Simulations lead to design of near-frictionless material

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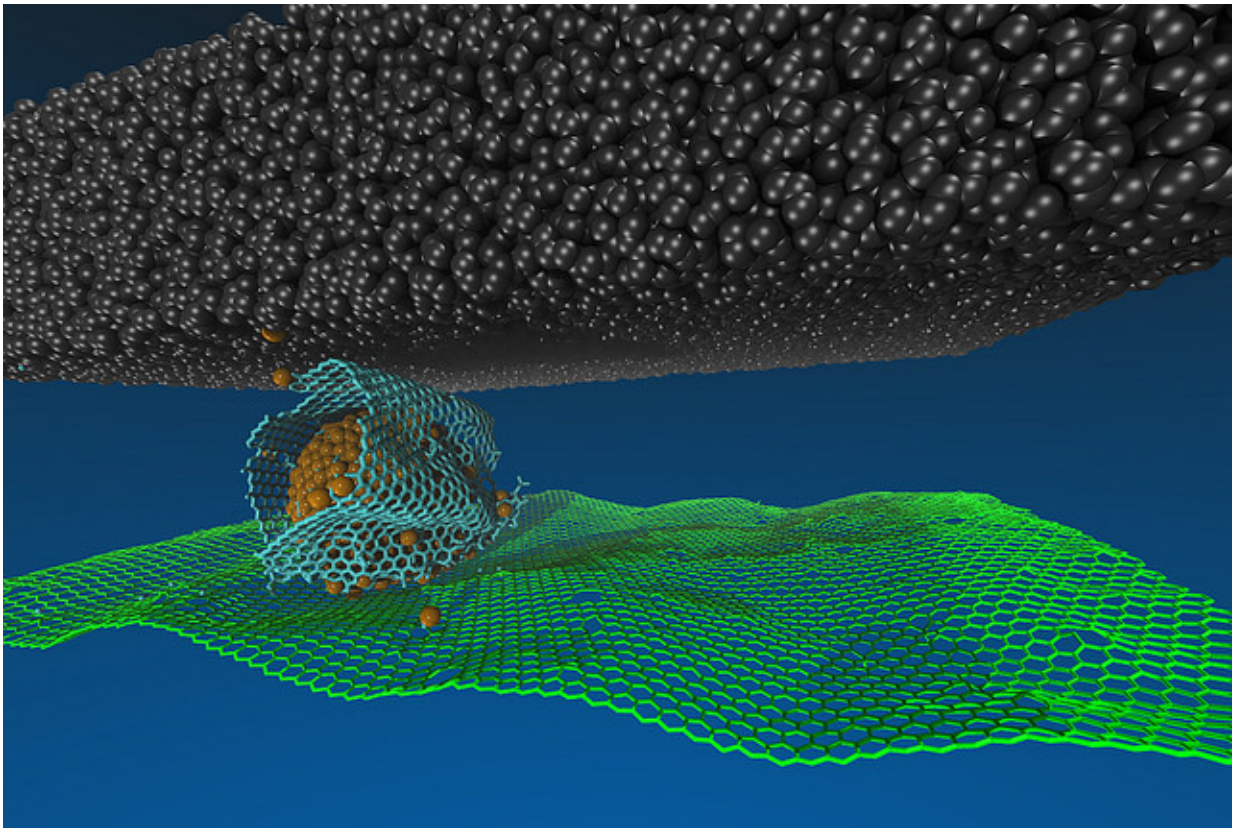

In this schematic of the superlubricity system, the gold represents nanodiamond particles; the blue is a graphene nanoscroll; green shows underlying graphene on silicon dioxide; and the black structures are the diamond-like carbon interface. Credit: Sanket Deshmukh, Joseph Insley, and Subramanian Sankaranarayanan, Argonne National Laboratory

Argonne scientists used Mira to identify and improve a new mechanism for eliminating friction, which fed into the development of a hybrid material that exhibited superlubricity at the macroscale for the first time. Argonne Leadership Computing Facility (ALCF) researchers helped enable the groundbreaking simulations by overcoming a performance bottleneck that doubled the speed of the team's code.

While reviewing the simulation results of a promising new lubricant material, Argonne researcher Sanket Deshmukh stumbled upon a phenomenon that had never been observed before.

"I remember Sanket calling me and saying 'you have got to come over here and see this. I want to show you something really cool,'" said Subramanian Sankaranarayanan, Argonne computational nanoscientist, who led the simulation work at the Argonne Leadership Computing Facility (ALCF), a DOE Office of Science User Facility.

They were amazed by what the computer simulations revealed. When the lubricant materials—graphene and diamond-like carbon (DLC)—slid against each other, the graphene began rolling up to form hollow cylindrical "scrolls" that helped to practically eliminate friction. These so-called nanoscrolls represented a completely new mechanism for superlubricity, a state in which friction essentially disappears.

"The nanoscrolls combat friction in very much the same way that ball bearings do by creating separation between surfaces," said Deshmukh, who finished his postdoctoral appointment at Argonne in January.

Superlubricity is a highly desirable property. Considering that nearly one-third of every fuel tank is spent overcoming friction in automobiles, a material that can achieve superlubricity would greatly benefit industry and consumers alike. Such materials could also help increase the lifetime of countless mechanical components that wear down due to incessant

friction.

