NUCLEAR ENERGY RESEARCH INITIATIVE

The Development of Models to Optimize Selection of Nuclear Fuel Materials through Atomic-Level Simulation

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Project Description

This project will develop an advanced fuel performance calculational platform based on the FRAPCON code. Detailed input about the properties of nuclear materials will be provided by databases determined from thermodynamic, atomic-level, and electronic-level calculations and simulations. Currently, all fuel performance codes are based on correlations derived from experimental data. The challenge is that these correlations cannot be extrapolated to operating conditions beyond the experimental points upon which the correlation is based, nor can they be used for materials lacking experimental data.

The objective of this project is to evaluate the possibility of extending performance codes to new materials based on databases developed from thermodynamic, atomistic, and first principles calculations. This project will create a prototype of a new generation of advanced fuel performance codes with inputs from state-of-the-art electronic-structure, atomic, and thermodynamic calculations. Pertinent input parameters will include material composition, temperature, density, closed porosity, surface roughness, fuel grain size, sintering temperature, and fractional cold work of the cladding. Development of this "first principles" based code will allow fuel development programs to reduce costly and time-consuming experimentation and transition to a selection process based on modeling, simulation, and analysis that will require only confirmatory irradiation testing.

Work Scope

This project will consist of two tasks:

- Task 1: Dissect and analyze FRAPCON to identify physical inputs; rebuild the code into a form that can use materials databases developed from atomic-level, electronic-structure, and thermodynamic calculations; and apply sensitivity analyses to identify properties on which fuel performance is most dependent.
- Task 2: Develop detailed databases of the U-Pu-O and U-Pu-N ternary systems and identify compositions that can meet key performance criteria.