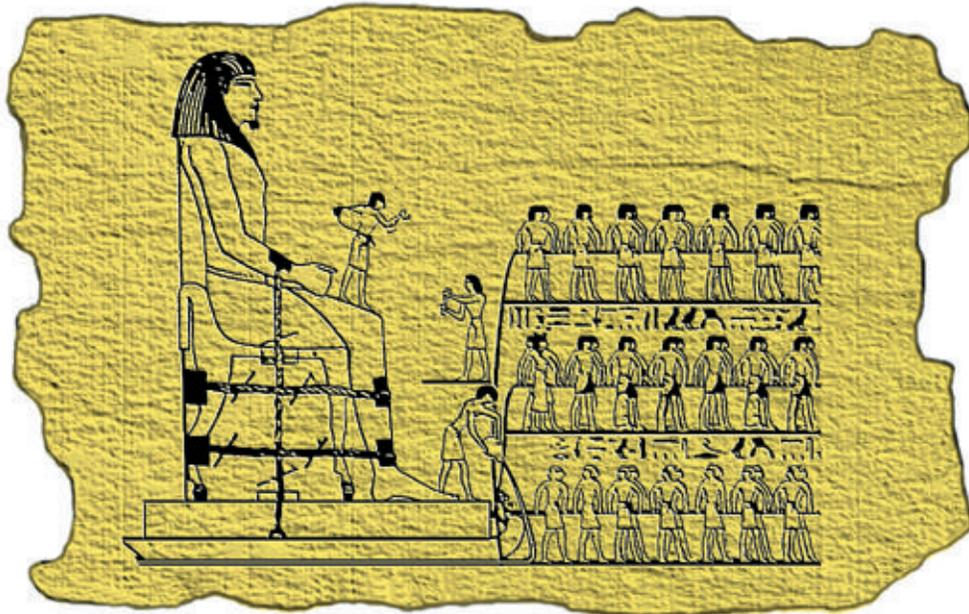


Nanotribology: Modeling Atoms When Surfaces Collide



Realistic computer simulations at the atomic level of detail are revealing new information about the basic processes that take place when materials are fabricated, as in cutting and grinding. With such increased understanding, we are developing more practical engineering guidelines for LLNL researchers and the industrial community.

TRIBOLOGY (friction, lubrication, and wear) is the science of interacting surfaces in relative motion. The word “tribology” is from the Greek *tribein*, meaning to rub. Although the term may be unfamiliar to many, its meaning is clearly conveyed among some of the oldest written records. An Egyptian painting dating back to 1880 B.C. depicts workers dragging a sled containing a heavy statue. One worker pours a liquid on the ground just before the runners to make the going easier. Leonardo da Vinci addressed the same problem when he wrote in 1519,

“All things and everything whatsoever however thin it be, which interposed in the middle between objects that rub together, lighten the difficulty of this friction.” An excellent source for further historical reading is Dowson’s *History of Tribology*.¹

We have first-hand experience with friction any time we walk on ordinary ground and compare the outcome with what happens when we try to walk on ice. Wear of mechanical parts—as every car owner knows—eventually leads to failure and is one of the most costly problems facing industry.

To design and engineer mechanical parts, we need a macroscopic understanding of tribological processes. However, today the tolerances of many components, such as optical devices, computer chips, and ultra-smooth surfaces, are approaching the microscopic (atomic) length scale. In fabricating such precise components, we can greatly benefit from an atomic-scale understanding of what happens when surfaces interact. The emerging field that lets us obtain this atomic-scale understanding of fundamental processes of surfaces in motion is called molecular tribology or

nanotribology. (A nanometer is one billionth or 10^{-9} of a meter; the size of an atom is about 0.3 nm.)

Recent progress in nanotribology is being driven by advances on several fronts. Of primary importance is the advent of probes that allow researchers to examine interacting surfaces at a microscopic level. One such probe is the atomic-force microscope, which has a very small tip with a radius of about 10 nm used to probe a surface. The surface force apparatus has also become a highly useful tool. Other major developments in the last decade are better models of interatomic forces, which, coupled with improved performance of computers, are giving researchers a new window into tip-surface interactions through computer simulations.

How Our Work Began

Scientists at the Laboratory became involved in the field of tribology as a result of work being done in precision engineering about a decade ago. At the time, we were exploring ways to cut materials with extreme accuracy and to obtain the best-quality surface in the process—one with very high smoothness and minimal surface damage. To meet the demand for extremely high tolerances, we developed a mechanical device called the single-point, diamond-turning machine.

Machines like the large-optics, diamond-turning machine (LODTM) at the Laboratory can routinely cut away as little as a few nanometers of material off a surface. Although diamond turning soon became a well-established technique, little was understood of the basic mechanisms that determine how the material is removed, how surface damage occurs, and how diamond tools themselves wear. Diamond turning was an obvious case where we could profit greatly

from an atomic-scale knowledge of underlying tribological processes.

For special applications, diamond-turning machines can cut materials at speeds of several hundred meters per second, and the entire process of chip formation takes place on time scales much less than a single microsecond (10^{-6} s). For these and other reasons, diamond turning is a good example of a mechanical device that lends itself well to atomistic computer modeling. Following the suggestion of John Holzhrichter and others at the Laboratory, we began to apply a type of modeling called molecular dynamics (MD) modeling, which explicitly takes into account interatomic motion. Such modeling gives us insights into the cutting process at very short time scales and length scales.

These days, we are using MD computer simulations to focus on several different aspects of nanotribology. For example, we are studying surface indentation of various metals and ceramics, high-speed metal cutting, and the growth of cracks in glass. LLNL has become a key player in the field of nanotribology, but it is only one of many institutions doing this type of research. Tribology issues being addressed today with MD simulations include wearless friction, adhesion and adhesive wear, and mechanical wear. Other problems range from boundary lubrication, to stick-slip phenomena (described later in this article), to junction formation and growth. For further reading on tribological processes in general, see [Reference 2](#). [Reference 3](#) is a review of recent progress in nanotribology.

