High-Pressure Structural Behavior and Bulk Modulus of $\text{U}_3\text{Si}_5$

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Light Water Reactors (LWR) commonly rely on uranium dioxide ($\text{UO}_2$) as a fuel choice, but in more recent years, potential accident-tolerant nuclear fuels such as uranium silicides ($\text{U-Si}$) 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 $\text{U}_3\text{Si}_5$ has a lower uranium density than $\text{UO}_2$ and U-rich $\text{U-Si}$ compounds, it possesses a higher thermal conductivity than $\text{UO}_2$ above 600 K, while having a lower thermal conductivity than USi and $\text{U}_3\text{Si}_2$$^{1-3}$. Additionally, the mechanical properties (i.e., bulk modulus) of $\text{U-Si}$ 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 $\text{U}_3\text{Si}_5$ 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 $126 \pm 4$ GPa, $173 \pm 8$ GPa, and $79.7 \pm 4.3$ 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 $\text{U}_3\text{Si}_5$ 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 $\text{U}_3\text{Si}_5$ 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.


