

Abstract Submitted
for the SHOCK09 Meeting of
The American Physical Society

Atomistic simulation of dislocation nucleation in aluminum ALEXEY YANILKIN, ALEXEY KUKSIN, GENRI NORMAN, PETER ZHILYAEV, Joint Institute for High Temperatures of RAS, Moscow, Russia — Homogeneous and defect induced dislocation nucleation are considered by means of molecular dynamics simulation. Different mechanisms of dislocation loop nucleation and growth are revealed. Dislocation nucleation starts from the formation of partial dislocation loop by thermally fluctuations. The dependence of the loop energy on shear stress and radius is obtained. It is in a good agreement with dislocation theory. Homogeneous nucleation rates are calculated at different temperatures and stress. During the loop growth the twinning is observed rather than second partial dislocation nucleation. Defects (void, precipitate) in crystal result in concentration of shear stress under deformation. Dislocations appear in the sites with the largest shear stress by formation of the part of dislocation loop. The ends of the dislocation line come together in the defect. The loop forms by rounding the defect like mechanism of Frank-Read source. The activation shear stresses of these mechanisms are obtained at different temperatures. This work was supported by the RAS programs # 11, 12 and SNL under the US DOE/NNSA ASC program.

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Date submitted: 17 Feb 2009

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