Experimental and theoretical studies on the elasticity of tungsten to 13.6 GPa

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Abstract

5d transition metal tungsten (W) is characterized by the highest melting point of all non-alloyed metals as well as high elastic properties. With its excellent mechanical and thermal strength, tungsten and its alloys have wide engineering and technology applications. At ambient conditions, tungsten crystallizes in a body-centered-cubic structure (space group number: 229, *Im-3m*). On the basis of its bcc stability up to extremely high pressure at room temperature, tungsten has attracted great interest in theoretical and experimental high pressure research. . 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 paper, we investigate the elasticity of W under pressure using both experimental methods and density functional theory (DFT) calculations. The compressional and shear wave velocities of polycrystalline W under quasi-hydrostatic pressure up to 13.6 GPa are measured with ultrasonic interferometry in a multi-anvil apparatus. The elastic bulk and shear moduli and their pressure derivatives are derived from the velocity data using fourth-order finite strain equations of state, yielding $K_{S0} = 315.5(16)$ GPa, $G_0 = 160.9(8)$ GPa, $K'_{S0} = 3.94(3)$, $G'_0 = 1.46(1)$, $K''_0 = -0.1219$ and $G''_0 = -0.0386$. The mechanical properties, such as Young's modulus, Poisson's ratio and ductility/brittleness (Pugh modulus ratio) of tungsten at ambient conditions are in good agreement with previous studies and their high pressure behavior have also been investigated. Complementary to the experimental data, the single crystal elastic constants, the elastic anisotropy, V_P and V_S as well as the bulk and shear moduli were computed using density functional theory (DFT) at pressures comparable to the current experiment. The present results offer a comprehensive dataset for the elasticity of polycrystalline bcc tungsten at room/high pressures and we believe these data will provide a consistent starting point for further theoretical modeling of the elastic, mechanical and electronic properties of tungsten and its alloys.