This article describes a variety of work we have recently done to model—that is, to simulate at the atomic level—the way material is removed by mechanical means. We have developed an MD model of the cutting process, studied the process of chip formation, and examined wear mechanisms for a diamond cutting tool. Recently, we

modeled the high-precision machining of glass surfaces. Our computer simulations of the indentation of a smooth glass surface are helping to explain how microscopic processes, such as the breaking and forming of interatomic bonds, give rise to macroscopic phenomena, like the plastic properties of silica glass and the ductile behavior it can exhibit under certain conditions. (In mechanics, plasticity refers to a permanent change in shape or size when a material is subjected to a stress; ductile behavior means plastic deformation without fracture.)

An underlying theme of our work is to study practical problems and materials and to ultimately transfer what we learn on the atomic scale to real-world applications that are important to the broader community of materials scientists and engineers. Molecular dynamics modeling is limited in terms of the size of the material and the period of time that can be studied. In particular, the length scale is limited by the number of atoms that can be stored in a computer's memory and the enormous amount of work required to calculate interatomic forces. For practical reasons, we typically study systems containing no more than 100 thousand atoms (a length scale of about 10 nm). In principle, however, systems containing more than 100 million atoms (100 nm) are now possible.

The time scale is limited by the time it takes for an atom to collide with a neighboring atom. This vibrational period is very short, only 10 to 100 femtoseconds (10^{-14} to 10^{-13} s). The single time step in an MD simulation must be a small fraction (about 1/25) of the vibrational period, leading to a time step of about one femtosecond. A typical long simulation runs for tens of millions of time steps (to simulate a total period of about 10 ns), requiring many days on a supercomputer.

In the next few years, we expect to routinely attain length scales of hundreds of nanometers (hundreds of millions of atoms) using more powerful parallel supercomputers. We use a parallel computer by dividing space so that each processor executes its own MD simulation for a small region. The [brief on pp. 6–7](#) gives more details on massively parallel computing. Unfortunately, to date, no one has determined how to exploit parallel computers to study longer time scales.

The Basics of Molecular Dynamics Modeling

The molecular dynamics method was originally developed at the Laboratory in the late 1950s to study the statistical mechanical properties of a collection of atoms at equilibrium. The method is now a well-established and important tool in the fields of physics, chemistry, biology, and engineering. Recent advances in computer hardware and software allow us to simulate relatively large systems using increasingly realistic models of the forces between atoms.

In principle, MD modeling is simple. We start by identifying the position and velocities of all atoms in a system we want to model. Then we calculate the force on every atom from its neighbors and advance the positions of the modeled atoms according to Newton's equations of motion (force = mass \times acceleration). During a simulation, we evaluate the response of a material—often copper, silicon, or silica glass—as it is subjected to an external force by following the response of each atom. Examples of external forces include stress fields, moving boundaries, and heat baths.

Despite the simplicity of MD modeling, the number of users and applications today remains limited; in addition, many researchers do not use

it to its full potential. The reason for this underuse is that this type of modeling can be “overkill” in that it is too expensive and requires too much detail for solving most practical problems. Furthermore, there is a certain art in selecting the appropriate boundary conditions and constructing interatomic-force models.

Consider, for example, [Figure 1](#), which shows the boundary conditions we use in many of our simulations of indentation and cutting of a clean metal surface by a diamond-like tool. In this figure, the dashed line forms a box surrounding all the atoms that are represented. This box is called a simulation cell, which is our “window” on the system being modeled. Both the metal surface and the V-shaped diamond tool above it have “handles” to position the surfaces

relative to one another. These are the dark circles forming the boundary. In practice, we keep the tool fixed in the rotational direction and slide the work surface from left to right during a simulation of cutting.

Immediately next to the boundary atoms is a region in which the atoms are constrained to be at room temperature. From an atomic point of view, temperature is a manifestation of the vibrational energy of the atoms. The role of the thermostat atoms in our tribology simulations is to draw away heat generated at the tip of the tool, mimicking a much larger piece of material than is represented in the illustration. The remaining atoms represented by open circles make up the Newtonian region, meaning that these atoms are free from further constraint and move according to

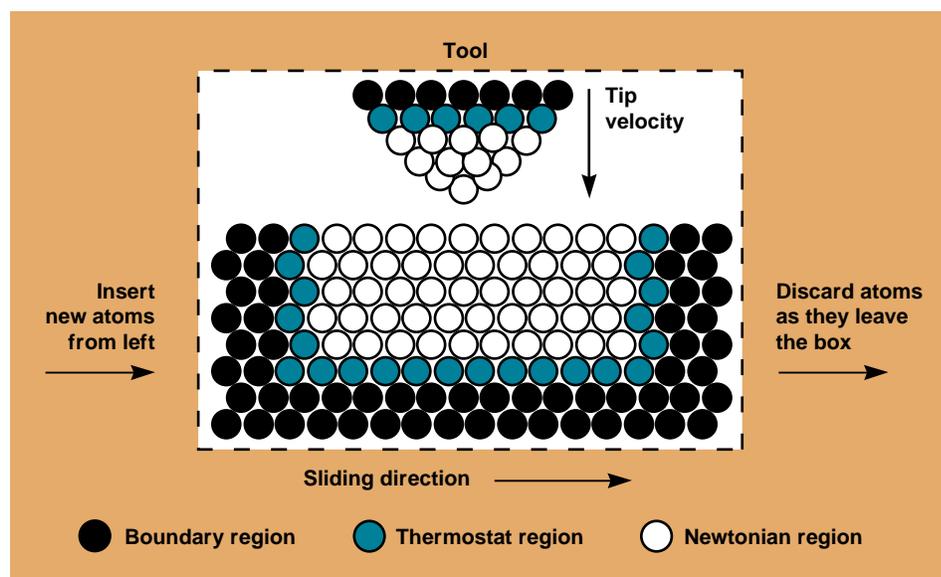


Figure 1. Geometry of a tool tip and work piece for a molecular dynamics (MD) simulation of indentation or cutting. The box, represented by the dashed line surrounding all the atoms, is our “window” into the system being modeled. Only the atoms in this box are evolved during an MD simulation. The top and bottom layers of boundary atoms (dark circles) are rigid and serve as “handles” to position the tool relative to the surface. The next layer of atoms (gray circles) are maintained at room temperature. Their purpose is to draw away heat produced at the tool tip. The remaining atoms (open circles) are free from constraint; that is, they obey Newton's equations of motion. Deformation processes in this interior region are the ones of interest in our MD simulations.

