Abstract Submitted
for the SHOCK09 Meeting of
The American Physical Society

Molecular Dynamics Simulation of Dynamic Response of Beryllium[1] AIDAN P. THOMPSON, J. MATTHEW D. LANE, MICHAEL I. BASKES, MICHAEL P. DESJARLAIS, Sandia National Laboratories — The response of beryllium to dynamic loading has been extensively studied, both experimentally and theoretically, due to its importance in several technological areas. Compared to other metals, it is quite challenging to accurately represent the various anomalous behaviors of beryllium using classical interatomic potentials. The spherically-symmetric EAM potential can not reproduce the observed c/a ratio for α-Be under ambient conditions, which is significantly smaller than the ideal HCP value. The directional-dependence of the MEAM potential overcomes this problem, but introduces additional complexity. We will compare predictions of these classical potentials to experimental measurements of beryllium at ambient conditions, and also to theoretical calculations at high temperatures and pressures. Finally, we will present initial results from non-equilibrium molecular dynamics simulations of beryllium under dynamic loading. This work is supported by the Laboratory Directed Research and Development program at Sandia National Laboratories.

[1]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.

Aidan Thompson
Sandia National Laboratories

Date submitted: 24 Feb 2009 Electronic form version 1.4