Abstract Submitted
for the SHOCK07 Meeting of
The American Physical Society

Energetic materials under mechanical shock and shear: Molecular dynamics simulation with reactive force field[1] SERGEY ZYBIN, PENG XU, ADRI VAN DUIN, WILLIAM GODDARD, California Institute of Technology
— The initial physical and chemical response of energetic materials under mechanical shock or shear loading has been investigated for RDX, PETN and HMX by molecular dynamics method with ReaxFF reactive force field parameterized from first-principles calculations. We study the propagation of a shock wave and shock-induced chemical reactions created by moving piston mimicked by a potential wall. We simulate both the continuous and impulsive piston loading to investigate its influence on the initiation and decomposition reactions in energetic materials as well as the orientational dependence using large-scale parallel ReaxFF-MD simulations. Besides, we perform a series of simulations of pure shear at high strain rate as well as static uniaxial compression of energetic crystals to study their transformation and decomposition under various loading conditions. The mechanism and evolution of chemical reactions induced by mechanical shock and pure shear is discussed along with the propagation of heat, mass, pressure, and reaction waves.

[1]Acknowledgements: supported by ARO and ONR grants.

Sergey Zybin
California Institute of Technology

Date submitted: 26 Feb 2007 Electronic form version 1.4