Abstract Submitted
for the SHOCK09 Meeting of
The American Physical Society

Molecular dynamics simulation of shock-induced phase transition in Germanium J. MATTHEW D. LANE, AIDAN P. THOMPSON, Sandia National Labs — Results from shock-wave and ramp-wave uniaxial loading of Germanium will be presented. Germanium is known to transition from ambient cubic diamond (cd) phase to the high-pressure body-centered tetragonal (bct) or β-tin phase at pressures between 10 and 12 GPa. Large-scale molecular dynamics (MD) simulations were used to study the phase transition in single-crystal Germanium under uniaxial compression along several different crystal axes. We observed that the transition from the cd phase to the bct phase nucleates through shear banding and advances to relieve uniaxial strain. The macroscopic properties are compared with experimental results for both the Modified Embedded Atom Method (MEAM) and Tersoff potentials. Simulation techniques included standard non-equilibrium MD, as well as alternative computational methods, such as the Continuous Hugoniot Method and homogeneous uniaxial ramp methods.

This work is supported by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

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Date submitted: 26 Feb 2009 Electronic form version 1.4