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Large scale NEMD simulations of polycrystalline Al sliding interfaces[1] JACQUELINE MILHANS, J.E. HAMMERBERG, R. RAVELO, T.C. GERMANN, B.L. HOLIAN, Los Alamos National Laboratory — We present the results of NonEquilibrium Molecular Dynamics (NEMD) simulations for the frictional force between polycrystalline Al samples. Polycrystalline Al samples of order 26M atoms with grain sizes from 10 - 20 nm at compressions of 15 GPa are condsidered as a function of sliding velocity . Typical sample dimensions are 58nm in the sliding and transverse directions and 116nm in the direction normal to the sliding interface. A constant temperature (300K) and constant tangential velocity boundary condition is imposed at the boundaries in the direction normal to the sliding plane. We discuss the modes of plastic deformation and polycrystalline deformation which determine the steady state frictional force and compare these results with results for defect free Al single crystals and highly defective Al single crystal samples.

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