Abstract Submitted
for the SHOCK05 Meeting of
The American Physical Society

Atomistic Simulations of Shock-Induced Melting in Iron Single Crystals K. KADAU, T.C. GERMANN, P.S. LOMDAHL, B.L. HOLIAN, Los Alamos National Laboratory — We report on non-equilibrium and Hugoniostat atomistic simulations of shock-induced melting in iron single crystals. The large-scale simulations show that the melting pressure varies by less than 10 GPa with the crystallographic shock direction. This is in contrast to a large dependence of more than 50 GPa in copper single crystal simulations. We discuss the different behavior of iron and copper and compare our theoretical results to experimental data. Acknowledgments: This work has been supported by the U.S. Department of Energy under contract no. W-7405-ENG-36 by the Advanced Simulation and Computing Program (ASC).

K. Kadau
Los Alamos National Laboratory

Date submitted: 28 Mar 2005 Electronic form version 1.4