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Molecular Dynamics Simulations of Shear Induced Transformations in Nitromethane JAMES LARENTZOS, Army Research Laboratory, BRAD STEELE, University of South Florida — Recent experiments demonstrate that NM undergoes explosive chemical initiation under compressive shear stress. The atomistic dynamics of the shear response of single-crystalline and bi-crystalline nitromethane (NM) are simulated using molecular dynamics simulations under high pressure conditions to aid in interpreting these experiments. The atomic interactions are described using a recently re-optimized ReaxFF-lg potential trained specifically for NM under pressure. The simulations demonstrate that the NM crystal transforms into a disordered state upon sufficient application of shear stress; its maximum value, shear angle, and atomic-scale dynamics being highly dependent on crystallographic orientation of the applied shear. Shear simulations in bi-crystalline NM show more complex behavior resulting in the appearance of the disordered state at the grain boundary.

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