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Large-scale molecular dynamics studies of sliding friction in nanocrystalline aluminum[1] TIMOTHY GERMANN, Los Alamos National Laboratory, RAMON RAVELO, University of Texas - El Paso, JAMES HAMMERBERG, Los Alamos National Laboratory — We present the results of 138 million-atom and 1.8 billion-atom non-equilibrium molecular dynamics (NEMD) simulations for Al-Al sliding friction at pressures of 15 GPa. Three-dimensional samples comprised of 4 nm, 20 nm and 50 nm grains were studied to times of 100 ns for the largest systems. We discuss the evolution of the initial grain size distribution to a steady state distribution that is statistically similar for all initial grain sizes. We compare the results for the frictional force to a rate dependent model that incorporates plasticity and discuss the relationships among grain size, grain morphology, dislocations and other defect structures, and plasticity.

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