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Atomistic Studies of Plastic Deformation and Dissipation in Crystalline HMX EUGENIO JARAMILLO, THOMAS D. SEWELL, Los Alamos National Laboratory, ALEJANDRO STRACHAN, Purdue University — We are using large scale molecular dynamics simulations of crystalline octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) to better understand the dominant fundamental mechanisms of inelastic deformation and other dissipative processes in anisotropic organic molecular crystals. A fully flexible force field (Smith, G. D. and Bharadwaj, R. K.; *J. Phys. Chem. B* 1999, 103, 3570) used in numerous preceding studies is used without modification in the present work. Our results, based on the results of simulations containing 25,000-250,000 molecules, indicate a large degree of directional anisotropy in response to compression, for both quasi-static and shock loading. Plastic deformation is observed for some loading directions whereas solid-solid phase transitions are observed for others. The emphasis of the present talk will be identifying and characterizing detailed molecular mechanisms and rate dependencies in those cases for which dislocation-induced plasticity occurs.

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