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Anisotropic Shock Response of Oriented Nitromethane Single Crystals LAN HE, THOMAS D. SEWELL, DONALD L. THOMPSON, University of Missouri-Columbia — Detailed anisotropic structural and mechanical responses of crystalline nitromethane subjected to shock loading along different crystallographic orientations have been studied using molecular dynamics (MD) simulations with a nonreactive force field. Single- and multi-particle properties prior to and following shock passage have been evaluated using a geometric binning approach that spatially and temporally resolves the shock-induced thermo-physical and geometric changes in the material. Initial partitioning and redistribution pathways of the energy imparted by the shock wave result in orientation-dependent structural relaxation processes among which are elastic deformation; crystal structure reordering; and plane-specific disordering phenomena, in which certain structural properties undergo changes from ordered to disordered states in some crystallographic planes but not others.

Thomas D. Sewell
University of Missouri-Columbia

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