Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Atomistic-based Dislocation Mobility Model for Material Strength at High Pressure[1] LIN H. YANG, JOHN A. MORIARTY, Lawrence Livermore National Laboratory — Understanding and predicting the mechanical behavior of materials at a range of temperatures, pressures, and strain rates require a detailed knowledge of the underlying mechanisms that govern plasticity. In this work, we focus on the high-pressure plastic deformation properties of bcc metals in which the plasticity is controlled by $a/2 < 111 >$ screw-dislocation behavior in the crystalline lattice. In particular, the finite-temperature motion of the screw dislocation is believed to be associated with the formation of mobile kinks on the screw dislocation line. Thus, the accurate prediction of kink-pair activation energetics is essential to the understanding and determination of the mobility of screw dislocations in these materials. In turn, an atomistic-based dislocation mobility model for $a/2 < 111 >$ screw dislocation is a key ingredient needed to develop predictive multiscale simulations of crystal plasticity for bcc metals. Based on the data obtained from atomistic simulations, we have developed a scaling relation and strength model for bcc metals under extreme conditions. The predicted flow stress as a function of temperature, strain rate and pressure for bcc Ta and Mo will be presented.

[1]This work was performed under the auspices of the U.S. DOE by

Lin H. Yang
Lawrence Livermore National Laboratory

Date submitted: 08 Dec 2004 Electronic form version 1.4