

## Fission Product Transport in TRISO Particle Layers Under Operating and Off-Normal Conditions

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## ABSTRACT

The objective of this project is to determine the diffusivity and chemical behavior of key fission products (Ag, Cs, I, Te, Eu and Sr) through SiC and PyC both thermally, under irradiation, and under stress, using fission-product introduction techniques that avoid the pitfalls of past experiments.

The experimental approach will rely on thin PyC-SiC couples containing the fission products in the PyC layer. The samples will be subjected to high-temperature exposures, to irradiation at high temperature, and to irradiation under stress at high temperature. The PyC serves as a host layer, providing a means of placing the fission product close to the SiC through ion implantation without damaging the SiC layer or losing the fission product during heating.

A variety of characterization tools will be used to track fission-product distribution as well as grain boundary structure in SiC. Rutherford backscattering spectrometry (RBS) will provide a coarse description of fission-product distribution, while cross-section transmission electron microscopy (TEM) will be used for a high-resolution characterization with a particular focus on fission-product distribution along grain boundaries. Atom probe tomography (APT) and TEM will be used to determine the state of the fission products and whether they form phases with the host. High resolution TEM and electron back-scatter diffraction (EBSD) will be used to determine grain boundary structure, which will serve as input for a first-principles modeling effort to study and elucidate fission-product diffusion mechanisms and rates along grain boundaries and in the bulk. Modeling will rely on density functional theory calculations together with kinetic Monte Carlo simulations of fission-product diffusion. The combination of detailed experimental characterization and first-principles computation will provide the capability to model fission-product transport through a TRISO particle in-reactor.