Abstract Submitted
for the SHOCK11 Meeting of
The American Physical Society

A multi-scale strength model with phase transformation N. BARTON, A. ARSENLIS, M. RHEE, J. MARIAN, J. BERNIER, M. TANG, L. YANG, Lawrence Livermore National Laboratory — We present a multi-scale strength model that includes phase transformation. In each phase, strength depends on pressure, strain rate, temperature, and evolving dislocation density descriptors. A donor cell type of approach is used for the transfer of dislocation density between phases. While the shear modulus can be modeled as smooth through the BCC to rhombohedral transformation in vanadium, the multi-phase strength model predicts abrupt changes in the material strength due to changes in dislocation kinetics. In the rhombohedral phase, the dislocation density is decomposed into populations associated with short and long Burgers vectors. Strength model construction employs an information passing paradigm to span from the atomistic level to the continuum level. Simulation methods in the overall hierarchy include density functional theory, molecular statics, molecular dynamics, dislocation dynamics, and continuum based approaches. We demonstrate the behavior of the model through simulations of Rayleigh Taylor instability growth experiments of the type used to assess material strength at high pressure and strain rate. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 (LLNL-ABS-464695).

N. Barton
Lawrence Livermore National Laboratory

Date submitted: 05 Jan 2011

Electronic form version 1.4