Experimental and First-principles Studies on the Elastic Properties of α-Hafnium Metal under Pressure

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Hafnium (Hf) has attracted great technological interest in nuclear science in recent years because of its excellent physical properties, such as exceptional corrosion resistance and high thermal neutron-capture cross-section, which makes hafnium a good material for reactor control rods. Much of our understanding about its structural phase stability and mechanical properties under extreme conditions of pressure and/or temperature is based on theoretical studies; experimental assessment of these properties, especially the elastic shear properties, is still limited to ambient conditions. In this study, for the first time, compressional and shear wave velocities of the α phase of hafnium have been measured up to 10.4 GPa at room temperature using ultrasonic interferometry in a multi-anvil apparatus. A finite strain equation of state analysis yielded K_{S0}=110.4 (5) GPa, G_0=54.7(5) GPa, K_{S0}'=3.7 and G_0'=0.6 for the elastic bulk and shear moduli and their pressure derivatives at ambient conditions. Complementary to the experimental data, the single crystal elastic constants, elastic anisotropy and the unit cell axial ratio c/a of α-hafnium at high pressures were investigated by Density Functional Theory (DFT) based first principles calculations. A c/a value of 1.605 is predicted for α-Hf at 40 GPa, which is in excellent agreement with previous experimental results. The low-pressure derivative of the shear modulus observed in our experimental data up to 10 GPa was found to originate from the elastic constant C_{44} which exhibits negligible pressure dependence within the current experimental pressure range. At higher pressures (>10 GPa), C_{44} was predicted to soften and the shear wave velocity trended to decrease with pressure, which can be interpreted as a precursor to the α - ω transition similar to that observed in other group IV elements (titanium and zirconium). The acoustic velocities, bulk and shear moduli, and the acoustic Debye temperature (θ_D=240.1 K) determined from the current experiments were all compared well with those predicted by our theoretical DFT calculations.