

NUCLEAR ENERGY RESEARCH INITIATIVE

Performance of Actinide-Containing Fuel Matrices under Extreme Radiation and Temperature Environments

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Project Description

This consortium will study fundamental details about the response of actinide-containing fuel matrices to the radiation and temperature environments within an advanced burner reactor. The work is comprised of two components: 1) an experimental component to study atomic-level details related to the influence of radiation damage and 2) a modeling component employing molecular dynamics (MD) and kinetic Monte Carlo (kMC) techniques to study the radiation damage processes.

Researchers will use thin films of uranium oxide and zirconium (UO_2 and U-10Zr) matrices in well-controlled, single-effect experiments and perform experiments to study the combined effects of several factors. The work will focus on the behavior of actinide surrogates (Ce, Nd), implanted non-volatile fission product surrogates (e.g., Mo), and fission gases (Xe) under the influence of high temperatures (to about 1400°C), displacement cascade damage, and microstructure defects (grain boundaries and other extended defects). Researchers will experimentally characterize the transport, segregation, and precipitation (or bubble formation in the case of Xe) and will study the processes with atomic-level detail using MD and kMC. The combination of the two components is anticipated to yield a knowledge database that currently does not exist related to the performance of the UO_2 and U-10Zr fuel matrices.

The specific objectives of the proposed research are the following:

1. To determine dependence of diffusivity and tendency for precipitation of *actinide surrogates* in UO_2 and U-10Zr with respect to heavy-ion radiation damage, UO_2 stoichiometry, initial actinide surrogate concentration, temperature, and microstructure
2. To determine dependence of diffusivity and tendency for bubble formation of implanted *nonvolatile fission product* surrogates in UO_2 and U-10Zr with respect to the above parameters
3. To determine dependence of diffusivity and tendency for bubble formation of implanted *fission gases* in UO_2 and U-10Zr with respect to the above parameters
4. To determine the synergistic effect between the actinides and fission products (including fission gases) on diffusivity, precipitation, and bubble formation

5. To determine the influence of the microstructure evolution (fission gas bubble formation, phase separation, lattice defect generation, and grain boundary area) on thermal conductivity as a function of temperature
6. To develop predictive theoretical/computational models that accurately describe the transport mechanisms at an atomistic level. This will include the effect of vacancy creation and diffusion on bubble formation and phase separation. The predictive models will permit extrapolation of fuel performance to environmental conditions not obtainable in the experimental phase of this work.