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Anisotropic Constitutive Relationships in Energetic Materials: TATB MIKALAI M. BUDZEVICH, AARON LANDERVILLE, MIKE CONROY, IVAN I. OLEYNIK, University of South Florida, CARTER T. WHITE, Naval Research Laboratory — One of the principal thrusts in energetic materials (EM) research is the acquisition of accurate equations of state (EOS) for various important classes of EMs. In the past, both theoretical and experimental studies concentrated on hydrostatic EOS. However, these isotropic EOS still need to be expanded to include anisotropic materials response, including uniaxial compression which are more relevant to shock initiation of detonation. To this end, we performed first-principles density functional calculations of the EOS for TATB, including uniaxial compressions in the [100], [010], [001], [110], [101], [011], and [111] crystallographic directions. Equilibrium properties, such as lattice parameters and elastic constants, as well as the hydrostatic EOS were calculated and compared with experimental results. Finally, we discuss the possible relationship between shear stresses induced by the uniaxial compression of TATB and the relative shock sensitivities of different crystallographic directions.

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