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Inelastic deformation in shock loaded pentaerythritol tetranitrate

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The mechanisms of shock-induced deformation in (100)- and (001)-oriented single crystals of pentaerythritol tetranitrate (PETN) were characterized at the atomic scale using classical molecular dynamics simulations with a fully flexible, non-reactive force field. Shock pressures P_{shock} ∼8.7 GPa in initially defect-free, thermalized crystals were studied in order to compare the mechanical behavior for these two orientations under conditions for which neglect of chemistry is a reasonable approximation on the time and space scales of the simulations. A two-wave structure was observed for the (100) shock whereas only elastic compression was observed for the (001) case. Spatially- and temporally-resolved responses for the two orientations were characterized using relative nearest-neighbor molecular displacements, orientational order parameters, dihedral angle distributions, and partitioning of kinetic energy between inter- and intramolecular degrees of freedom. The differences in mechanical response for the two orientations are qualitatively consistent with expectations based on the steric hindrance model of initiation anisotropy.

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