: $900,000 Award Period Covered: 01/01/10-12/31/12	
Total Award Amount to PI's Research:	
Describe Synergies and/or overlaps with This Proposal/Award:	
Person-Months Per Year Committed to Project: 1.0 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr.	

Investigator: Simon Phillpot	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **High Temperature Reactivity: Methods and Mechanisms**	
Source of Support: National Science Foundation Location of Project: University of Florida	
Total Award Amount: $500,000 Award Period Covered: 10/01/10-09/30/13	
Total Award Amount to PI's Research:	
Describe Synergies and/or overlaps with This Proposal/Award:	
Person-Months Per Year Committed to Project: 1.0 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr.	

Investigator: Simon Phillpot	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **Fuel Performance Experiments on the Atomistic Level, Studying Fuel Through Engineered Single Crystal UO_2**	
Source of Support: Idaho State University Location of Project: University of Florida	
Total Award Amount: $300,000 Award Period Covered: 10/01/10-09/30/13	
Total Award Amount to PI's Research: $	
Describe Synergies and/or overlaps with This Proposal/Award:	
Person-Months Per Year Committed to Project: 1.5 Pers. Months; Specify: Cal., Acad., or Sumr: Acad.	

Investigator: Simon Phillpot	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **The Consortium for Advanced Simulation of Light-water Reactors (CASL)**	
Source of Support: Oak Ridge National Laboratory Location of Project: University of Florida	
Total Award Amount: $120,170 Award Period Covered: 09/01/10-12/16/11	
Total Award Amount to PI's Research: $	
Describe Synergies and/or overlaps with This Proposal/Award:	
Person-Months Per Year Committed to Project: 1.0 Pers. Months; Specify: Cal., Acad., or Sumr: Acad.	

Investigator: Simon Phillpot	Other Agencies to which this proposal has been/will be submitted:
Support: Pending	
Project/Proposal Title and grant number, if appropriate: **Novel Materials Design and Characterization for Validation**	
Source of Support: ARL – University of Texas Location of Project: University of Florida	
Total Award Amount: $883,819 Award Period Covered: 02/01/12-01/31/16	
Total Award Amount to PI's Research: $	
Describe Synergies and/or overlaps with This Proposal/Award:	
Person-Months Per Year Committed to Project: .3 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr.	

Investigator: Simon Phillpot	Other Agencies to which this proposal has been/will be submitted:
Support: Current	
Project/Proposal Title and grant number, if appropriate: **The Computational Alloy Design for Fusion Applications**	
Source of Support: DOE – Purdue Location of Project: University of Florida	
Total Award Amount: $100,000,000 Award Period Covered: 06/01/12-05/31/17	
Total Award Amount to PI's Research: $	
Describe Synergies and/or overlaps with This Proposal/Award:	
Person-Months Per Year Committed to Project: .5 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr.	

Investigator: Simon Phillpot	Other Agencies to which this proposal has been/will be submitted:
Support: Pending	
Project/Proposal Title and grant number, if appropriate: **FRG: Collaborative Research: A nanoscale Field Theory and Computational Analysis of Flexoelectric Materials**	
Source of Support: National Science Foundation Location of Project: University of Florida	
Total Award Amount: $254,549 Award Period Covered: 05/01/12-04/31/15	
Total Award Amount to PI's Research: $	
Describe Synergies and/or overlaps with This Proposal/Award:	
Person-Months Per Year Committed to Project: .5 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr.	