Newton's equations. The tribological processes in this region are of interest in the MD simulation.

In many cases, we would like to simulate cutting or scraping over lengths that are far greater than the dimensions of the dozen or so atoms shown in Figure 1. However, as mentioned earlier, following the motion of a large number of atoms is prohibitive in terms of computer time and cost. To help overcome this problem, we use a relatively simple approach. We allow atoms to leave the simulation cell at the "downstream" end (to the right in Figure 1 as the simulated work piece moves under the tool). At the same time, we periodically insert new atoms from the left at the upstream boundary. This approach restricts the population of atoms simulated at any given time, while allowing us to model nanotribological processes in a much larger work piece. The extension

of this model from two to three dimensions is straightforward.

MD Simulations at LLNL

Indenting Surfaces

One of our first simulations involved the indentation of a metal surface by a blunted, triangular diamond tip moving vertically at a constant velocity ranging from 1 to 1000 m/s. Keep in mind that in this and all of our subsequent work, our objective is to understand—at a more microscopic, atomistic level than was previously possible—what is happening when surfaces in relative motion interact with one another.

Figure 2a is a "snapshot" of what happens when the tool indents the first three layers of metal. The interatomic forces in a metal arise from two effects: the interaction between electrons localized on the atoms, and the interaction of atoms with free electrons.

We use an embedded-atom model of the metal that incorporates both of these effects. In this figure, the atoms are shaded by the local value of stress. At first, the surface responds elastically (deforms without permanent loss of size or shape), and we see circular regions of constant stress, called the Hertzian stress field, which is well known from elasticity studies of contact mechanics. When the tool is pushed in further to indent six layers of metal, as in Figure 2b, the surface begins to flow plastically, and we obtain shear and discontinuity. (See Reference 4 for an introduction to dislocations and plastic deformation.) In a 2D simulation like this one, dislocation edges are clearly visible within the metal along the darker-colored slip bands that appear at ± 60 -degree angles with the surface. In a close-packed metal such as this, the atoms behave like hard spheres (for example, billiard balls), and slip

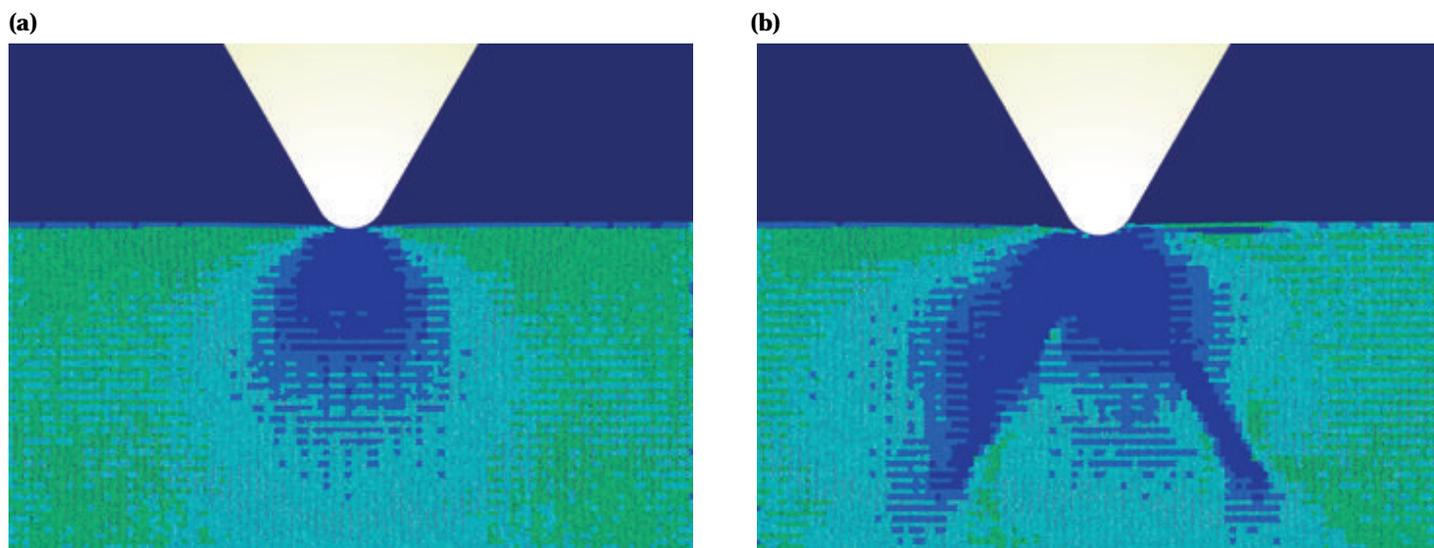


Figure 2. Two frames from our two-dimensional MD simulation of the indentation of a metal surface. The atoms are shaded by the local value of stress. (a) When the tip is pressed three layers into the surface, the response is entirely elastic; that is, there is no permanent change in size or shape of the material. The circular regions of stress are well known from continuum elasticity studies of contact mechanics. (b) When the tip is pressed six layers into the surface, the material yields plastically by creating dislocations along slip bands visible at ± 60 degrees from the horizontal surface of the metal. The plastic deformation means that the metal's change in shape remains when the tool tip is removed from the surface.

is analogous to sliding stacks of billiard balls over each other.

