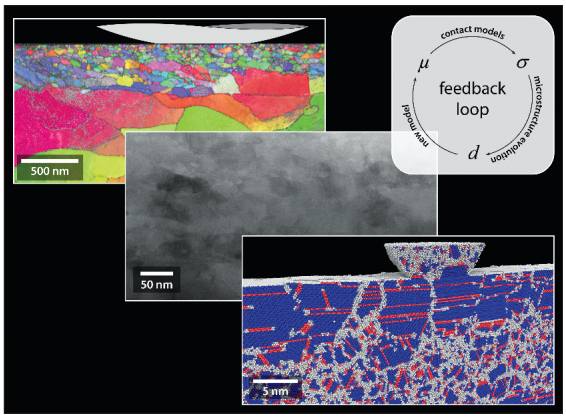
Nano Focus

## Sliding metals: A quantitative roadmap for low-friction materials

What happens when one metal rubs against another? Typically, the surfaces undergo processes such as cold-welding and galling, generating high friction and wear. This eventually leads to material degradation, heating, loss of luster, and, ultimately, structural failure. While lubricants and tribological coatings can often be used to counter these problems, the development of wear-resistant coatings offers many advantages for highly efficient engineering solutions. Researchers are therefore exploring the fundamental properties of materials that contribute to friction in order to develop strategies that mitigate these effects. Systems of pure metals that slide against each other are of particular interest. The microstructures of these materials evolve in different ways in low-friction and high-friction regimes. However, to date, studies have neither completely mapped out these conditions nor developed a comprehensive framework that may predict this behavior.

Researchers from Sandia National Laboratories (SNL) decided to tackle this challenge. Nicolas Argibay and Michael Chandross of SNL's Material, Physical and Chemical Sciences Center relied on a combination of experimental characterization and molecular dynamics simulations to describe a structure–property relationship that yields exceptionally low coefficients of friction between metals. In collaboration with researchers from Virginia Polytechnic Institute and State University, they published the results in a recent issue of the *Journal of Materials Science* (doi:10.1007/s10853-016-0569-1).

Chandross says, "This is one of those great collaborations where everything just comes together perfectly; the mechanisms we initially predicted purely from simulations turned out to be validated by experiments. That allowed us to develop the structure–property relationships that link atomic-scale deformation mechanisms to macroscale friction." Argibay adds, "This work gives us a new way to think about friction in metals. Instead of relying on phenomenological explanations of friction, like the engineering rule-of-thumb that 'harder is better,' we can now begin to think about materials design in a more rigorous way."




The transmission Kikuchi diffraction pattern, transmission electron microscopy, and molecular dynamics simulation results that describe the effect of grain size on friction. The proposed model is a feedback loop that ties together key materials properties to explain the resulting tribological properties. Credit: *Journal of Materials Science*.

Chandross and Argibay first detected a low-friction regime for metals from tribological experiments involving self-mated contacts of two different copper- and gold-metal systems. They applied a normal force of up to 100 mN between metal balls and flat coupons, and sheared them at 1 mm/s. They detected a low-friction regime (friction coefficient less than 0.4), a low-to-high transition region (friction coefficient between 0.5 and 1.0), and a steady high-friction region (coefficient above 1.0). They found a very thin (few tens of nanometers) nanocrystalline film that accommodates any plastic strain. While fine-grained (<~20 nm) surface layers corresponded with lower friction, coarser grains (>~20 nm) yielded high-friction regimes.

The researchers built on these findings and developed molecular dynamics (MD) models to identify the key parameters that contribute to low-friction behavior. They simulated pure silver and its alloys and predicted grain growth and high friction for pure metals and soluble alloys, where sliding occurred along fcc slip planes. In contrast, insoluble alloys exhibit grain refinement and allow low-friction grain-boundary sliding. Alloys can minimize the damaging dislocation-mediated deformation process and suppress grain reorientation and coarsening. In turn, this effect allows low-friction sliding.

The researchers' MD simulations estimated the coefficients of friction ratio between the low-friction disordered grain-boundary sliding and high-friction intragrain slip to be approximately 1:3. This value matched both the research team's own experimental results and previously documented low/high friction coefficients for metal systems. Chandross and Argibay further determined that each metal system exhibits a unique critical grain size that governs the stress-, temperature-, and time-resolved transition between grain-boundary sliding and dislocation-mediated plasticity. Applied stress drives the grain size toward the equilibrium dislocation splitting distance (the zero-stress separation between two Shockley partial dislocations, or DSD), and the material's stacking-fault energy determines the properties of the slip system. The research team, subsequently, named and defined two material property limits: the Beilby limit (reduced stress is 0.5, grain size is less than the DSD diameter) and the Hall–Petch limit (reduced stress is 1.0, grain size is more than twice that of the DSD diameter). The researchers mapped out the friction regime for metals in the range between these two extremes.

The researchers expanded on existing deformation models and discussed additional properties of real-life systems that follow-up research efforts must consider. Metallic contacts and moving parts are present in a broad range of applications, including nanoscale electronics, sensors, actuators, and Ohmic switches. These systems, in particular, are highly vulnerable to frictional heating and could stand to benefit from conditions that minimize shear-induced wear and tear. The efforts by Chandross, Argibay, and their collaborators present a promising path toward that goal.

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