<table>
<tr><td>Investigator: Simon Phillpot</td><td>Other Agencies to which this proposal has been/will be submitted:</td></tr>
<tr><td colspan="2">Support: Pending</td></tr>
<tr><td colspan="2">Project/Proposal Title and grant number, if appropriate:
Unit Defect and Microstructural Processes at Metal/Dielectric Interfaces: An Integrated Experimental and Simulation Approach</td></tr>
<tr><td colspan="2">Source of Support: National Science Foundation
Location of Project: University of Florida</td></tr>
<tr><td colspan="2">Total Award Amount: $976,906
Award Period Covered: 05/01/12-04/30/16</td></tr>
<tr><td colspan="2">Total Award Amount to PI's Research: $</td></tr>
<tr><td colspan="2">Describe Synergies and/or overlaps with This Proposal/Award:</td></tr>
<tr><td colspan="2">Person-Months Per Year Committed to Project: .5 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr.</td></tr>
<tr><td>Investigator: J. W. L. Pang</td><td>Other Agencies to which this proposal has been/will be submitted:</td></tr>
<tr><td colspan="2">Support (XCurrent, Pending, Submission Planned in Future or Transfer of Support):</td></tr>
<tr><td colspan="2">Project/Proposal Title and grant number, if appropriate:
Center for Materials Science of Nuclear Fuel Energy Frontier Research Center (ERKCM58). This project is part of the INL Energy Frontier Research Center by this name, but direct funded to Oak Ridge National Laboratory under ERKCM58)</td></tr>
<tr><td colspan="2">Source of Support: DOE BES Location of Project: Idaho National Lab.</td></tr>
<tr><td colspan="2">Total Award Amount: $ 2 M/yr Total Award Period Covered: FY 07-14</td></tr>
<tr><td colspan="2">Total Award Amount to PI's Research: $266 K</td></tr>
<tr><td colspan="2">Describe Synergies and/or overlaps with This Proposal/Award:
Develop predictive computational models, validated by experiments, for the thermal and mechanical behavior of analogues to nuclear fuel. Investigator's role involves inelastic neutron scattering and interaction with theory. Work by the investigator is synergistic with research in ERKCS73, but the research direction is distinct from work in this project.</td></tr>
<tr><td colspan="2">Person-Months Per Year Committed to Project: _9_ Pers. Months; Specify: XCal., Acad., or Sumr:</td></tr>
<tr><td>Investigator: J. W. L. Pang</td><td>Other Agencies to which this proposal has been/will be submitted:</td></tr>
<tr><td colspan="2">Support (XCurrent, Pending, Submission Planned in Future or Transfer of Support):</td></tr>
<tr><td colspan="2">Project/Proposal Title and grant number, if appropriate:
X-Ray and Neutron Scattering and Microscopy (ERKCS73)</td></tr>
<tr><td colspan="2">Source of Support: DOE BES Location of Project: Idaho National Laboratory</td></tr>
<tr><td colspan="2">Total Award Amount: $ 1675 K/yr Total Award Period Covered: FY 10-12</td></tr>
<tr><td colspan="2">Total Award Amount to PI's Research: $ 89 K</td></tr>
<tr><td colspan="2">Describe Synergies and/or overlaps with This Proposal/Award:
Study the underlying structure, dynamics, and microstructural basis for materials properties and test first-principles and multi-scale models with first-of-their-kind x-ray and neutron experiments. Investigator's role involves x-ray and neutron scattering that is synergistic with research in the Center, but the research is distinct from the research in this project.</td></tr>
<tr><td colspan="2">Person-Months Per Year Committed to Project: _3_ Pers. Months; Specify: XCal., Acad., or Sumr:</td></tr>
<tr><td colspan="2">Other Agencies to which this proposal has been/will be submitted:</td></tr>
<tr><td colspan="2">Support (Current, Pending, Submission Planned in Future or Transfer of Support):</td></tr>
<tr><td colspan="2">Project/Proposal Title and grant number, if appropriate:</td></tr>
<tr><td colspan="2">Source of Support: Location of Project:</td></tr>
<tr><td colspan="2">Total Award Amount: $ Total Award Period Covered:</td></tr>
<tr><td colspan="2">Total Award Amount to PI's Research: $</td></tr>
<tr><td colspan="2">Describe Synergies and/or overlaps with This Proposal/Award:</td></tr>
<tr><td colspan="2">Person-Months Per Year Committed to Project: ____ Pers. Months; Specify: Cal., Acad., or Sumr:</td></tr>
</table>

Investigator: Jian Gan (Todd Allen; David Hurley)	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Energy Frontier Research Center, Center for Materials Science of Nuclear Fuel**	
Source of Support: DOE Basic Energy Sciences Location of Project: Idaho National Lab	
Total Award Amount: $2M/year Total Award Period Covered: 2009-2014	
Total Award Amount to PI's Research: $185K	
Describe Synergies and/or overlaps with This Proposal/Award: Develop fundamental understanding of the irradiated microstructure on thermal conductivity in UO2	
Person-Months Per Year Committed to Project: 1.5_ Pers. Months; Specify: Cal., Acad., or Sumr: Cal.	

