High-Pressure Structural Behavior and Bulk Modulus of U_3Si_5

Jason L. Baker[1], Josh T. White[2], Robert C. Roback[1], Changyong Park[3], and Hongwu Xu[1]

[1]*Earth and Environmental Sciences Division, Los Alamos National Laboratory (LANL), Los Alamos, NM 87545, USA*
[2]*Materials Science and Technology Division, LANL, Los Alamos, New Mexico 87545, USA*
[3]*High-Pressure Collaborative Access Team, X-Ray Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA*

Light Water Reactors (LWR) commonly rely on uranium dioxide (UO_2) as a fuel choice, but in more recent years, potential accident-tolerant nuclear fuels such as uranium silicides (U-Si) have been garnering a great deal of interest due to their higher thermal conductivities at operating temperatures and, in some cases, higher uranium densities. Although U_3Si_5 has a lower uranium density than UO_2 and U-rich U-Si compounds, it possesses a higher thermal conductivity than UO_2 above 600 K, while having a lower thermal conductivity than USi and U_3Si_2[1-3]. Additionally, the mechanical properties (i.e., bulk modulus) of U-Si compounds have been recently studied (USi and USi_2)[4] using high-pressure X-ray diffraction (HPXRD) measurements. HPXRD measurements probe the intrinsic mechanical properties of materials, and are useful for understanding mechanical integrity, which is an important parameter in evaluation of potential nuclear fuels.

Here we present investigations of the structural behavior and mechanical properties of U_3Si_5 under high-pressures up to 17 GPa using angle-dispersive powder XRD and Raman spectroscopy coupled with a diamond anvil cell (DAC). The ambient hexagonal structure with the space group *P6/mmm* remains stable up to the maximum pressure tested. The bulk modulus, *a* and *c*-axial moduli have been determined from equations of state to be 126 ± 4 GPa, 173 ± 8 GPa, and 79.7 ± 4.3 GPa, respectively. An anisotropy in compressibility is observed between the *a* and *c*-axis with the *a*-axis being approximately 2.2 times less compressible than the *c*-axis. A comparison of the bulk modulus of U_3Si_5 to those of other U-Si compounds has revealed a trend of decreased compressibility with increased U content, where USi_2 is the least compressible (140 GPa)[4] and U_3Si_5 is the second least compressible. The HPXRD and Raman spectroscopy data, the trend in bulk moduli, and the observed anisotropy in compressibility will be discussed.

[1] J. T. White *et al*., *J. Nucl. Mater.*, 2015, **456**, 442-448.
[2] J.T. White *et al.*, *J. Nucl. Mater.*, 2016, **471**, 129-135.
[3] J.T. White *et al*. *J. Nucl. Mater.*, 2015, **464**, 275-280.
[4] S. Yagoubi *et al*., *J. Alloys and Compounds*, 2013, **546**, 63-71.