Georgia Tech

Research News

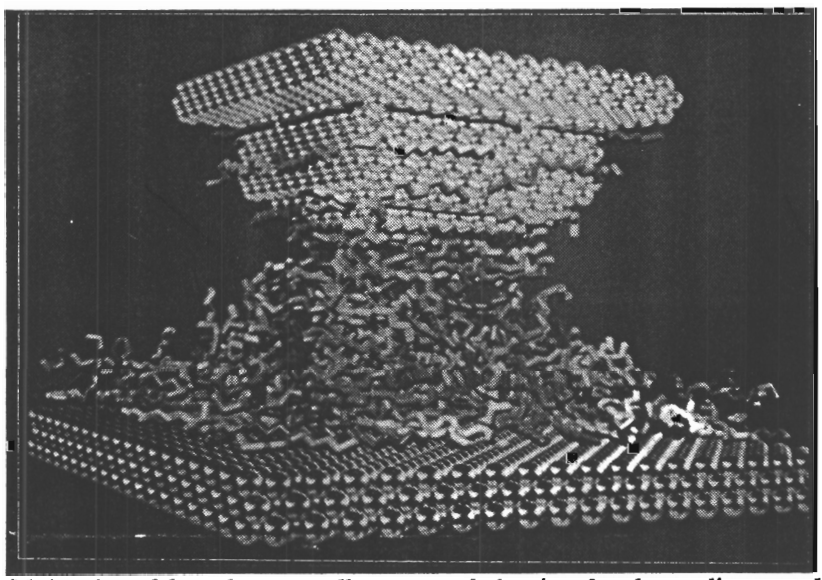
Georgia Institute of Technology
Research Communications Office
Atlanta, Georgia 30332-0800
404•894•3444

Embargoed For Release 10 a.m.
April 10, 1992

IN THE WORLD OF THE VERY SMALL: STUDY OF MOLECULAR & ATOMIC INTERACTION GIVES NEW INSIGHTS INTO MECHANICAL CONTACTS

Wriggling hydrocarbon molecules well up toward the microscopic tip of an approaching metal probe. As the probe presses on the molecules, they first flow up its side, then begin organizing themselves into neatly-structured layers. Under high pressure, the layers squeeze out until just a single blanket of molecules separates the tip from a gold sheet underneath.

Created on a powerful supercomputer, such molecular dynamics simulations are giving Georgia Institute of Technology physicists dramatic new insights into the complex molecular and atomic-scale interactions that occur when materials come into contact. By visualizing the complex behavior, the research could lead to development of improved lubricants and a better understanding of a wide range of mechanical contact phenomena.



Molecules of hexadecane well up toward the tip of a descending metal probe in this simulation of the microscopic interactions which occur when materials come into contact. (Color/B&W Available).

"By looking at the response to stress and load on the molecular level, we can get ideas about the type of molecular architecture needed to make lubricants that wear less or work better under extreme conditions," explained Dr. Uzi Landman, professor in Georgia Tech's School of Physics. "This work gives us a rational way of looking at how to make better materials. To make the next jump in materials, we need to know the structure and dynamic response characteristics on the atomic scale."

Landman will present recent results of the research

- OVER -

FOR MORE INFORMATION:

ASSISTANCE/PHOTO: John Toon or Lea McLees, (404) 894-3444
RESEARCHER: Dr. Uzi Landman, (404) 894-3368 or (404) 894-5219
WRITER: John Toon

April 10 at the Spring meeting of the American Chemical Society in San Francisco.

In a paper published two years ago in Science, Landman and Research Scientist Dr. W. David Luedtke -- in collaboration with experimental researchers from the Naval Research Laboratory in Washington, D.C. -- described the peculiar atomic behavior that occurs when a nickel probe approaches a crystalline gold surface. When the probe is approximately four Angstroms away, gold atoms leap up to coat the tip of the probe.

When the probe is then raised, the gold responds plastically and forms a thin connecting neck which is drawn out like a wire until it finally breaks, leaving a damaged gold surface. Formation of these contacts, said Landman, explains the source of friction that occurs between unlubricated metal surfaces.

Since then, Landman and Luedtke have explored how thin films of hydrocarbon lubricants work to reduce friction by preventing formation of the junctions. Their simulations of a long-chain hydrocarbon lubricant known as hexadecane reveals a dramatic sequence of activity which has been captured on videotape.

"When you bring the tip of the probe toward the surface, the film of lubricant forms a bulge toward the probe, wetting its surface," Landman explained. "When we squeeze on the film, there is molecular-scale drainage of the molecules from under the tip. Then the liquid confined between the tip and the substrate begins to exhibit properties that are very different from either the bulk liquid or the thin film. The confined molecular film has structural, dynamic and transport properties which appear to be a new phase of the liquid."

As the pressure exerted by the tip continues to increase, the once homogenous film of molecules forms a layered structure. "The molecules orient themselves in a way which affects the viscosity and the transport properties of the film," he noted.

Under high pressure, all but a few of the molecules slip out of their confinement -- but enough remain to prevent the materials from creating the kinds of contacts seen in bare metal.

Formation of the junctions and the strange antics of the hydrocarbon molecules illustrate how the consequences of physical laws change at unseen boundaries in the microscopic world. "Each atom feels not only the atom next to it, but also a whole environment of other atoms. It is not a simple interaction, but one governed by the quantum-mechanical electronic charge distributions," Landman added.

Such atomistic simulations give scientists new knowledge about the behavior of materials on the microscopic scale.

"On a really small level, certain classical theories of materials properties become inadequate and then we have to provide a different description," said Landman. "But if you know where your continuum mechanics description holds or how to modify and extend it, you don't always have to do the supercomputer simulations. This makes a connection between the macroscopic and microscopic worlds."

The simulations and related visualizations have implications for such analytical techniques as scanning tunneling microscopy (STM) and atomic force microscopy (AFM), which rely on the proximity of a probe to a surface to reveal features of a material under study. The interactions between the probe and the surface and the possible formation of contacts could modify the material being investigated and therefore affect the experimental results, Landman warned.

The simulations and visualizations also have application to development of atomic-scale switches, which use electrical voltage to affect the atomic jumping phenomena, opening and closing the junction.

The simulations are based on a detailed set of physical laws and interactions that describe the behavior of atoms and molecules. A powerful supercomputer allows the researchers to deduce the consequences of these interactions in complex systems of up to 100,000 atoms.

"We integrate equations of motion and we provide the full detail of the evolution of a system," Landman explained. "We look atom by atom at this motion, and then we extract information about the behavior of the system."

Other scientists have partially verified these simulations by experimental means using atomic force microscopes able to measure the forces involved in the formation and properties of the junctions.

This research was sponsored by the U.S. Department of Energy, the U.S. Air Force Office of Scientific Research and the National Science Foundation.