Investigator: Jian Gan (Dennis Keiser; Dan Wachs)	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of 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 Lab
Total Award Amount: $ ~ 24M/year	Total Award Period Covered: FY2012
Total Award Amount to PI's Research: $250K	
Describe Synergies and/or overlaps with This Proposal/Award: My RERTR work mainly focus on TEM characterization of irradiated U-Mo based nuclear fuels for research and test reactors.	
Person-Months Per Year Committed to Project: 8 Pers. Months; Specify: Cal., Acad., or Sumr: Cal.	

Investigator: Jian Gan	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Fiber Optical Sensor for In-Pile Temperature Monitoring**	
Source of Support: DOE/LDRD	Location of Project: Idaho National Lab
Total Award Amount: $ 510K	Total Award Period Covered: 2010-2012
Total Award Amount to PI's Research: $ 255K	
Describe Synergies and/or overlaps with This Proposal/Award: This research project is to develop a fiber optical sensor for in-pile irradiation temperature monitoring for nuclear reactor.	
Person-Months Per Year Committed to Project: 1 Pers. Months; Specify: Cal., Acad., or Sumr: Cal.	

Investigator: Jian Gan (James Cole)	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Develop Advanced Coating for Cladding Inner Wall as a Diffusion Barrier to Mitigate the Fuel/Cladding Interaction**	
Source of Support: DOE/NE	Location of Project: Idaho National Lab
Total Award Amount: $ 700K	Total Award Period Covered: FY2012
Total Award Amount to PI's Research: $ 50K	
Describe Synergies and/or overlaps with This Proposal/Award: This project is to develop a diffusion barrier coating on the inner wall of the advanced fast reactor cladding to mitigate the fuel-cladding interaction.	
Person-Months Per Year Committed to Project: 1 Pers. Months; Specify: Cal., Acad., or Sumr: Cal.	

Investigator: Jian Gan (James Stubbins; Michell Barsoum)	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of 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: $??	Total Award Period Covered: FY 2012
Total Award Amount to PI's Research: $ 25K	
Describe Synergies and/or overlaps with This Proposal/Award: This project is to conduct post-irradiation examination on TEM characterization of irradiated metals and ceramics.	
Person-Months Per Year Committed to Project: 0.5 Pers. Months; Specify: Cal., Acad., or Sumr: Cal.	

Investigator: Xianming Bai (Leading PI: Todd Allen)	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Energy Frontier Research Center, Center for Materials Science of Nuclear Fuels**	
Source of Support: DOE Basic Energy Sciences Location of Project: Idaho National Laboratory	
Total Award Amount: $2M/year Total Award Period Covered: 2009-2014	
Total Award Amount to PI's Research: ~$240K/year	
Describe Synergies and/or overlaps with this Proposal/Award: Using atomistic modeling methods to study microstructural evolution in UO2 under irradiation environments.	
Person-Months Per Year Committed to Project: 9.8 Pers. Months; Specify: Cal., Acad., or Sumr: Cal.	

Investigator: Xianming Bai	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Protectiveness and stability of the zirconium oxide in early-phase corrosion of zirconium alloys - predictive relations to surface structure and composition**	
Source of Support: INL/LDRD	Location of Project: Idaho National Lab
Total Award Amount: $ 217.3K/year	Total Award Period Covered: 10/3/11 – 09/30/14
Total Award Amount to PI's Research: $97/year (the rest will be subcontracted to Massachusetts Institute of Technology)	
Describe Synergies and/or overlaps with This Proposal/Award: No direct overlap. The computational methods developed in this project may benefit the Energy Frontier Research Center. The plan is to hire a postdoc with 50% of time to work on this project.	
Person-Months Per Year Committed to Project: 0.02 Pers. Months; Specify: Cal., Acad., or Sumr: Cal.	

