Center for Materials Science of Nuclear Fuel (CMSNF)
EFRC Director: Todd Allen
Lead Institution: Idaho National Laboratory

Mission Statement*: To develop an experimentally validated multi-scale computational capability for the predictive understanding of the impact of microstructure on thermal transport in nuclear fuel under irradiation, with ultimate application to UO_2 as a model system.*

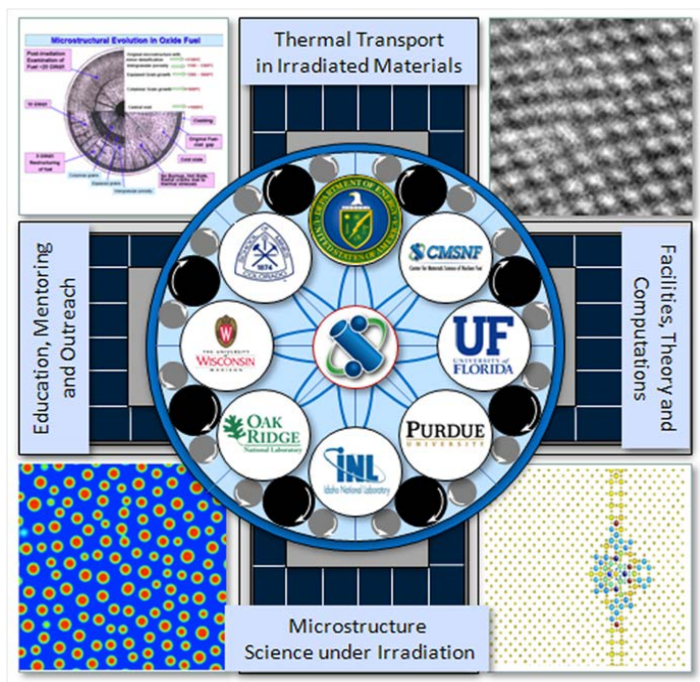
Research Direction: The Center will enrich the scientific basis of thermal transport in the ceramic materials (UO_2) used as nuclear fuel, based on an understanding of phonon transport through the unique microstructures formed under radiation at high temperature. Although there is significant interaction 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. This thrust area will also conduct measurements of lattice dynamics and conductivity 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, which will form a foundation for attaining these broader objectives. These scientific questions are:

- **Thermal Transport**
  - How do anharmonicity, fission product impurities, and chemical stoichiometry impact phonon lifetimes and thermal transport as a function of temperature in single crystal UO_2?
  - How do microstructural features such as grain boundaries, dislocations, interfaces, voids and bubbles affect thermal transport in UO_2 before and after irradiation?



At the Center for Materials Science of Nuclear Fuel, we integrate the physics of thermal transport in crystalline solids with the microstructure science under irradiation to understand the impact of irradiation on thermal transport in nuclear fuel. The Center thus introduces a new paradigm of basic research in the field of radiation materials science.

- **Microstructure under Radiation**
  - What type of clusters are produced by irradiation of UO_2 what do we need to understand the energies and kinetic paths of formation of clusters in UO_2, and predict atomic scale mechanisms of nucleation in UO_2?
  - What is the impact of temperature and oxygen environment on the stoichiometry of single and polycrystalline UO_2 before and after irradiation?
  - How do dislocation loops and gas bubbles form and grow in irradiated UO_2?

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 Idaho National Laboratory, University of Florida, and Purdue 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, Intermediate Voltage Electron Microscope, and Advanced Photon Source.

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