Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Developing an Embedded Atom Method Potential for Copper BEN STORTENBECKER, BRIAN DEMASKE, VASILY ZHAKHOVSKY , IVAN OLEYNIK, University of South Florida — A new embedded-atom method (EAM) interatomic potential for copper has been developed in order to improve upon the predictive power of atomistic simulations under extremes of pressures and temperatures induced by shock compression and ultrashort laser irradiation. Several candidate potentials were fit to a database consisting of *ab initio* cold pressure tensor components calculated for a wide range of hydrostatic and uniaxial deformations as well as experimental properties near equilibrium conditions. The close relationship between the stress tensor and interatomic forces under naturally-occurring material states ensures the accuracy of the potential without the need for a large number of fitting points. After fitting, the candidates were then screened against the experimental melting point in order to select a single best potential. This final potential will be verified against the experimental melting line, liquid-vapor coexistence curve, and the shock Hugoniot.

Ben Stortenbecker
University of South Florida

Date submitted: 09 Nov 2012 Electronic form version 1.4