A 3D simulation of the indentation of copper gives us a slightly different picture. **Figure 3a** is an image we obtained after copper was indented at a rate of 1 m/s, and the simulated tool was withdrawn from the surface. (Slower rates, typical of experiments performed in the laboratory, are beyond the current capabilities of MD simulations.) In a 3D simulation, we do not see the distinctive bands of dislocation that were observed in a 2D simulation. Moreover, there is relatively little distortion at the metal surface. Instead, we find a small pileup of atoms on the metal surface, a few atoms in interstitial positions (between regular lattice positions), and a small dislocation loop (observable in **Figure 3a** as the “step” or ledge of atoms on the surface) extending to the bottom of the crater.

Figure 3b helps to explain the difference between our 2D and 3D simulations. Here, the atoms are colored according to the initial layering before the computer experiment. This cross section at the moment of full indentation of the copper surface shows that very little surface distortion has actually occurred. Remarkably few atoms have bulged out around the tool. Instead of distinctive dislocation bands, we see disorder only within a few layers of the sides and bottom of the tool tip. This localized disorder arises from point mechanisms (interstitials, vacancies, and so forth) of plasticity.

There are many other ways to display the results for such a simulation. One of the best and most revealing is by means of a graph, called a loading curve. **Figure 4** shows the load (instantaneous force in nanoNewtons) on the diamond-like tool as a function of depth of indentation (shown here as the number of layers indented) for the simulation in **Figure 3a**. The very rapid

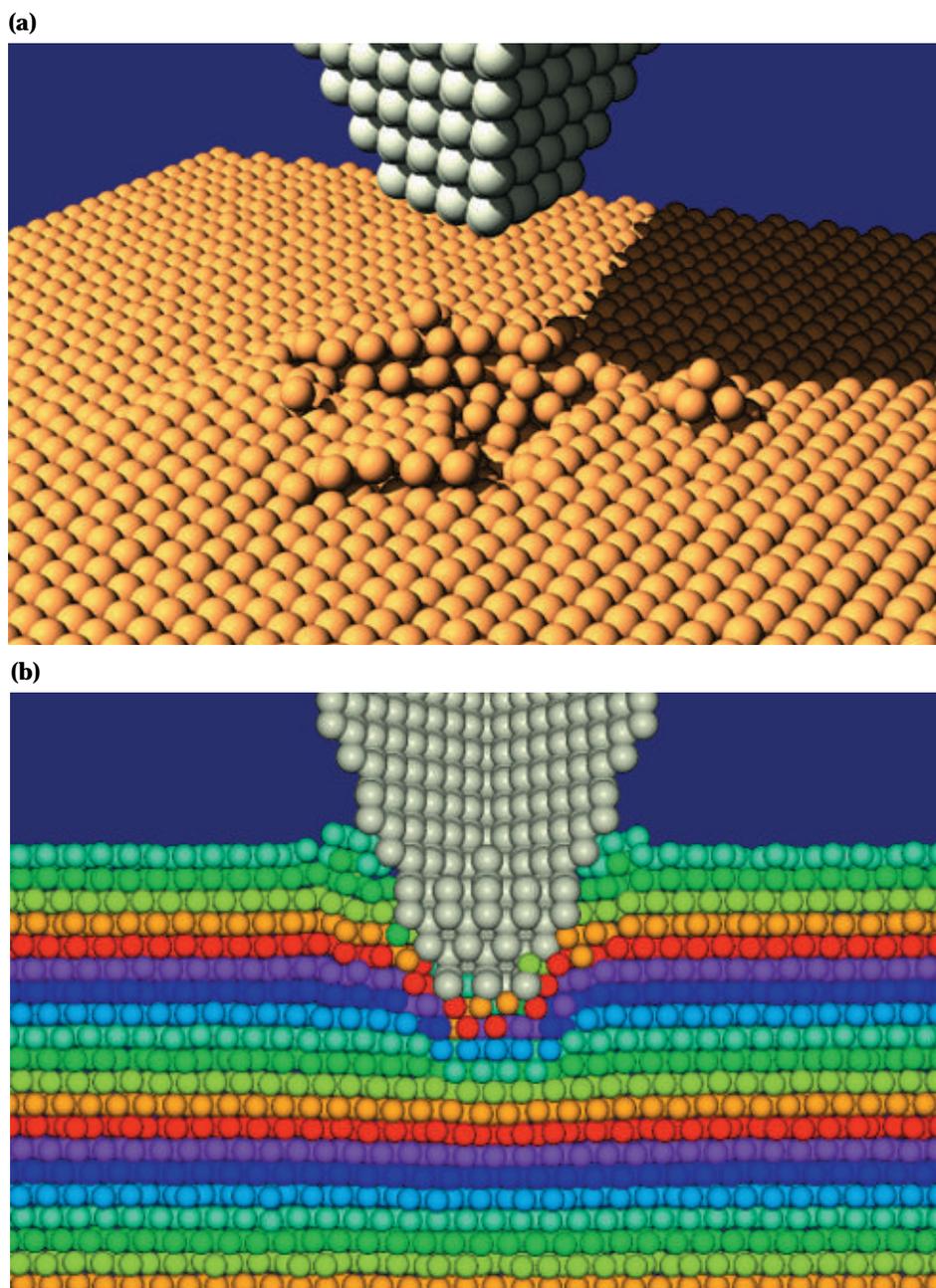


Figure 3. (a) Three-dimensional simulation of the indentation of a clean copper surface. The tool was pressed into the surface to a depth of seven atomic layers and removed to the position shown. The mechanisms of plastic deformation (permanent change in shape) include a small pileup of atoms on the metal surface, a few atoms in interstitial positions, and a small dislocation loop (observable as the “step” of atoms on the surface in front of the indent) extending to the bottom of the indent. (b) Cross section through the center of the tool for the simulation shown in (a). The copper atoms are shaded according to their initial depth. (The shading pattern repeats every eight layers.) Remarkably few atoms have bulged out onto the surface around the tool. Through elastic and plastic deformation, the surface is able to accommodate nearly the entire volume of the tool.

fluctuations in load—which look like “noise” on the curve—arise from the rapid motion of surface atoms repeatedly colliding against the tool atoms. The larger peaks and valleys are far more interesting in terms of what they reveal.

