NUCLEAR ENERGY RESEARCH INITIATIVE

Fission Product Transport in TRISO-Coated Particle Fuels: Multi-Scale Modeling and Experiment

PI: Izabela A. Szlufarska, University of Winsconsin-Madison

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Program Area: Generation IV

Collaborators: None

Project Description

The objective of this project is to develop a multi-scale computational model of transport of fission products through tri-isotopic (TRISO)-coated particles. This model will be capable of predicting diffusion constants and concentration profiles based on experimental images of coating's microstructure. Researchers will employ this model to discover mechanisms underlying fast diffusion of silver through silicon carbide layer, which is a primary barrier for fission products.

Previous models did not take into account the details of the underlying silicon-carbide (SiC) microstructure. The pathway of silver (Ag) transport in the SiC layer is likely to be governed by grain boundary diffusion, which researchers will by model through the molecular dynamics (MD) technique. Simulated microstructures will be benchmarked against experimental results. The MD-derived diffusion constants will be compared to diffusion constants calculated from kinetic Monte-Carlo and based on energy barriers estimated in full *ab-initio* calculations for select microstructures. The diffusion constants will be optimized based on both of these methods and incorporated into diffusion equations, which will be then employed to predict silver concentration profiles in experimental structures derived from transmission electron microscopy (TEM) images. In order to validate the model, predicted concentration profiles will be compared to experimental profiles determined by means of electron backscatter diffraction (EBSD). This approach will provide a reliable model for transport based solely on the fuel microstructure, with no reliance on historical measurements of diffusion.

Workscope

This project consists of the following primary tasks:

- Set up atomistic models of SiC bulk and grain boundaries (MD simulations)
- *Ab-initio* calculation of diffusion in bulk crystalline SiC
- Fit Ag-SiC potential (*ab-initio*, MD) and implement into MD code
- Build diffusion couple apparatus and perform initial EBSD characterization of SiC
- Initiate diffusion equation framework
- MD simulations of diffusion pathways and activation energies
- *Ab-initio* calculations of activation energies for diffusion along grain boundaries
- KMC model development

- Heat treatments on diffusion couples and initial EBSD characterization; continue diffusion equation framework
- Develop KMC model and perform simulations of diffusion along grain boundary
- Complete EBSD characterization and perform TEM examinations of selected samples
- Set up SiC specific diffusion equations and calculate diffusion profiles in experimentally derived structures