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Atomistic simulations of quasi-static and shockwave loading of HMX crystals THOMAS SEWELL, EUGENIO JARAMILLO, Los Alamos National Laboratory, ALEJANDRO STRACHAN, Purdue University — We have recently undertaken non-equilibrium molecular dynamics studies to aid our understanding of dynamical processes in the high explosive HMX, in particular the inelastic, anisotropic response of crystalline HMX subjected to quasi-static and shock loading. The same force field used by Sewell and co-workers in preceding simulations of HMX equilibrium properties is employed for the present research. The overarching goal of this work is to provide information that can serve as a foundation in basic science for the formulation of improved mesoscale constitutive models for the constituent materials in selected energetic formulations. The medium-term scientific challenge that stands as a prerequisite to this larger objective is to carefully identify, characterize, and quantify the dominant mechanisms of localization and dissipation in such materials, under a variety of prescribed quasi-static and dynamic loading scenarios. The focus of the present talk will be the shock response of structurally perfect, but properly thermalized, α -HMX crystal shocked in the (100) direction, with specific discussion of results for loading below the hughoniot elastic limit, in the two-wave elastic-plastic region, and for overdriven shocks.

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