Theoretical simulations reveal how nanoscale lubricating systems can ease friction between surfaces

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Diamond-like-carbon (DLC) coatings are an innovative technology, exhibiting the twin properties of mechanical toughness and ultralow friction. These features, which are desirable in abrasive environments, have led to the widespread adoption of DLC films in microelectromechanical systems, such as hard disk drives. But because these coatings contain amorphous carbon atoms that produce rough, nanoscale textures, it is difficult to optimize their friction properties using classical theories designed for macroscopic objects.

By performing atom-level simulations of nanoscale friction, Ling Dai and co-workers from the A*STAR Institute of High Performance Computing in Singapore have now uncovered critical clues for designing better systems to lubricate and protect DLC coatings.

Perfluoropolyether (PFPE) is a Teflon-like polymer that is commonly sandwiched between DLC-coated substrates to reduce friction and protect against damage. Understanding the friction mechanisms between these ultrathin films is tricky; these materials have contrasting hard and soft mechanical properties, and the sandwich arrangement obscures any direct observation of atomic structure and activity.

To better understand how nanoscale lubrication works in microdevices, the researchers constructed an atomic DLC–PFPE–DLC triple layer using a three-dimensional computer modeling program. They set one DLC slab as a substrate and the other as a 'slider'. They then used molecular dynamics techniques to simulate how the lube film responds when the slider moves. However, it was challenging to describe the atomic interactions in this complex material, and so Dai's team developed hybrid computations that combined several potential energy expressions to replicate the many-body forces in this system.

Simulating frictional motions at different speeds and PFPE film thicknesses revealed that the lubricating film behaves as a solid—the polymer retained its shape without deforming from internal shearing. However, the lubricating film displayed two distinct and competitive modes of motion at an interface: a 'stick–slide' action that produced jerky, stepwise displacements, and a continuous motion that caused the film to slide with fluctuating velocities. The team's analysis showed that these two types of motions switched on or off depending on adhesion factors, such as thermal vibrations and the interfacial roughness.

After mapping the local friction forces along the sliding interfaces, the researchers discovered a way to link the law describing macroscopic friction to the nanoscale using a simple mathematical modification—a finding with practical importance for the surface engineering of DLC coatings.

"Because our model closely resembles the materials used in industrial applications, this work can serve as a guide for future experimental developments," says Dai.

More information: Dai, L., Sorkin, V., Sha, Z. D., Pei, Q. X., Branico, P. S. & Zhang, Y. W. Molecular dynamics simulations on the frictional behavior of a perfluoropolyether film sandwiched between diamond-like-carbon coatings. *Langmuir* 30, 1573–1579 (2014). dx.doi.org/10.1021/la404680v

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