Abstract Submitted
for the SHOCK11 Meeting of
The American Physical Society

Simulation and theory of high-rate plastic deformation of polycrystalline bcc metals[1] ROBERT RUDD, Lawrence Livermore National Laboratory — High-rate plastic deformation is the subject of increasing experimental activity. High power laser platforms such as the NIF offer the possibility to study plasticity at extremely high rates in shock waves and shockless ramp waves. Here we report on the results of molecular dynamics (MD) simulations of these processes at the atomistic level and related analytic theory. These theories are compared with experiment, the MD simulations and other plasticity models. In the MD simulations we focus on the high-rate deformation of multi-million atom (nanoscale) polycrystalline tantalum and vanadium systems at pressures up to a few Mbar. The simulations span several orders of magnitude in strain rate, allowing us to analyze the rate dependence and the effect of the rate on the mechanisms of plasticity. We also compare the simulations to single crystal simulations. The vanadium simulations explore the pressure range of a recently reported rhombohedral phase. Rhombohedral variant formation contributes to the plastic flow, and we show the interaction of variant nucleation and growth with dislocation flow. We also report an analytic theory of the rate of plastic relaxation associate with dislocation flow and compare it to the MD simulations.

[1]This work was performed under the auspices of the US Dept. of Energy by LLNL under Contract DE-AC52-07NA27344.

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Date submitted: 11 Feb 2011 Electronic form version 1.4