

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Molecular-dynamics analysis of the mechanical behavior of face-centered cubic metallic ultrathin films KEDARNATH KOLLURI, M. RAUF GUNGOR, DIMITRIOS MAROUDAS, Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003-3110 — We report results of large-scale molecular-dynamics simulations for the dynamic deformation under biaxial tensile strain of nanometer-scale-thick films of various face-centered cubic metals. Our results indicate that films of metals with moderate to high propensity for formation of stacking faults (e.g., Ni and Cu) exhibit an extended easy glide regime followed by a sharp increase in the material stress, whereas those with low propensity for stacking-fault formation (such as Al) exhibit a monotonic increase in the stress during dynamic loading. We find that the plastic strain rate in Cu and Ni thin films is far greater than that in Al thin films, leading to stress dissipation and an extended easy glide regime. Analysis of defect interaction mechanisms during dynamic deformation reveals dislocation annihilation, which is due to stacking-fault-mediated cross-slip mechanisms in Ni and Cu films and due to collinear interactions between dislocations in Al films.

Kedarnath Kolluri
Department of Chemical Engineering,
University of Massachusetts, Amherst, MA 01003-3110

Date submitted: 11 Dec 2008

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