Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Reactive Molecular Dynamics Studies of Thermal Induced Chemistry in HMX[1] JASON QUENNEVILLE, TIMOTHY GERMANN, THOMAS SEWELL, EDWARD KOBER, Los Alamos National Laboratory — Equilibrium molecular dynamics (MD) simulation of high explosives can provide important information on their thermal decomposition by helping to characterize processes with timescales that are much longer than those attainable with non-equilibrium MD shock studies. A reactive force field is used with MD to probe the chemistry induced by intense heating ('cook-off') of octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX). The force field (ReaxFF) was developed by van Duin, Goddard and coworkers[1] at CalTech and has shown promise in predicting the chemistry in a variety of systems, including RDX and TATB under either shock compression or intense heat. In the current work, we investigate the effect of initial equilibration temperature (1000 to 1500 K), volumetric compression, crystal polymorph (β and δ), and system size (ranging from 150 to 1200 molecules) on the reaction rate and reaction products. Finally, we will compare these results with those from our previous work on TATB. [1]A. C. T. Van Duin, *et al*, *J. Phys. Chem. A*, **1005**, 9396 (2001).

[1]This work was performed at Los Alamos National Laboratory under U.S. Department of Energy contract DE-AC52-06NA25396.

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Date submitted: 20 Nov 2007 Electronic form version 1.4