Abstract Submitted
for the TSF16 Meeting of
The American Physical Society

Strain-Rate Dependence of Material Strength: Large Scale Atomistic Simulations of Defective Cu and Ta Crystals[1] JAYALATH ABEYWARDHANA, Computational Science, University of Texas at El Paso TX, TIMOTHY GERMANN, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM,, RAMON RAVELO, Physics Department, University of Texas at El Paso TX, X-Computational Physics Division, Los Alamos National Laboratory, Los Alamos, NM — Large−Scale molecular dynamics (MD) simulations are used to model shock wave (SW) and quasi−isentropic compression (QIC) in defective copper and tantalum crystals. The atomic interactions were modeled employing embedded−atom method (EAM) potentials. Quasi−isentropic uniaxial compression is achieved by incorporating a strain rate function in the positions and velocities equations of motion. In this new formalism the change in internal energy is exactly equal to the work done in compression. We examined the deformation mechanisms and material strength for strain rates in the $10^8 - 10^{12} s^{-1}$ range for both Cu and Ta defective crystals. Near and far−field X−ray diffraction simulations were also performed to infer the required resolution for resolving defect densities.

[1]Part of this work supported by the Department of Energy under contract DE-AC52-06NA25396 and by the Air Force Office of Scientific Research under AFOSR Award No. FA9550-12-1-0476.

Jayalath Abeywardhana
Computational Science, University of Texas at El Paso TX

Date submitted: 23 Sep 2016 Electronic form version 1.4