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Elastic response of shocked aluminum single crystals: a continuum analysis of molecular dynamics simulations J.A. ZIMMERMAN, Sandia National Laboratories, J.M. WINEY, Y.M. GUPTA, Washington State University — Molecular dynamics (MD) simulations were used to examine elastic shock wave propagation in aluminum single crystals along [100], [110] and [111] directions using four different embedded-atom method potentials. Continuum variables extracted from MD results show that stresses, densities, and temperatures for [100] shock propagation are significantly different for the various potentials, while the results for [110] and [111] propagation are similar for three of the four potentials. Overall, the recent potential by Winey, Kubota and Gupta [*MSMSE* **17**, 055004 (2009)] provides the best agreement with nonlinear elastic calculations that include elastic constants up to fourth order. Our MD-continuum approach provides a key step in establishing the applicability of classical MD potentials for dynamic compression. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

J.A. Zimmerman
Sandia National Laboratories

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