Crystal Structure Characterization of Uranium-Silicides Accident Tolerant Fuel by High Temperature Neutron Diffraction

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Abstract:
The uranium-silicide compound, U_3Si_2, is one of the fuel forms currently being developed as an accident tolerant fuel (ATF) for light water reactors. Despite the body of work characterizing both fresh and irradiated U_3Si_2 fuel, crystallographic studies are sparse, especially when compared to UO_2. In this study we investigated the crystal structure of U_3Si_2 from 25°C to 1100°C using high temperature time-of-flight neutron diffraction on the High Pressure Preferred Orientation (HIPPO) diffractometer at Los Alamos Neutron Science Center (LANSCE). To test predictions based on thermodynamic models that any excess Si in U_3Si_2 should lead to precipitation of additional phases, a stoichiometric $U_3Si_{2.00}$ sample and a hyper-stoichiometric $U_3Si_{2.01}$ sample were studied. Specimens were prepared by arc-melting the constituents of depleted uranium and silicon and annealing the resulting ingots at 1250°C for 20 hours. Neutron diffraction data were collected at 25 temperatures during heating and cooling. The HIPPO time-of-flight neutron diffractometer provides detectors arranged on rings with 145° (highest resolution $\Delta d/d$, lowest count rate), 120°, 90°, 60°, and 40° (lowest resolution $\Delta d/d$, highest count rate) nominal diffraction angles. The simultaneous Rietveld refinement of five histograms from the five HIPPO detector rings allowed us to study lattice parameters, anisotropic atomic displacement parameters, and atomic positions as a function of temperature. This data is compared to predictions from atomistic simulations.

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