At first, the load rises linearly as the metal surface responds elastically. After indenting about 1.5 layers of copper, the load drops abruptly when the elastic stress is relieved. This abrupt drop, called “critical yielding,”

is reminiscent of what is observed in the laboratory. The first yielding in the simulation corresponds to a single copper atom popping out onto the surface from under the tool tip and relieving the stress energy. With more indentation, more of these point events take place. After indenting seven layers of copper, the tool is stopped. At this point, the surface accommodates nearly all the tip through elastic and plastic deformation, and there is little pileup of atoms around the tip, as

observed in the cross section in [Figure 3b](#). When the direction of the tool is reversed (lifted from the surface), the load quickly drops to zero, as expected. However, the load suddenly rises once again as the tool is removed further. This unexpected rise is caused by annealing at the surface of the metal so that the material returns to more intimate contact with the tool, and the load rises.

Our results from simulations using silver as the indented material are quite similar to those just described for copper. However, because silver is softer, the yielding occurs at a smaller load than for copper.

Cutting and Chip Formation

Cutting is a widely used process in fabricating components. To obtain a more basic understanding of what happens when a metal is cut, we use a simplified geometry. We idealize our model slightly by limiting the motion to two dimensions or thin, periodic slabs in three dimensions. This idealization, known as orthogonal cutting, assumes that the material being cut is sufficiently wide that edge effects have essentially no influence on the results.

We have simulated orthogonal cutting in both two and three dimensions. The 2D simulations more accurately model the length scales and time scales that are common in laboratory experiments using single-point, diamond-turning machines. In this type of simulation, cutting speeds range from about 10 to 100 m/s. We have also varied the sharpness of the rigid tool tip used for cutting. We have used tool-edge radii of curvature ranging from 1 to 20 nm. Our bluntest tip (20 nm) approaches the sharpest real-life tool tip, which has a radius of curvature of about 35 nm.

[Figure 5a](#) is a single frame from a computer-animated movie of our three-dimensional MD simulation of orthogonal cutting. The copper

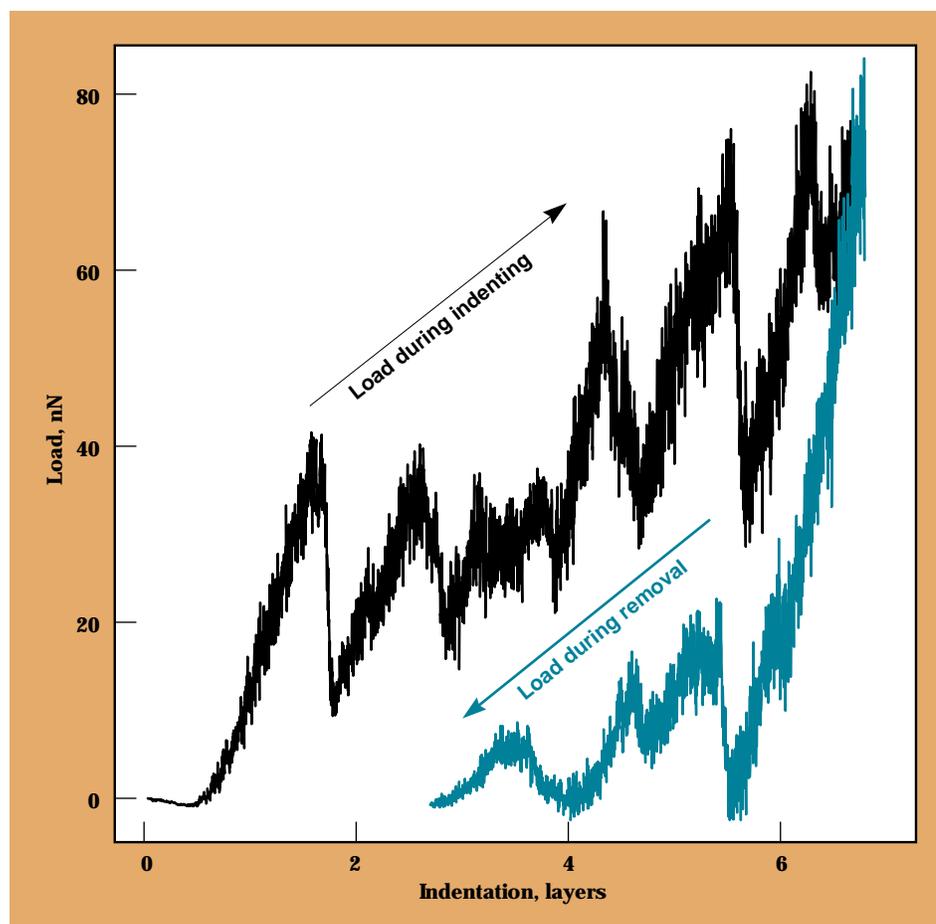


Figure 4. The load (normal force in nanoNewtons) on the diamond tool as a function of depth of indentation for the simulation shown in [Figure 3a](#). The abrupt drops in the loading curve correspond to individual plastic events, such as an atom popping out onto the surface from beneath the tool tip. After indenting seven layers, the direction of the tool is reversed, and the load quickly drops to zero as is expected. However, on further removal, the load suddenly rises again. This unexpected rise is caused by annealing at the surface so that the material returns to more intimate contact with the tool, and the load rises again.

material flows from left to right at 100 m/s. In this simulation, the carbon atoms in the diamond-like tool are not permitted to move, so they serve as our fixed frame of reference.

