Nonequilibrium molecular dynamics simulations of grain dynamics at ductile metal interfaces

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ABSTRACT

We discuss the results of very large scale Non-Equilibrium Molecular Dynamics simulations for polycrystalline Al-Al and Al-Ta interfaces. Initial grain sizes of 13, 20, and 50 nm were considered with maximal sample sizes of 1.8 B atoms and maximal times to 10 s of ns. We observe independence of the frictional force to initial grain size in the velocity regime of 20-4000 m/s for nominal material pressures of 15 GPa. The steady sliding state is characterized by a quasi-periodic sequence of grain growth and refinement which we discuss. A scaling analysis in terms of a power scaling for the frictional force as a function of $v/v_c$ for $v/v_c > 1$, which characterized single crystal sliding, remains valid for the polycrystalline materials.