Abstract Submitted
for the SHOCK11 Meeting of
The American Physical Society

Molecular dynamics simulation of dynamic response of beryllium[1]

AIDAN P. THOMPSON, J. MATTHEW D. LANE, MICHAEL P. DESJARLAIS, Sandia National Laboratories, ALBERT P. BARTOK, GABOR CSANYI, University of Cambridge, UK — 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. We have used large-scale classical molecular dynamics simulations to study the response of single-crystal beryllium to high-strain rate uniaxial loading. We compare results from two different types of interatomic potential. A MEAM potential was constructed to reproduce properties of beryllium at ambient conditions. A potential based on the recently-developed GAP approach was fit to quantum simulations of solid and liquid beryllium phases near the shock-melting line.

[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: 22 Feb 2011 Electronic form version 1.4