Figure 5b is a projection in two dimensions of all the atomic positions in Figure 5a. This type of projection makes it easier to see some important effects. During our simulation of cutting, the system forms a chip. The chip is reminiscent of what is actually observed during real experiments. The chip remains crystalline, but it has an orientation different from that of the surface. Regions of disorder among the atoms are apparent in front of the tool tip and on the surface in front of the chip. Unlike our 3D studies of point indentation, dislocations readily form during orthogonal cutting. Unlike the single point in our indentation simulations, the cutting tool in the orthogonal cutting geometry forms an infinite line, like a knife edge. This geometry provides much more energy for the creation of dislocations.

Our calculations show that the cutting force strongly depends on the sharpness of the tool. This relation is also observed experimentally. Dull tools (those with a large tip radius) require larger forces to achieve the same depth of cut as sharp tools. A good measure to quantify our observations is the work (force \times distance) performed by the cutting tool divided by the volume of material removed, also known as the specific energy. This energy increases dramatically with decreasing depths of cut. For our shallowest (nanometer-scale) cut, the specific energy exceeds the energy required to vaporize the material, though the material remains a solid.

The dependence of specific work on depth of cut has been observed in macroscopic metal cutting for many years and is known as the size effect. However, the macroscopic size effect

is much less dramatic than the size effect observed in our simulations or in experiments using single-point, diamond-turning machines. The transition between macroscopic and microscopic behavior occurs at a length scale of a few micrometers, comparable to the average grain size in most metals. We interpret this

result as a change in the mechanisms of deformation, from grain-boundary sliding and motion of *existing* dislocations at the macroscopic scale to the creation of *new* dislocations and other point mechanisms of deformation at the microscopic, atomic scale. These dislocation-creation and point mechanisms of deformation consume

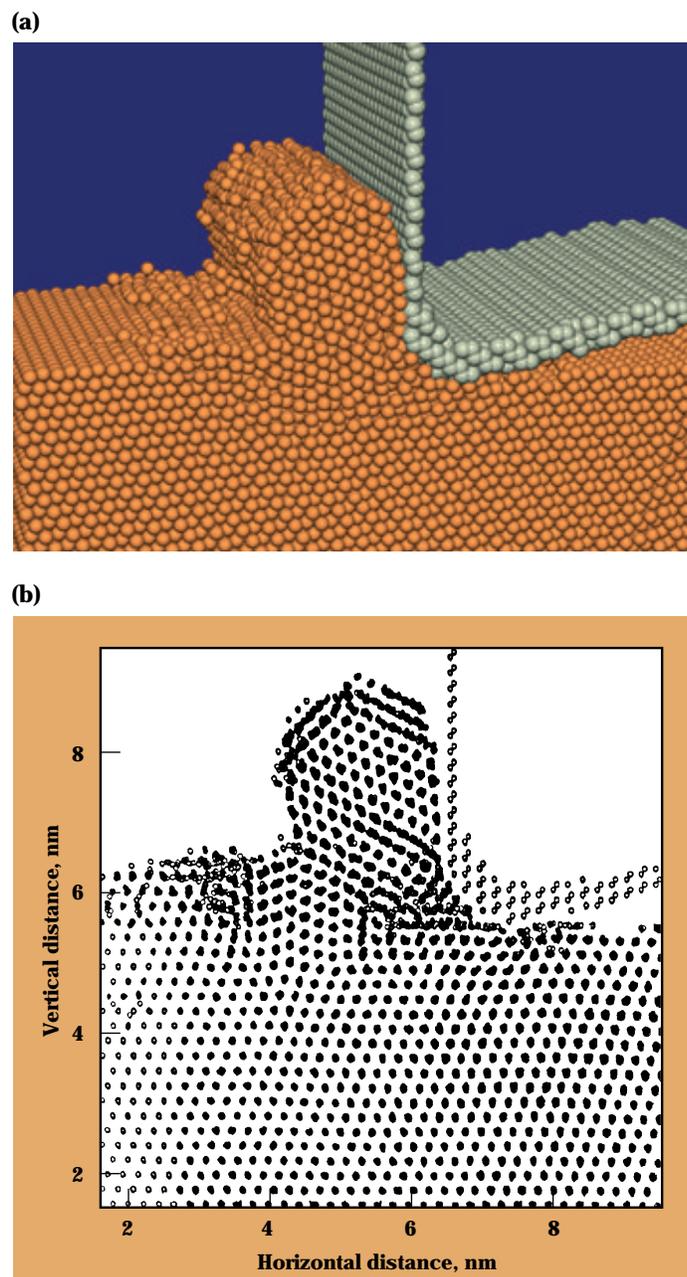


Figure 5. A 3D simulation of orthogonal cutting of copper (a) after the formation of a chip and (b) with all atomic positions projected into two dimensions. In this MD simulation, the carbon atoms in the tool are not permitted to move, and the copper material is flowing from left to right. The chip remains crystalline, and regions of disorder are seen in front of the tool tip and on the surface in front of the chip. These regions of disorder, clearest in (b), are connected by a zone of intense shear.

significantly greater energies, leading to the observed size effect.

In contrast to copper, materials like silicon and iron are not considered machinable with diamond tools. The reason is that the diamond tool wears rapidly, and it becomes difficult to maintain contour accuracy. The increased wear occurs for all materials that form strong chemical bonds (covalent bonds) with carbon. We have investigated and identified some of the underlying processes that give rise to these effects.

In covalent materials like silicon, the nature of interatomic forces is much different from that in metals. The strength of a covalent bond depends on the local environment, and the material forms an open structure. Our basic method is the same as that for cutting copper, except that now we evolve not only the silicon surface material but also the carbon atoms in the diamond tool to allow for tool wear. We have found that both copper and silicon show ductile behavior during cutting; however, the underlying

mechanisms that allow this behavior are very different for the two materials. Whereas a copper chip remains crystalline, a silicon chip is transformed into a completely different state.

