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Anisotropic constitutive relationships in energetic materials: PETN and HMX MICHAEL CONROY, IVAN OLEYNIK, University of South Florida, SERGEY ZYBIN, California Institute of Technology, CARTER WHITE, Naval Research Laboratory — One of the important goals in energetic materials (EM) research is predicting EM properties from first principles based upon underlying atomic structure. Special attention is being focused on obtaining accurate equations of state for several important classes of EMs. In this presentation, we will discuss the results of first-principles density functional theory calculations of the energetic materials PETN and HMX. For each material, we have simulated both hydrostatic compression and uniaxial compression in the crystallographic directions [100], [010], [001], [110], [101], [011], and [111] up to $V/V_0 = 0.50$ ($\sim$40-50 GPa). We will examine the equations of state for each material and other structural properties of the unit cell as a function of volume and compare with available experimental results. Also, we will discuss the correlation between calculated shear stresses upon uniaxial compression with experimentally observed anisotropies in sensitivity to shock-induced detonation.

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