Investigator: Jiangou Yu (Leading PI: Todd Allen)	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Energy Frontier Research Center, Center for Materials Science of Nuclear Fuels**	
Source of Support: DOE Basic Energy Sciences Location of Project: Idaho National Lab	
Total Award Amount: $2M/year Total Award Period Covered: 2009-2014	
Total Award Amount to PI's Research: $240K/year	
Describe Synergies and/or overlaps with this Proposal/Award: Using atomistic modeling methods to study microstructural evolution in UO2 under irradiation environments.	
Person-Months Per Year Committed to Project: 9.8 Pers. Months; Specify: Cal., Acad., or Sumr: Cal.	

Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Synthesis of Prototype Magnesium Alloys**	
Source of Support: Questek Location of Project: University of Florida	
Total Award Amount: $ 4,000 Total Award Period Covered: 09/19/11-10/18/11	
Total Award Amount to PI's Research: $ 4,000	
Describe Synergies and/or overlaps with This Proposal/Award: There are no synergies and/or overlaps with this proposal/award.	
Person-Months Per Year Committed to Project: **0** Pers. Months; Specify: Cal., Acad., or Sumr:	

Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **CAREER: Towards Room Temperature Formability in Magnesium Alloys (DMR 0845868)**	
Source of Support: NSF	Location of Project: University of Florida
Total Award Amount: $ 400,000	Total Award Period Covered: 02/01/09 – 01/31/14
Total Award Amount to PI's Research: $ 400,000	
Describe Synergies and/or overlaps with This Proposal/Award: There are no synergies and/or overlaps with this proposal/award.	
Person-Months Per Year Committed to Project: **1** Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Center for Materials Science of Nuclear Fuel**	
Source of Support: INL	Location of Project: University of Florida
Total Award Amount: $ 1,000,000	Total Award Period Covered: 10/08/09-09/30/14
Total Award Amount to PI's Research: $ 500,000	
Describe Synergies and/or overlaps with This Proposal/Award: Current Award	
Person-Months Per Year Committed to Project: 1 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **REU Site: Infrastructure Materials (DMR 1062674)**	
Source of Support: NSF	Location of Project: University of Florida
Total Award Amount: $ 300,000	Total Award Period Covered: 01/01/11-12/31/13
Total Award Amount to PI's Research: $ 0	
Describe Synergies and/or overlaps with This Proposal/Award: There are no synergies and/or overlaps with this proposal/award.	
Person-Months Per Year Committed to Project: 0 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Ultrafine-Grained TiAl-Based Alloys for High Temperature Applications (DMR 0856622)**	
Source of Support: NSF	Location of Project: University of Florida
Total Award Amount: $ 534,432	Total Award Period Covered: 09/15/2009 – 08/31/11
Total Award Amount to PI's Research: $ 534,432	
Describe Synergies and/or overlaps with This Proposal/Award: There are no synergies and/or overlaps with this proposal/award.	
Person-Months Per Year Committed to Project: 1 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Pending	
Project/Proposal Title and grant number, if appropriate: **Advanced Materials Design and Processing Development**	
Source of Support: UCF	Location of Project: University of Florida
Total Award Amount: $ 609,811	Total Award Period Covered: 08/01/11-07/31/16
Total Award Amount to PI's Research: $ 609,811	
Describe Synergies and/or overlaps with This Proposal/Award: There are no synergies and/or overlaps with this proposal/award.	
Person-Months Per Year Committed to Project: 1 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **MRI: Acquisition of a Scanning X-ray Photoelectron Spectrometer with Ultraviolet Photon Source and C60 Ion Gun**	
Source of Support: NSF	Location of Project: University of Florida
Total Award Amount: $ 897,153	Total Award Period Covered: 09/01/11-08/31/14
Total Award Amount to PI's Research: $ 0	
Describe Synergies and/or overlaps with This Proposal/Award: There are no synergies and/or overlaps with this proposal/award.	
Person-Months Per Year Committed to Project: 0 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Pending	
Project/Proposal Title and grant number, if appropriate: **Magnetic Field Processing: Enabling Customized Lightweight Nano Composites and Cast Materails for Transportation and Energy Transmission Applications**	
Source of Support: Oak Ridge National Laboratory	Location of Project: University of Florida
Total Award Amount: $ 251,099	Total Award Period Covered: 10/01/11 – 09/30/14
Total Award Amount to PI's Research: $ 251,099	
Describe Synergies and/or overlaps with This Proposal/Award: There are no synergies and/or overlaps with this proposal/award.	
Person-Months Per Year Committed to Project: 1 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **IRES: Australian International Research Experience for Students: Materials for Energy Technologies**	
Source of Support: NSF	Location of Project: University of Florida
Total Award Amount: $ 146,880	Total Award Period Covered: 10/01/11-09/30/14
Total Award Amount to PI's Research: $ 146,880	
Describe Synergies and/or overlaps with This Proposal/Award: There are no synergies and/or overlaps with this proposal/award.	
Person-Months Per Year Committed to Project: 0 Pers. Months; Specify: Cal., Acad., or Sumr:	

Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Pending	
Project/Proposal Title and grant number, if appropriate: **Novel Materials Design and Characterization for Validation and Verification of Advanced Computational Models**	
Source of Support: Army Research Office	Location of Project: University of Florida
Total Award Amount: $ 850,000	Total Award Period Covered: 02/12 – 01/17
Total Award Amount to PI's Research: $ 850,000	
Describe Synergies and/or overlaps with This Proposal/Award: There are no synergies and/or overlaps with this proposal/award.	
Person-Months Per Year Committed to Project: **1** Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: Michele Manuel	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Pending	
Project/Proposal Title and grant number, if appropriate: **Brain-Susceptibility-Matched Electrodes and Cannula**	
Source of Support: NIH	Location of Project: University of Florida
Total Award Amount: $168,917	Total Award Period Covered: 09/11-08/13
Total Award Amount to PI's Research: $168,917	
Describe Synergies and/or overlaps with This Proposal/Award: There are no synergies and/or overlaps with this proposal/award.	
Person-Months Per Year Committed to Project: ____ Pers. Months; Specify: Cal., Acad., or Sumr:	

Investigator: Jianliang Lin	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Thick Ta Coatings of Gun Barrels using MPP**	
Source of Support: US Army Benet Labs Location of Project: Colorado School of Mines	
Total Award Amount: $160K Total Award Period Covered: 10/1/08 – 09.30/11	
Total Award Amount to PI's Research: $$160K	
Describe Synergies and/or overlaps with This Proposal/Award: The aim of this project is to deposit thick (>100 μm) alpha Ta coatings for Gun Barrels protection against the high temperature and wear during firing using the novel modulated pulsed power magnetron sputtering technique. Some results could provide useful information on the thick CeO_2 and UO_2 coating depositions for the Energy Frontier Research Center project.	
Person-Months Per Year Committed to Project: 2 Pers. Months; Specify: Cal., Acad., or Sumr: Cal	

Investigator: Jianliang Lin	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Development of CrA1AgN Coatings for Bolt Carriers and Bolts**	
Source of Support: Army ARDEC Location of Project: Colorado School of Mines	
Total Award Amount: $65K	Total Award Period Covered: 05/01/11 – 09/30/11
Total Award Amount to PI's Research: $25K	
Describe Synergies and/or overlaps with This Proposal/Award: The aim of this project is to develop a highly wear resistant nanocomposite coating based on CrAlNAg for high temperature tribological applications. There are no synergies and/or overlaps with this proposal.	
Person-Months Per Year Committed to Project: 2 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: Jianliang Lin	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Energy Frontier Research Center, Center for Material Science of Nuclear Fuel**	
Source of Support: DOE Basic Energy Sciences	Location of Project: Colorado School of Mines
Total Award Amount: $2M/yr	Total Award Period Covered: 01/2009 – 01/2014
Total Award Amount to PI's Research: $ 150K	
Describe Synergies and/or overlaps with This Proposal/Award: None	
Person-Months Per Year Committed to Project: 1 Pers. Months; Specify: Cal., Acad., or Sumr: Cal	

