Friction Flicks

Computer animation offers insights into friction's molecular underpinnings

By JANET RALOFF

As the room darkens, jazz strains break the silence and a surreal scene emerges: A mat of multicolored spaghetti covers a field of gold. Some short distance above hovers a large silver object — a truncated, upside-down pyramid of tightly packed, metallic balls. Suddenly the spaghetti strands begin wiggling, and it becomes clear that the rainbow-hued objects are sleeping snakes.

Before long, one of the writhing creatures rises like a hoodless, purple cobra from the serpentine sea. Reaching up from the backs of its teeming brethren, it grabs hold of and climbs onto the bottom of the inverted pyramid. Defying gravity, it slithers back and forth across the bottom of this silvery structure. Seconds later, a green snake joins it, followed in turn by orange and yellow comrades. In time, a mass of the slithering bodies covers the lower end of the pyramid.

So begins the latest of Uzi Landman's animated short subjects.

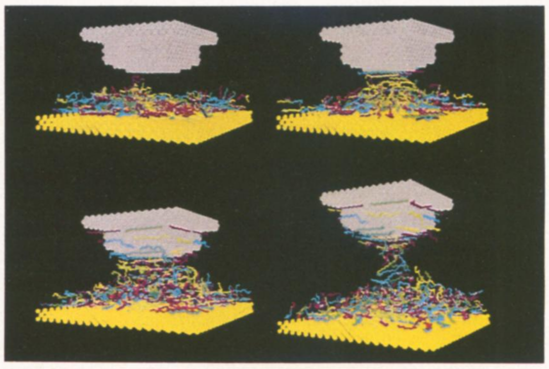
Director of the Center for Computational Materials Science at the Georgia Institute of Technology in Atlanta, Landman explores the interactions that define tribology — the science of friction, wear and lubrication — on an atomic scale. So while this physicist makes every effort to wed music and animation into a production that entertains the eye and ear, his primary objective remains the creation of moving pictures that stretch scientific frontiers.

Landman's team provides a Cray supercomputer with a cast of characters whose personalities are determined by the physical and chemical forces that govern how they interact with their neighbors. Then the scientists set a theoretical stage and allow the simulated characters to improvise their way through a hypothetical scene.

The protagonists in their serpentine video — which played to packed rooms at an American Physical Society meeting in March and at the spring meeting of the American Chemical Society last month — are individual 16-carbon-atom molecules of a short-chained paraffin lubricant. The story line follows the adventures of these writhing antiheroes as they become locked in a life-and-death struggle to escape two large, opposing forces: the nickel tip of an atomic force microscope (played by the inverted pyramid) and the plane of gold.

A camera records the evolving choreography of these silent players — a complex drama simulating reactions on a scale beyond resolution by the human eye, motions that occur on stage sets measured in billionths of a meter. By replaying this drama over and over — some portions in frame-by-frame slow motion — tribologists are gleaning insights into how lubricants function.

For instance, although the lubricant's interwoven mat of snake-like hydrocarbons starts out like an ordinary liquid, as the tip of the atomic force microscope (AFM) begins to squeeze the lubricant against the larger, gold surface, the paraffin starts to undergo structural changes. Essentially, the pressure forces order out of the chaos.



Four frames from serpentine video. Upper two show lubricant welling up to eventually cover hovering AFM tip. Lubricant continues to bridge the metal surfaces even as AFM tip begins pulling up and away (lower right).

Landman

When the AFM tip forces the jumbled mix of paraffin molecules down to a thin film just four or five molecules thick, "you start to get layering," Landman observes. Along the enclosing nickel and gold horizontal walls, the strands begin orienting themselves into parallel rows of molecules parked head-to-tail. As the tip squeezes down harder, the mix of molecules sandwiched between the outer layers also successively separates into strata of ordered strands.

Unique to confined liquid thin films, "this is a very, very new type of thing," Landman says, one "we didn't expect to emerge in such a dramatic manner." Essentially, the liquid undergoes "alterations that immediately change its elasticity, flow and viscosity — and consequently its lubricating abilities."

Together with W. David Luedtke, Landman directed the hypothetical AFM tip to squeeze down even harder. While it doesn't appear in this movie, the resulting simulation showed the paraffin strands begin to drain out — but not in an orderly, straight line. They snake out with a reptilian wiggle — a motion called reptation. Additional pressure on the AFM tip squeezes out all but a one-molecule-thick layer of the lubricant. Still the tip presses on, until it finally dents the golden plate. Yet to the end, a monolayer of paraffin remains sandwiched between the metal surfaces.