Figure 6 is a cross-sectional view, just as the one in Figure 5b, but this time of a silicon-cutting simulation. In this case, the diamond wedge is cutting at a speed of 540 m/s. Although no wear of the tool is apparent yet, a single layer of silicon atoms has coated the diamond tip. Chip formation occurs between this layer of silicon atoms and the crystalline surface. In related simulations of diamond asperities (abrasive tips) scraping a silicon surface (as in grinding processes), we found that the diamonds wear by forming small clusters of silicon carbide, which remain on the silicon surface.

In Figure 6, the silicon material in the chip and in the first few layers of newly cut surface appears to be amorphous or possibly to have melted. The temperature in the chip, calculated from the vibrational motion of silicon atoms, is comparable to the melting temperature of bulk silicon. However, the silicon atoms in the chip are not diffusing, which demonstrates that the material is, indeed, in a solid state.

We have developed the following idea to explain chip formation in crystalline silicon. Because of the nature of covalent bonds in crystalline silicon, the energy needed to shear the crystal is enormous. In fact, less energy is required to transform the crystal into an amorphous solid and to shear the amorphous solid than to shear the crystal. The interplay between the energetics of different deformation processes and the dependence on length scale may explain the transition from brittle to ductile behavior that is observed in ceramic materials.

How Cracks Propagate in Glass

The ability to precisely machine ceramic surfaces like silica glass affects

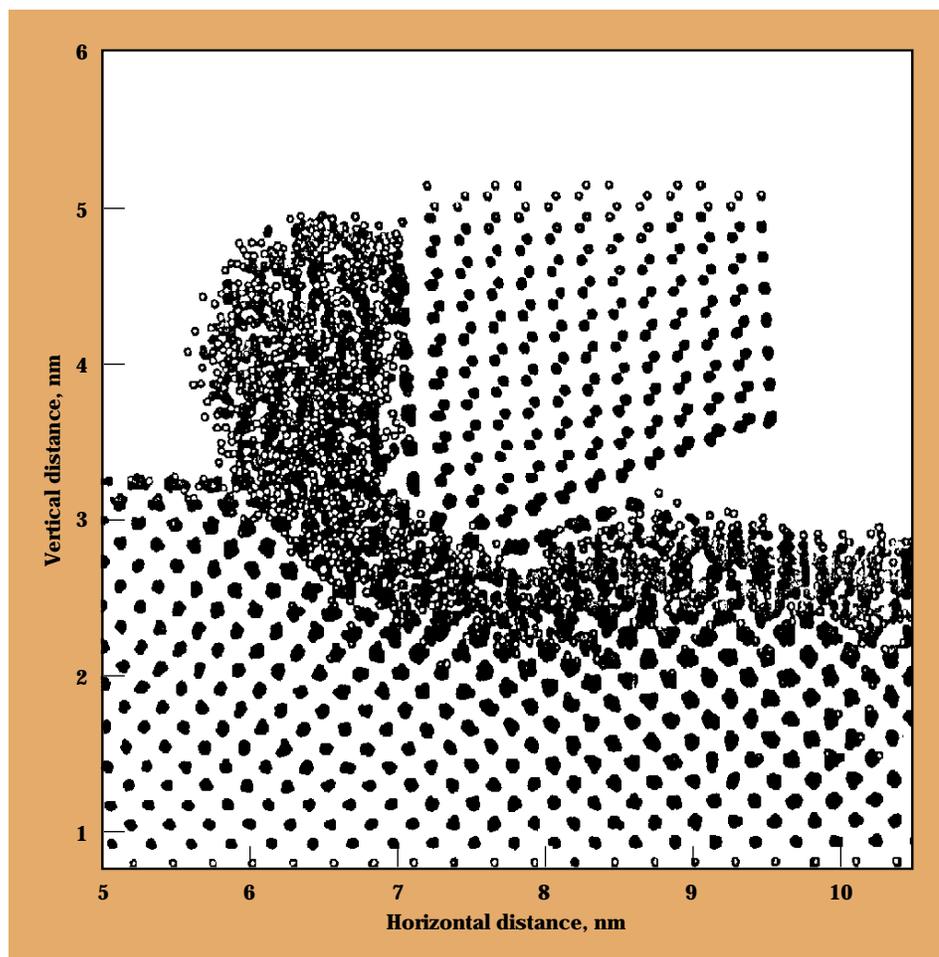


Figure 6. A 3D simulation of orthogonal cutting of silicon. As in Figure 5b, all the atomic positions are projected into two dimensions to make certain features more visible. Unlike copper, silicon is transformed from a crystalline state into an amorphous state during cutting. Both the chip and the first few layers of newly machined surface are amorphous. A thin layer of silicon atoms also coats the diamond tool. The chip forms between the bulk silicon and this thin coating.

many different fabrication technologies and is central to constructing a wide range of sophisticated optics systems. At LLNL, the Laser Program needs to make very high-quality mirrors, and we need to know more about special materials, such as ceramics, used in modern devices and equipment. We are applying MD methods to examine deformation processes at the atomic scale in these materials.

The main difficulty is that glass and ceramic materials are brittle. Anyone who has seen a rock impact a windshield or a pane of window glass knows about the property of brittleness. This property can result in cracking, subsurface damage, and other kinds of costly damage during precision machining. However, a growing body of experimental evidence suggests that glass and ceramics can exhibit both ductile and brittle behavior during grinding, depending on the size of the abrasive used. In particular, there is an abrupt change in the surface smoothness of glass with a smaller abrasive size. In other words, with a smaller depth of cut, even glass can behave in a ductile manner. If we could better understand and manipulate this ductile-to-brittle transition, we could improve the economics associated with fabricating ceramic components.