Investigator: Jianliang Lin	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Deposoitions of Nanocrystalline Si iand SiC Fils Using Pulsed DC and Modulated Pulsed Power Magnetron Sputtering**	
Source of Support: US Army Benet Labs Location of Project: Colorado School of Mines	
Total Award Amount: $160K/6 months	Total Award Period Covered: 9/1/11 – 12/30/11
Total Award Amount to PI's Research: $160K	
Describe Synergies and/or overlaps with This Proposal/Award: Optimize the deposition conditions for nanocrystalline Si and SiC thin film depositions using pulsed dc and MPP technique, respectively. There are no synergies and/or overlaps with this proposal.	
Person-Months Per Year Committed to Project: 2 Pers. Months; Specify: Cal., Acad., or Sumr: Sumr	

Investigator: Jianliang Lin	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Lubricant Free Die Coatings**	
Source of Support: Department of Energy Location of Project: Colorado School of Mines	
Total Award Amount: $300K/3 years	Total Award Period Covered: 12/30/11 – 12/30
Total Award Amount to PI's Research: $300K	
Describe Synergies and/or overlaps with This Proposal/Award: Development of two self-lubricant nanocomposite 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: 3 Pers. Months; Specify: Cal., Acad., or Sumr: Cal	

Investigator: Marat Khafizov	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Energy Frontier Research Center, Center for Materials Science of Nuclear Fuel**	
Source of Support: DOE Basic Energy Sciences Location of Project: Idaho National Laboratory	
Total Award Amount: $2,000,000 Total Award Period Covered: FY 2009-2014	
Total Award Amount to PI's Research: $	
Describe Synergies and/or overlaps with This Proposal/Award:	
Person-Months Per Year Committed to Project: 8.5 Pers. Months; Specify: Cal., Acad., or Sumr: Cal	

Investigator: Marat Khafizov	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Observation Of Zirconium Oxidation At Atomic Level Using Non-Linear Optical Spectroscopy**	
Source of Support: Laboratory Directed Research and Development Location of Project: Idaho National Laboratory Idaho	
Total Award Amount: $190,600	Total Award Period Covered: FY 2012-2014
Total Award Amount to PI's Research: $75,000	
Describe Synergies and/or overlaps with This Proposal/Award: none	
Person-Months Per Year Committed to Project 1.50 Pers. Months; Specify: Cal., Acad., or Sumr: Cal	

Investigator: Marat Khafizov	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of Support): Current	
Project/Proposal Title and grant number, if appropriate: **Characterization Of Intergranular Corrosion Using Thermal Wave Imaging**	
Source of Support: Laboratory Directed Research and Development Location of Project: Idaho National Laboratory Idaho	
Total Award Amount: $ 200K	Total Award Period Covered: FY 2012
Total Award Amount to PI's Research: $70K	
Describe Synergies and/or overlaps with This Proposal/Award: Development of laser based experimental methodology to detect temperature discontinuity in a thermal wave profile	
Person-Months Per Year Committed to Project: 1.75 Pers. Months; Specify: Cal., Acad., or Sumr: Cal	

Investigator: Marat Khafizov	Other Agencies to which this proposal has been/will be submitted:
Support (Current, Pending, Submission Planned in Future or Transfer of 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: Idaho National Laboratory Location of Project: University of Wisconsin	
Total Award Amount: $104.8K	Total Award Period Covered: FY 2011-2013
Total Award Amount to PI's Research: $ 5K	
Describe Synergies and/or overlaps with This Proposal/Award: none	
Person-Months Per Year Committed to Project: 0.25 Pers. Months; Specify: Cal., Acad., or Sumr: Cal	

8. ATTACHMENTS

Attachment 1, Staffing and Budget Tables

Attachment 2, Copies of Journal Publications

Attachment 3, Letters of Commitment from Unfunded Key Personnel/Senior Investigators or Institutions.

