Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Ab initio simulations of grain boundary sliding in aluminum and nickel JIVTESH GARG, Department of Mechanical Engineering, Massachusetts Institute of Technology, NICOLA MARZARI, Department of Materials Science and Engineering, Massachusetts Institute of Technology — The Hall-Petch relationship predicts an increase in material yield strength with decreasing grain size. However, a breakdown has been reported at smaller grain sizes, where plastic deformation gradually becomes grain-boundary dominated. Studying grain-boundary sliding processes is therefore key to understanding the mechanical properties of polycrystalline materials. In the present work, we use density-functional theory to examine the microscopic processes that accompany grain boundary sliding in aluminum and nickel for different grain boundary structures. Sliding of tilt boundaries is also accompanied with grain boundary migration, where grain boundary movement normal to the boundary surface takes place. The effect of adding W to the sliding process in Ni-W alloys is also reported.

Jivtesh Garg
Department of Mechanical Engineering, Massachusetts Institute of Technology

Date submitted: 30 Nov 2007 Electronic form version 1.4