Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

Molecular Simulation of the Free Energy for the Accurate Determination of Phase Transition Properties of Molecular Solids[1] MICHAEL SELLERS, US Army Rsch Lab - Aberdeen, MARTIN LISAL[2], Laboratory of Chemistry and Physics of Aerosols, Institute of Chemical Process Fundamentals of the ASCR, JOHN BRENNAN, US Army Rsch Lab - Aberdeen — Investigating the ability of a molecular model to accurately represent a real material is crucial to model development and use. When the model simulates materials in extreme conditions, one such property worth evaluating is the phase transition point. However, phase transitions are often overlooked or approximated because of difficulty or inaccuracy when simulating them. Techniques such as super-heating or super-squeezing a material to induce a phase change suffer from inherent timescale limitations leading to "over-driving," and dual-phase simulations require many long-time runs to seek out what frequently results in an inexact location of phase-coexistence. We present a compilation of methods for the determination of solid-solid and solid-liquid phase transition points through the accurate calculation of the chemical potential. The methods are applied to the Smith-Bharadwaj atomistic potential's representation of cyclotrimethylene trinitramine (RDX) to accurately determine its melting point (Tm) and the alpha to gamma solid phase transition pressure. We also determine Tm for a coarse-grain model of RDX, and compare its value to experiment and atomistic counterpart. All methods are employed via the LAMMPS simulator, resulting in 60-70 simulations that total 30-50ns.

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Date submitted: 28 Jan 2015 Electronic form version 1.4