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Shear stresses in shock compressed energetic materials SERGEY ZYBIN, California Institute of Technology, IVAN OLEYNIK, TAHIR CAGIN, Texas A&M University — There are numerous experimental indications of orientational dependence of shock-induced detonation phenomena in energetic materials (EM). The initial response of EM to shock wave loading can be related to such fundamental characteristics of EM as its elastic properties upon uniaxial compression. It is well-known in the case of covalent solids that shear stresses are the driving forces of shock induced plasticity and the formation of point and extended defects but their effect on shock induced deformations and chemical reactions in molecular crystals of EM is not certain. We report results of combined first-principles density functional theory (DFT) and reactive force field (ReaxFF) study of shear stresses in uniaxially compressed EM such as PETN, RDX and HMX as a function of crystalline orientation and the compression ratio of the load. The steric effects, changes in the bond lengths and angles, relative contribution of inter and intra-molecular interactions and possibilities of phase transitions are discussed in relation to experimental observations of orientational sensitivity of EM.

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