Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Multi-Scale Shock Compression Simulations of Metals and Metallic Phase Transitions[1] NIR GOLDMAN, LARRY FRIED, Lawrence Livermore National Laboratory — We present a straightforward method for efficient molecular dynamics (MD) simulation of shock compression of materials that experience thermal electronic excitations at high pressure and temperature. Previous studies have shown that exclusion of the electronic temperature at extreme conditions can result in incorrect computation of dynamic and equation of state properties. The Multi-Scale Shock Technique (MSST) is a simulation methodology based on the Navier–Stokes equations for compressible flow that enables MD simulation of a shock wave with relatively small computational cost. We extend MSST to allow for changes in the electronic entropy during shock compression while conserving Hugoniot conditions. This allows for simulation of significantly higher shock velocities than previously possibly with MSST. We have used our simulation methodology in density functional tight binding simulations of shock compressed silicon. We observe that at high shock velocities inclusion of a non-zero electron temperature results in lower computed shock Hugoniot temperatures and pressures. Our methodology is well suited for shock compression simulations of any material that experiences changes in its electronic entropy under extreme thermodynamic conditions.

[1]Prepared by LLNL under Contract DE-AC52-07NA27344.

Nir Goldman
Lawrence Livermore National Laboratory

Date submitted: 18 Nov 2010 Electronic form version 1.4