SHOCK17-2017-020005

Abstract for an Invited Paper
for the SHOCK17 Meeting of
the American Physical Society

Cross-scale MD simulations of dynamic strength of tantalum

VASILY BULATOV, Lawrence Livermore National Laboratory

Dislocations are ubiquitous in metals where their motion presents the dominant and often the only mode of plastic response to straining. Over the last 25 years computational prediction of plastic response in metals has relied on Discrete Dislocation Dynamics (DDD) as the most fundamental method to account for collective dynamics of moving dislocations. Here we present first direct atomistic MD simulations of dislocation-mediated plasticity that are sufficiently large and long to compute plasticity response of single crystal tantalum while tracing the underlying dynamics of dislocations in all atomistic details. Where feasible, direct MD simulations sidestep DDD altogether thus reducing uncertainties of strength predictions to those of the interatomic potential. In the specific context of shock-induced material dynamics, the same MD models predict when, under what conditions and how dislocations interact and compete with other fundamental mechanisms of dynamic response, e.g. twinning, phase-transformations, fracture.

In collaboration with: Luis Zepeda-Ruiz, Lawrence Livermore National Laboratory; Alexander Stukowski, Technische Universitat Darmstadt; Tomas Oppelstrup, Lawrence Livermore National Laboratory.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.