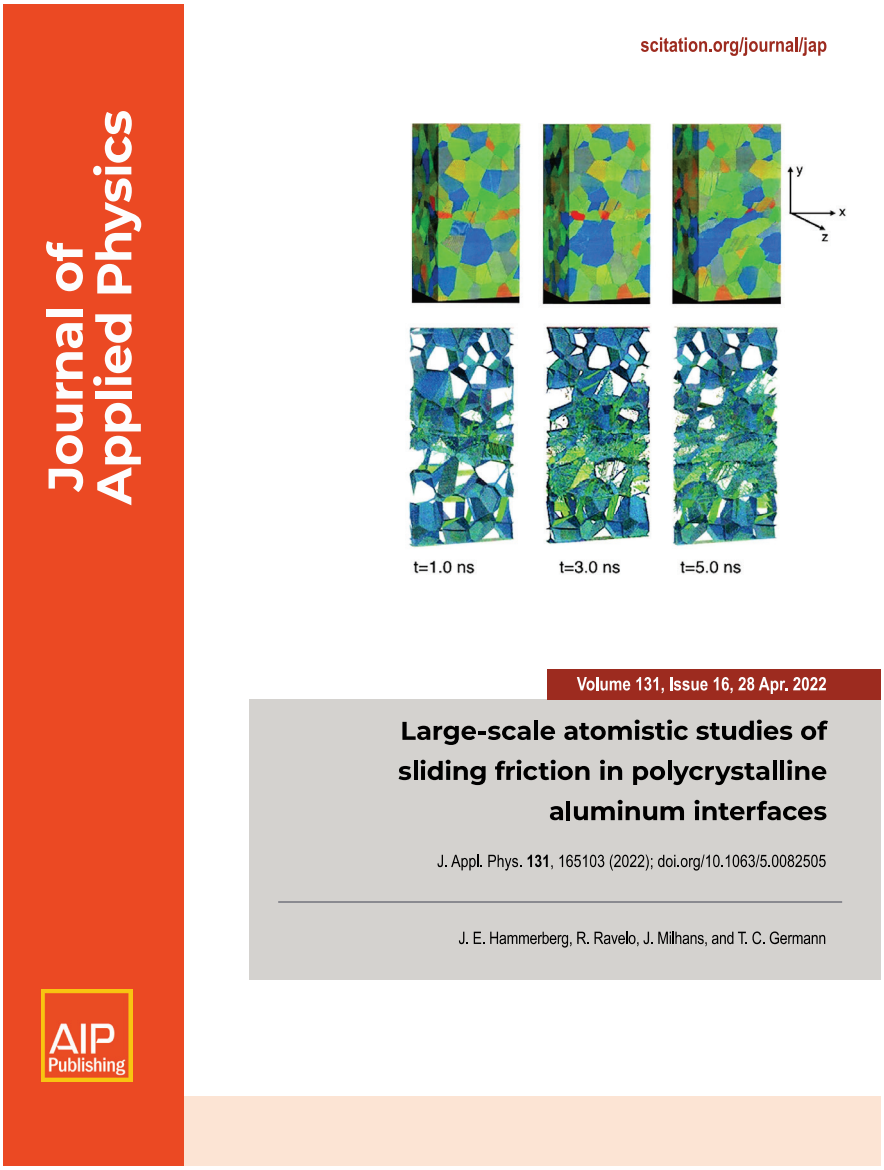
Microstructural Evolution and Friction at Sliding Metal Interfaces

Molecular dynamics simulations of ductile metal sliding at polycrystalline aluminum interfaces provide insight into the interplay between microstructural evolution and the steady-state frictional force.



The image featured on the cover of the *Journal of Applied Physics* shows the early time evolution of grain structure and plastic deformation of a nanocrystalline aluminum sample with an initial 50 nm grain size, and 60 m/s sliding velocity. The top images are colored according to the local face-centered-cubic (fcc) crystal orientation. The bottom images only show defective (non-fcc) atoms.

The Science

The physics of frictional interactions at ductile metal interfaces is complex, involving material mixing, grain structure transformation, and the formation of graded microstructures. At high sliding speeds, the frictional force typically exhibits velocity weakening, i.e., a decrease in the frictional force with increasing velocity with melting occurring at very high velocities. Large-scale non-equilibrium molecular dynamics (NEMD) simulations provide a window into the microscopic world of frictional dissipation. Such simulations, pioneered at LANL in the 1990s by Jim Hammerberg and Brad Holian, have provided insight into each of the phenomena mentioned above, but require extremely large length scales to model realistic polycrystalline materials, and long time scales to reach a steady state frictional heating and resistance. Only now have modern supercomputers and high-performance scalable codes made this possible.

The Impact

Experimental studies of frictional interactions have provided *post situ* evidence of material mixing, grain structure transformation, and the formation of graded microstructures, but the processes are too fast, and occur on length scales that are too short, to observe experimentally. Atomistic simulations fill this gap, and enable a systematic study of the effects of loading conditions and initial microstructure, thus enabling the development of a strain, strain rate, and grain size model that can be deployed in continuum-scale simulations.

Summary

We have used large-scale non-equilibrium molecular dynamics (NEMD) simulations, following billions of atoms for tens of nanoseconds using LANL's SPaSM molecular dynamics code on LLNL's Sequoia supercomputer, to study ductile metal sliding. A series of simulations of sliding friction of polycrystalline aluminum interfaces compressed to a nominal pressure of 15 GPa, typical of plate impact or explosively driven experiments, and for sliding velocities in the range of 10–2000 m/s. The effect of initial grain size was systematically studied by utilizing (initially) mono-dispersive grain distributions with initial mean grain sizes of 4, 13, 20, and 50 nm, which translates into atomistic systems containing between a few hundred million atoms and up to 2 billion atoms. The original grain structure evolves under shear strain and frictional heating, leading to a steady sliding state very different from the initial structure, characterized by grain growth and refinement at high rates of plastic deformation and large values of plastic strain. The results of these simulations have identified a variety of physical mechanisms that are important in determining the steady-state frictional force for a wide range of velocities at compressed metal–metal interfaces. These include grain growth and refinement, the evolution of large plastic strains and strain rates, material mixing, and melting. These phenomena can be included in a strain, strain rate, and grain size model that gives good agreement with the NEMD simulations and can be applied to macroscopic continua.

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Publication

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