Abstract Submitted
for the SHOCK13 Meeting of
The American Physical Society

Large-scale Molecular Dynamics Simulations of Shock-induced Plasticity and Twinning in bcc Nb and Ta TIMOTHY GERMANN, RUIFENG ZHANG, Los Alamos National Laboratory, RAMON RAVELO, University of Texas at El Paso — Large-scale classical molecular dynamics (MD) simulations are used to investigate dislocation slip and twinning activity in bcc metals under shock compression. We will discuss both the orientation-dependent response of Nb and Ta single crystals, as well as the more complex response of nanocrystalline samples. Of particular importance as MD simulations are becoming applied to model more complex materials, we will discuss issues related to the interatomic potential description and the analysis of the deformation response. Embedded atom method (EAM) potentials for shock compression studies must properly describe the energy landscape under the pressure range of interest; and an orientation imaging map technique is described for following the plastic response of fcc and bcc metals.

Timothy Germann
Los Alamos National Laboratory

Date submitted: 22 Feb 2013 Electronic form version 1.4