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Atomistic simulations of orientation effects during shock compression and decomposition of energetic materials[1] SERGEY V. ZYBIN, LUZHENG ZHANG, ADRI VAN DUIN, SIDDHARTH DASGUPTA, WILLIAM A. GODDARD III, California Institute of Technology — Several experiments have indicated that the shock sensitivity of single crystal energetic materials can depend on the crystallographic direction. For example, sensitivity of PETN strongly correlates with orientational anisotropy of elastic precursor strength as well as steric hindrance to shear in some slip directions. In particular, deformation and excitation of energetic molecules can be affected by different slip systems and mechanisms of elastic-plastic transition for different directions. To study the orientational effects in material transformation and initiation of chemical events related to the detonation we have performed a series of reactive molecular dynamics (MD) simulations using the ReaxFF reactive force field, capable to reproduce the quantum chemical (QM)-derived relative energies of the reactants, products, intermediates and transition states related to the RDX and HMX unimolecular decomposition. Our analysis shows that the sensitivity, pathways, and products of shock-induced decomposition in these single energetic crystals are dependent on the shock orientation.

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