In this drama, then, the protagonist paraffins triumph in their appointed mission. Despite great duress, they prevent the nickel and gold from touching. And that constitutes a happy ending, Landman says, because even the lightest touch could have opened a devastating wound on the weaker metal — a lesion that might even have welded the nickel and gold into an unwanted, lifelong embrace.

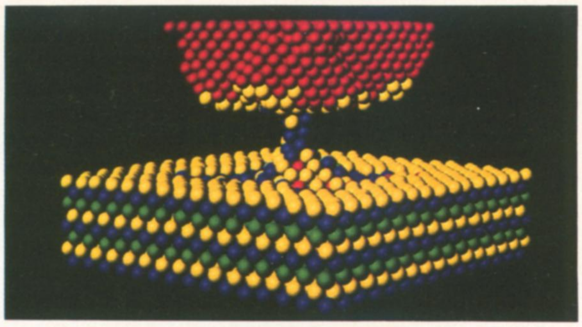
Fiction? No, a number of researchers say. Indeed, Landman says, although the movie cannot yet quantitatively depict the real world, qualitatively "it's not far off."

For instance, experimental physicist C. Mathew Mate and his co-workers at the IBM Almaden Research Center in San Jose, Calif., have confirmed that lubricant molecules caught between two rigid surfaces "do wriggle out" like a snake. However, he says that they've yet to confirm the untangling of tightly pressed lubricant molecules, because their experimental setup is "not sensitive enough to see the ordering effect."

But surface scientist Jacob Israelachvili and his co-workers at the University of California, Santa Barbara, have witnessed experimental evidence of an unexpected ordering in thin films of lubricant liquids. Tribologists had suspected that, compared to a liquid in bulk form, thin films of a lubricant – on the order of about five molecules, or 20 angstroms, thick – might become perhaps twice as viscous. But Israelachvili says "no one expected [the viscosity increase his group detected] of about five orders of magnitude."

"Even more interesting, the liquid [lubricant] changes its properties qualitatively. It can undergo a phase change . . . and take on properties of a solid or liquid crystal."

Moreover, "we have found that even if a phase change does not occur, the molecules can be forced to align in a certain way." Imagine the tangled molecules of the lubricant suddenly lining up like rows of parallel logs. "They become more ordered and structured," he says – characteristics usually associated with solids. "But ordered this way, they can also roll more easily, making the lubrication more effective and, therefore, dynamically more like a liquid."



Landman

Frame from earlier movie shows gold-surface defect created as thin gold wire forms to bridge two nearly touching, clean-metal surfaces.

In an earlier movie, Landman's team modeled what would happen when two pristine metals – again a nickel AFM tip and a gold plate – approached one another but did not touch. To their surprise, when the metals reached some critical distance – about 2 angstroms apart – atoms of the gold suddenly broke loose from the plate, creating a surface crater, and welled up to coat the bottom of the nickel tip. At the time, this unexpected phenomenon – termed dry wetting – struck Landman as nothing less than "bizarre."

"When we asked ourselves why this might happen," recalls Richard J. Colton, a surface chemist at the Naval Research Laboratory, "we realized that the nickel's surface energy [the forces binding it together] was greater than the gold's, so gold should have wet the nickel. But that was hindsight. We didn't think of that until we saw the movie."

Colton was not content to accept that the portrayed phenomenon merely made sense, however. He set up an experiment at his laboratory in Washington, D.C., to emulate the movie. When it was over, "we looked at the tip and found gold was indeed present."

That earlier Georgia Tech movie also indicated a few other phenomena not previously observed. For instance, once the gold jumped to the nickel, the team asked their model what would happen if they slowly began lifting the AFM tip away from the newly formed gold junction.

"A sort of connective neck started to form," Landman says. "It looked like an atomic-dimensional wire."

As the nickel tip pulled away, the thin gold wire connecting the surfaces held for just so long before undergoing an instability – a physical change that allowed the wire to suddenly thin and elongate. With further pulling, the process repeated itself again and again.

The atoms within this wire are bonded together. "And those bonds can take just so much force pulling them apart before they all of a sudden break," Colton explains. "That's when the wire lengthens." Then the strand narrows as the metal's bonds rearrange into unstressed configurations. With continued pulling, the bonds again stretch until they break and can reconfigure.

