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Nonlinear anisotropic response for shocked single energetic crystals[1] SERGEY V. ZYBIN, California Institute of Technology, TAHIR CAGIN, Texas A&M University, WILLIAM A. GODDARD III, California Institute of Technology — The response of energetic materials to the shock loading determines the initiation of chemical reactions and transition to detonation. The sensitivity of single energetic crystals can depend on shock orientation and correlate with their elastic properties, the strength of elastic precursor, and the mechanisms of shock-induced plasticity. In a continuum framework, the elastic-plastic response of materials is usually described by the constitutive relations coupling linear elastic response to a viscoplastic flow in a single crystal. However, for stronger shocks or more compliant crystals the resulting response at the shock front may be complicated by: 1) large compressions leading to a nonlinear elastic response, 2) highly anisotropic strains requiring the use of non-hydrostatic constitutive relations (equation of states), 3) very high strain rates which may affect the mechanism of plasticity. Here, we present the results of ab initio and reactive force fields (ReaxFF) calculations of nonlinear mechanical response of energetic materials under large anisotropic (e.g. uniaxial) strains typical for the conditions at the shock front.

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