Experimental origins

Prior to the computational work, Argonne scientists Ali Erdemir, Anirudha Sumant, and Diana Berman were studying the hybrid material in laboratory experiments at Argonne's Tribology Laboratory and the Center for Nanoscale Materials, a DOE Office of Science User Facility. The experimental setup consisted of small patches of graphene (a two-dimensional single-sheet form of pure carbon) sliding against a DLC-coated steel ball.

The graphene-DLC combination was registering a very low friction coefficient (a ratio that measures the force of friction between two surfaces), but the friction levels were fluctuating up and down for no apparent reason. The experimentalists were also puzzled to find that humid environments were causing the friction coefficient to shoot up to levels that were nearly 100 times greater than measured in dry environments.

To shed light on these mysterious behaviors, they turned to Sankaranarayanan and Deshmukh for computational help. Using Mira, the ALCF's 10-petaflops IBM Blue Gene/Q supercomputer, the researchers replicated the experimental conditions with large-scale molecular dynamics simulations aimed at understanding the underlying mechanisms of superlubricity at an atomistic level.

This led to their discovery of the graphene nanoscrolls, which helped to fill in the blanks. The material's fluctuating friction levels were explained by the fact that the nanoscrolls themselves were not stable. The researchers observed a repeating pattern in which the hollow nanoscrolls would form, and then cave in and collapse under the pressure of the load.

"The friction was dipping to very low values at the moment the scroll formation took place and then it would jump back up to higher values when the graphene patches were in an unscrolled state," Deshmukh said.

The computational scientists had an idea to overcome this issue. They tried incorporating nanodiamond particles into their simulations to see if the hard material could help stabilize the nanoscrolls and make them more permanent.

Sure enough, the simulations proved successful. The graphene patches spontaneously rolled around the nanodiamonds, which held the scrolls in place and resulted in sustained superlubricity. The simulation results fed into a new set of experiments with nanodiamonds that confirmed the same.

"The beauty of this particular discovery is that we were able to see sustained superlubricity at the macroscale for the first time, proving this mechanism can be used at engineering scales for real-world applications," Sankaranarayanan said. "This collaborative effort is a perfect example of how computation can help in the design and discovery of new materials."

Not slippery when wet

Unfortunately, the addition of nanodiamonds did not address the material's aversion to water. The simulations showed that water suppresses the formation of scrolls by increasing the adhesion of graphene to the surface.

While this greatly limits the hybrid material's potential applications, its ability to maintain superlubricity in dry environments is a significant breakthrough in itself.

The research team is in the process of seeking a patent for the hybrid material, which could potentially be used for applications in dry environments, such as computer hard drives, wind turbine gears, and mechanical rotating seals for microelectromechanical and nanoelectromechanical systems.

Adding to the material's appeal is a relatively simple and cost-effective deposition method called drop casting. This technique involves spraying solutions of the materials on moving mechanical parts. When the solutions evaporate, it would leave the graphene and nanodiamonds on one side of a moving part, and diamond-like carbon on the other side.

However, the knowledge gained from their study is perhaps even more valuable, said Deshmukh. He expects the nanoscroll mechanism to spur future efforts to develop materials capable of superlubricity for a wide range of mechanical applications.

For their part, the Argonne team will continue its computational studies to look for ways to overcome the barrier presented by water.

"We are exploring different surface functionalizations to see if we can incorporate something hydrophobic that would keep water out," Sankaranarayanan said. "As long as you can repel water, the graphene nanoscrolls could potentially work in humid environments as well."

Simulating millions of atoms

The team's groundbreaking nanoscroll discovery would not have been possible without a supercomputer like Mira. Replicating the experimental setup required simulating up to 1.2 million atoms for dry environments and up to 10 million atoms for humid environments.

The researchers used the LAMMPS (Large-scale Atomic/Molecular

Massively Parallel Simulator) code to carry out the computationally demanding reactive molecular dynamics simulations.

With the help of ALCF catalysts, a team of computational scientists who work directly with ALCF users, they were able to overcome a performance bottleneck with the code's ReaxFF module, an add-on package that was needed to model the chemical reactions occurring in the system.

The ALCF catalysts, in collaboration with researchers from IBM, Lawrence Berkeley National Laboratory, and Sandia National Laboratories, optimized LAMMPS and its implementation of ReaxFF by adding OpenMP threading, replacing MPI point-to-point communication with MPI collectives in key algorithms, and leveraging MPI I/O. Altogether, these enhancements allowed the code to perform twice as fast as before.

"With the code optimizations in place, we were able to model the phenomena in real experimental systems more accurately," Deshmukh said. "The simulations on Mira showed us some amazing things that could not be seen in laboratory tests."

And with the recent announcement of Aurora, the ALCF's next-generation supercomputer, Sankaranarayanan is excited about where this line of research could go in the future.

"Given the advent of computing resources like Aurora and the wide gamut of the available two-dimensional materials and nanoparticle types, we envision the creation of a lubricant genome at some point in the future," he said. "Having a materials database like this would allow us to pick and choose lubricant materials for specific operational conditions."

The researchers recently published their findings from this project in a

Science Express.

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