Landman's team saw these periodic, quantized jumps in the force and energy curves related to their lengthening wire. While Colton's subsequent experiment showed no similar "fine structure," new work by Mate's team at IBM has.

As with the modeled prediction that gold would wet a somewhat distant nickel tip, this development of very thin atomic strands between nearly touching, unlubricated surfaces "is one of those things that, once you know the answer, you realize is not surprising," Mate told SCIENCE NEWS. But prior to Landman's movie, it was "not obvious that would happen."

It now appears "that friction has its origins in these small contacts that form when you bring two materials close together," Landman says, because to slide one surface along another, "you essentially have to break these contacts." Moreover, to the extent that these microscopic contacts can open up atomic-scale surface flaws, they also contribute to surface wear.

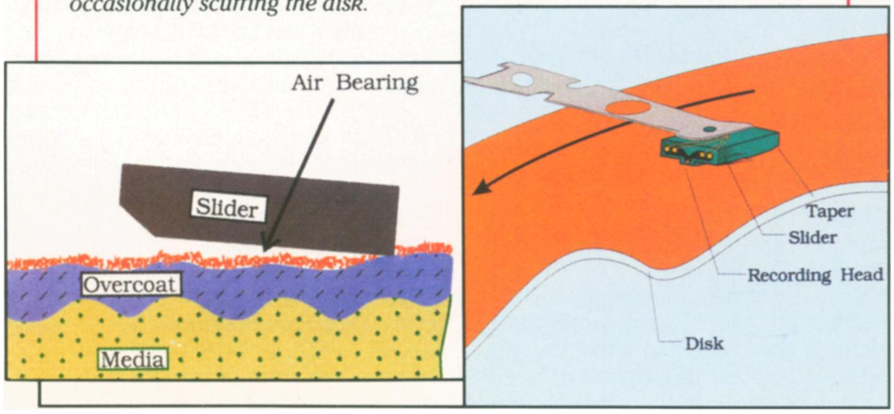
"One of the major roles of lubricants, then, is to separate two materials and prevent this junction formation," he continues. As such, these findings have important implications for the fundamental understanding of friction and wear.

Colton agrees. Humans have been aware of friction, wear and lubrication for ages. But until a couple of years ago, he says, "we never knew what happened on an atomic scale," where most of these phenomena have their roots.

Nor are these developing atomic-scale insights of merely academic interest. They promise near-immediate payoffs in a number of high-tech products, including high-density disk drives for computers.

As it hovers a short distance above a computer's rapidly rotating hard disk, a small magnetic-recording "head" (see diagram) employs a magnetic field to read and write information. The lower the head flies above the disk, the narrower the spread of its magnetic field across that disk and the smaller the area required to store each bit of data. To increase a disk's data-storing capacity, computer designers are attempting to fly heads ever closer to the disk surface. But every time a disk starts or stops rotating, or the head hits a piece of surface contamination, the head contacts the disk and risks wearing away some of its magnetic coating. Worse, the head and disk

Cross-section (left) of surface of hard drive. Only a thin layer of lubricant – depicted in gold – keeps the slider and its recording head (see right) from occasionally scuffing the disk.



IBM Almaden

Order from chaos: Three diagrams depict paraffin's structure in top (far left), middle and bottom layers as AFM tip presses down.

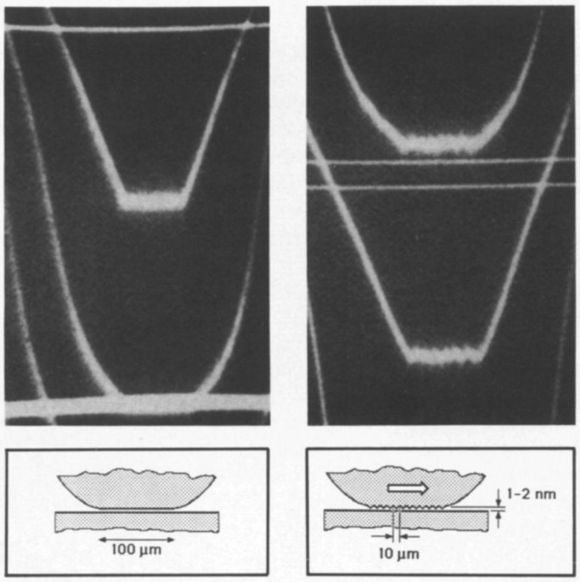
Landman

might develop cold-weld contacts, as seen in Landman's movie of unlubricated surfaces.