Attachment 1

Staffing and Budget Tables

Attachment 1 will be provided under separate cover.

Attachment 2

Copies of Journal Publications

Attachment 2 will be provided under separate cover.

Attachment 3

Letters of Commitment from Unfunded Key Personnel/Senior Investigators or Institutions

Dr. Jim Stubbins and Dr. Brent Heuser, University of Illinois
Dr. W. J. L. (Bill) Buyer, National Research Council of the Atomic Energy Canada Limited (AECL)
Dr. Andrew Nelson, Los Alamos National Laboratory
Dr. Rory Kennedy, Idaho National Laboratory

UNIVERSITY OF ILLINOIS
AT URBANA-CHAMPAIGN

**Department of Nuclear, Plasma,
And Radiological Engineering**

216 Talbot Laboratory
104 South Wright Street
Urbana, IL 61801

November 2, 2011

Professor Todd Allen
University of Wisconsin
Scientific Director, ATR National Scientific User Facility
Director, Center for Material Science of Nuclear Fuels, Idaho National Laboratory

Dear Todd,

This letter is to confirm my group's participation in the Center for Materials Science of Nuclear Fuel EFRC as an unfunded collaborator. We have been supporting the Center for approximately one year. This support consists of the supply of single crystal UO_2 films for analysis by members of the Center, specifically Dr. David Hurley at INL and Prof. Michele Manuel at the University of Florida. We look forward to our continuing collaboration with Center personnel and support of the Center via the supply of additional samples.

Best regards,

Brent J. Heuser

Brent J. Heuser, Ph.D.
Associate Professor

telephone (217)333-3598 • *fax* (217)333-2906

National Research Council Canada
Canadian Neutron Beam Centre

Conseil national de recherches Canada
Le centre canadien de faisceaux de neutrons

NRC·CNRC

Chalk River Laboratories
Chalk River
Ontario K0J 1J0
Canada

November 20, 2011

To: Prof. Todd Allen, Director
Center for Materials Science of Nuclear Fuel (CMSNF)

Re: Letter of collaboration on thermal conductivity in UO_2 in the CMSNF EFRC

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

As a retired Principal Research Officer of the National Research Council of Canada (NRC), I am currently affiliated with the NRC's 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 measurements of neutron scattering. I have considerable experience in experimental phonon methods dating from the sixties and seventies.

Moreover I provided a high-quality, massive single crystal of uranium dioxide as a loan to my Oak Ridge collaborators. 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. Early results, now available, have enabled a direct comparison with ambitious theoretical approaches, and pointed the way in which the latter should be improved.

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. Since the research is of personal interest to me, and I have excellent collaborators to work with at MST, HFIR and SNS at ORNL, I therefore require no salary or fee.

W. J. L. Buyers

Canada

Idaho National Laboratory

November 15, 2011

Professor Todd Allen
University of Wisconsin
Scientific Director, ATR National Scientific User Facility
Director, Center for Material Science of Nuclear Fuels, Idaho National Laboratory

Dear Todd,

Idaho National Laboratory is both a funded and unfunded collaborator in the Center for Materials Science of Nuclear Fuel EFRC. Our unfunded participation in the Center reflects our commitment to the success of the Center and consists of the supply of feedstock UO2 for single crystal growth and other sample preparation. These materials will be studied by Dr. Ben Larson (ORNL), Dr. Jian Gan (INL), Dr. David Hurley (INL), and Prof. Todd Allen (University of Wisconsin). We look forward to our continuing support for the Center and collaboration with Center personnel.

Best regards,

J. Rory Kennedy, Ph.D.
Manager, Fundamental Fuel Properties Department
Nuclear Fuels and Materials Division
Idaho National Laboratory

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Battelle Energy Alliance, LLC