Abstract Submitted
for the SHOCK05 Meeting of
The American Physical Society

Shock induced decomposition and sensitivity of energetic materials by ReaxFF molecular dynamics[1] S.V. ZYBIN, L. ZHANG, A.C. VAN DUIN, S. DASGUPTA, W.A. GODDARD III, Caltech — Shock sensitivity of single crystal energetic materials can depend on the crystallographic direction. For example, sensitivity of PETN strongly correlates with orientational anisotropy of elastic precursor strength as well as steric hindrance to shear in some slip directions. In particular, deformation and excitation of energetic molecules can be affected by different slip systems and mechanisms of elastic-plastic transition for different directions. To study the influence of shock/impact orientation on initiation and decomposition of energetic materials we have performed a series of reactive molecular dynamics (MD) simulations using the ReaxFF reactive force field, capable to reproduce the quantum chemical (QM)-derived relative energies of the reactants, products, intermediates and transition states related to the RDX and HMX unimolecular decomposition. Our analysis shows that the sensitivity, pathways, and products of shock-induced decomposition in these single energetic crystals are dependent on the shock orientation as well as crystalline phases of energetic materials.

[1]Supported by DARPA-PROM, ONR, and ARO-MURI

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Date submitted: 23 May 2005 Electronic form version 1.4