However, heads can even stick to lubricated disks, notes G. Bryan Street, a materials technologist at the IBM Almaden Research Center. Because the surface of the disk and the "slider" that carries the head are both very smooth, any liquid between them can cause a form of adhesion known as stiction. Street compared the phenomenon to a drop of water between two glass microscope slides: "It's easy to slide one off the other, but to pry them apart is very difficult."

As a result, Street notes, the industry is puzzling over how to work out a compromise between disk durability and stiction. "For durability you want a lot of lube; for stiction you want to have as little lubricant as possible," he says. "It turns out that this compromise ends up being one or two layers of lubricant" – a coating just 20 or 30 angstroms thick.

But with so little lubricant, there's always the risk that it may erode quickly, leaving the surface exposed again. This begs for another compromise: a lubricant that wants to bind tightly enough to the surface that it doesn't wear off easily, but that remains plastic – indeed, liquid – enough to flow back and heal areas that have experienced some wear.



Optically produced fringe patterns (upper photos) depict two solid surfaces, pressed together and separated by two-molecule-thick layer of lubricant (as drawn in lower diagrams). At rest (left pair), the surfaces are in continuous contact. Corregated fringe shows how surface contact changes under motion – and stick/slip friction. Here, slip phases occur at regular, 10 micron intervals.

Israelachvili

Mate and Israelachvili are among experimentalists attempting to understand not only how lubricants function, but also the attributes that help them endure. Mate's most recent experiments suggest that attaching little branch-like side chains to those snake-like lubricant molecules may improve their adherence to the disk surface.

At the American Chemical Society meeting last month, he reported that the addition of branched, alcohol end groups increases the lubricant's attraction for the disk surface. The result? "You have to provide a much larger force . . . to get the molecules to squeeze out."

Branching increases a lubricant's viscosity. Because the branches also facilitate molecular entanglement, many researchers assumed the higher viscosity traced to greater entanglement.

However, Israelachvili says, "That is not the whole story. It's not even an important part of the story. What happens is that the branched molecules are more irregular in shape and therefore cannot easily solidify in a thin film." As a result, he's found, "these molecules remain liquid under conditions where other straight-chain molecules would solidify. And the last thing you want is for your lubricant to solidify – to seize up."

Over the past three years, tribologists have come increasingly to rely on the simulations by Landman and others. These models are "providing us the between steps – the interactions that take place that lead to the atomic or molecular modifications that we observe," says chemical physicist Phaedon Avouris at the IBM Thomas J. Watson Research Center in Yorktown Heights, N.Y. For instance, looking at the pictures that Landman generates, "you get a microscopic description of lubrication phenomena at the single-molecule level. And that's very important in building intuition" – perspectives that will drive future experimental inquiries.

Adds Colton, even the best experiments cannot record materials changes in three dimensions. But when simulations generate the same numerical changes for a modeled surface that experiments have recorded, "then we can fairly confidently believe that the motion of the atoms that we see in a movie is indeed what happened when we actually did the experiment."

Israelachvili offers another example. Everything from a squeaking door to an earthquake results from a phenomenon known as stick-slip friction. For decades, physicists have assumed that stick-slip friction arises from the fact that friction falls with increasing sliding velocity. "But what people like Landman and others have shown is that it's the other way around," Israelachvili says: "It's that stick-slip is the *cause* of friction appearing to fall with sliding velocity."

Any point along two surfaces is either sticking or sliding. Along the course of two opposing surfaces at any point in time, there will be thousands of individual points sticking or sliding. "And as you increase the speed at which things move," Israelachvili explains, "those little contacts will be spending more time in the slipping state than in the sticking state." So it's really the distribution of surface points in the sticking state versus the slipping one that changes with velocity.

The growing dependence on molecular modeling has even given rise to a new journal – COMPUTATIONAL MATERIALS SCIENCE – to debut in August. But because the written word and still pictures cannot convey dynamics and trends nearly as well as motion pictures, this journal is encouraging its authors to supplement their submitted texts with movies – and even the raw data used to develop those simulations. Readers can then obtain copies of the videos "for some rather minimal cost," Landman says, or download the raw data – together with related computer programs and subroutines – free of charge from a pair of new electronic bulletin boards.

Landman and his colleagues never set out looking for film careers. But increasingly, they find, materials designers are encouraging theoreticians like them to become directors of the computer stage and screen. ☐