Abstract Submitted
for the SHOCK07 Meeting of
The American Physical Society

Atomistic simulations of fracture in nanocrystalline copper under high strain rates[1] ALEXEY YANILKIN, ALEXEY KUKSIN, GENRI NORMAN, VLADIMIR STEGAILOV, Joint Institute for High Temperatures of RAS, Moscow, Russia — Structural features of nanocrystalline materials attract continuous attention due to their unique properties and prospects for various technological applications. In this work microscopic mechanisms of plasticity and fracture in nanocrystalline copper are considered at the atomistic level by molecular dynamics method. The EAM potential model [Y. Mishin et al // PRB 63 (2001) 224106] is used to describe interatomic potential. The initial structure is created by filling random Voronoi polyhedra with different orientations of lattice and subsequent equilibration. Three ways of the high strain rate (10^8 – 10^{10} s^{-1}) plastic deformation and fracture processes modeling are compared: hydrostatic and uniaxial strain and shock wave loading in the impacor-target model. The dependence of the results on the average grain size, orientation and shape is studied.

[1]This work was partially supported by the RFBR grant 05-08-65423, RAS programs # 3, 9 and 14, and SNL under the US DOE/NNSA ASC program.

Alexey Yanilkin
Joint Institute for High Temperatures of RAS, Moscow, Russia

Date submitted: 28 Mar 2007 Electronic form version 1.4