

Abstract Submitted
for the SHOCK05 Meeting of
The American Physical Society

Atomistic Simulations of Shocks in HMX Crystals. EUGENIO JARAMILLO, ALEJANDRO STRACHAN, THOMAS D. SEWELL, Los Alamos National Laboratory — We are using large scale molecular dynamics simulations to study HMX crystals under shock compression. The objective is to obtain a fundamental understanding on the molecular scale of the dominant mechanisms of plastic relaxation and other dissipative processes in anisotropic 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. Initial results indicate that plastic deformation occurs even for weak shocks (~ 4 GPa) on a time scale that is accessible to atomistic molecular dynamics (~ 100 ps for a 66,561 molecule system).

Eugenio Jaramillo
Los Alamos National laboratory

Date submitted: 22 Apr 2005

Electronic form version 1.4