Fission Product Transport in TRISO Fuel

PI: Fei Gao, University of Michigan

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Collaborators: Zhijie Jiao, University of Michigan; Gary Was, University of Michigan; Blaise Collins, Idaho National Laboratory; Isabella van Rooyen, Idaho National Laboratory

ABSTRACT:

The objective of this research is to measure diffusion coefficients of fission product (FP) for thermal and irradiation conditions, as well as synergistic effects of radiation damage and fission products at IPyC/SiC interface and in SiC. First-principles approaches (*ab initio* calculations and molecular dynamics simulations) will be used to validate experimental data and determine the atomistic diffusion mechanisms to further improve empirical models in Idaho National Laboratory's (INL) fuel performance modeling code PARFUME to predict FP release in TRISO fuel. In particular, the efforts will focus on understanding both thermal and irradiation-enhanced diffusion of Ag, I, Pd, and Ru in the bulk and along grain boundaries in SiC.

We propose to use a multi-layered diffusion couple developed at the University of Michigan to investigate the diffusion of FPs, which consists of a SiC substrate that is coated with a thin layer of PyC, ion implanted with the FP of interest, and then sealed with a final layer of low temperature SiC. Diffusion couples will be annealed at operating high temperature gas reactor (HTGR) temperature and accident conditions to investigate the behavior of the FPs at the PyC-SiC interface and thermal transport of these fission products in SiC. Heavy ion beam irradiations will then be conducted to investigate the effect of radiation-enhanced diffusion. The dose rate will be varied to investigate the applicability of the ion irradiations to the neutron irradiations performed on fuel at ATR. In addition, co-implantation of fission products will also be used to investigate synergistic effects on diffusion and FP solubility.

Atomic-level computational methods will be used to assist in the interpretation of experimental results, determine activation energies and pathways for diffusion, and predict enhanced diffusion behavior under ion-beam irradiation conditions for comparative validation and under in-reactor operating conditions to provide data for design and performance assessments. ***Thus*, *the goal is to develop a comprehensive atomic-level understanding of the dynamics of FPs and provide physics-based diffusion kinetics to further improve empirical models used in the PARFUME code at INL, which will be benchmarked against data obtained from INL's Advanced Gas Reactor (AGR) Fuel Development and Qualification Program.***

The collaborations between university and national laboratory will also provide a unique platform for the workforce development in which the graduate students or young scientists can be exposed to a dynamic research environment to interact with top scientists nationally and internationally.