To address this problem, in 1993 we began simulating fused silica glass with no impurities. In silica, four oxygen atoms surround each silicon atom to form a tetrahedron. Each oxygen atom is shared with two silicon atoms to form connected tetrahedra. Amorphous silica glass is a random network of these interconnected tetrahedra. To study the nanometer-scale deformation of fused silica, we pushed a diamond tip with a radius of about one nanometer into a smooth silica surface, as shown in [Figure 7](#). We found that the silica surface responds much more elastically than did either the copper or silicon surfaces. For indentations up to

1.25 nm, we observe no plastic deformation. At an indentation of 1.25 nm, a significant rearrangement of the silica network occurs directly beneath the tool tip. This rearrangement, an example of which is shown in [Figure 8](#), leads to a decrease in the slope of the loading curve. When the tool is removed, the unloading curve does not follow the loading curve, as it does for elastic indentations up to 1.25 nm. The area between the two curves is a measure of the work performed by the tool in rearranging the silica network. These calculated loading and unloading curves are strikingly similar to those observed experimentally.

It is essential to learn more about cracks for a better understanding of deformation in glass. To simulate the

propagation of a crack into a silica surface, we put a notch on the top surface of the glass and let the computer simulation pull apart the sample at a constant velocity. The critical stress for crack propagation depends on the geometry and length of a pre-existing crack. Longer cracks, for example, yield at lower applied stress than do shorter cracks. In the simulation shown in [Figure 9](#), we observed the crack length to elongate by 30%, stop, and then yield again at lower stress. This “stick-slip” phenomenon has been observed during crack propagation in fiber-reinforced materials. The sticking is determined by the microstructure. In our case, the crack stopped after entering a large void. The void permits additional stress relaxation,

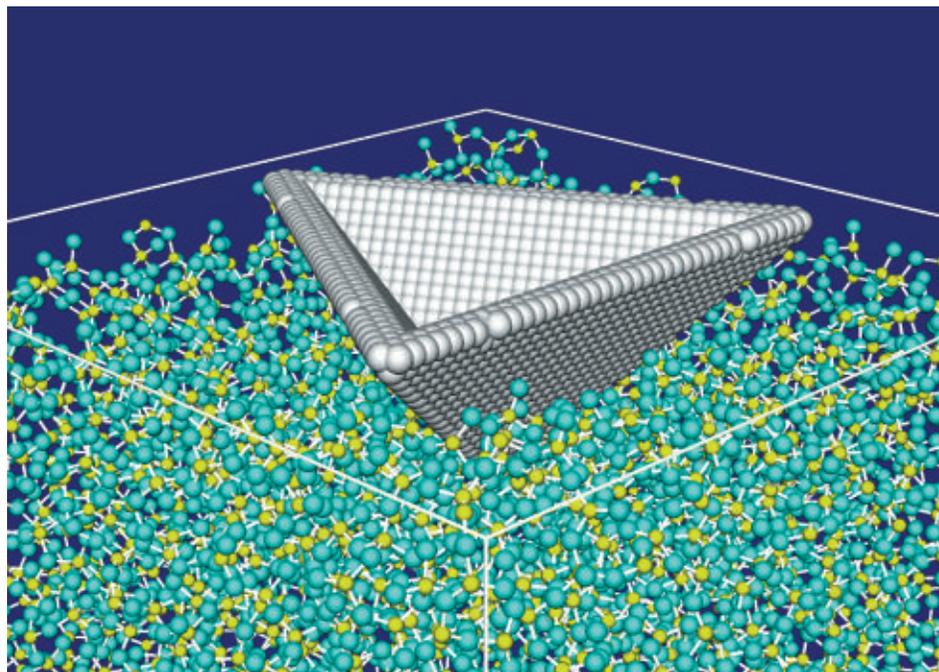


Figure 7. Surface indentation of fused silica (glass). Amorphous silica glass forms a random network of interconnected tetrahedra. A silicon atom (shown here as a yellow ball) is located at the center of each tetrahedron; an oxygen atom (blue ball) is located at each of the four corners. During our simulated indenting of a silica surface, we do not observe the abrupt drops in the loading curve that were seen in copper ([Figure 4](#)). Instead, the response of a silica surface is almost entirely elastic up to 1.25 nm. After 1.25 nm, there is a slight change in slope of the loading curve, indicating the onset of plastic deformation.

and the crack tip halts until sufficient stress builds up again.

In related new work, we are modeling crack propagation in silica in the presence of water. Water has the interesting property of enhancing the propagation of cracks in silica by replacing silicon–oxygen bonds with terminal hydrogen atoms.

New Directions: Bridging the Gap

Our atomic-scale simulations of deformation in materials such as copper, silicon, and glass are beginning to give us new insight into specific microscopic processes. However, most macroscopic processes—those we must understand to engineer mechanical parts—are a complicated mix of many different microscopic processes. Orthogonal cutting with a single-point, diamond-turning machine is an almost unique exception to the rule. The reason we are able to model this type of cutting so realistically is that both the length scale (tens of nanometers) and time scale (tens of nanoseconds for cutting speeds of up to 100 m/s) overlap in actual diamond-turning experiments and computer simulation.

Another important example of such overlap is friction and wear at the interface between a computer hard disk and the head used to read and

write information on the disk. The space between a flying head and a spinning magnetic disk is less than 100 nm in today's technology, and the space will soon shrink to about 10 nm. A problem this size fits into the main memory of modern parallel supercomputers, allowing us to simulate all the atoms and molecules at the head–disk interface and their response when the head collides with the surface. Moreover, because modern disks spin at high rates of about 5000 rpm, collisions occur on the nanosecond time scale attainable in MD modeling. Extending our MD model to this industrial process could lead to greatly increased storage capacity for next-generation computers, as is described in more detail on pp. 4–5.

In the future, we plan to apply the microscopic, atomic scale, understanding that we have been acquiring to solve macroscopic engineering problems. To do so, we need a bridge between the microscopic world of atoms and the macroscopic world of our everyday experience.

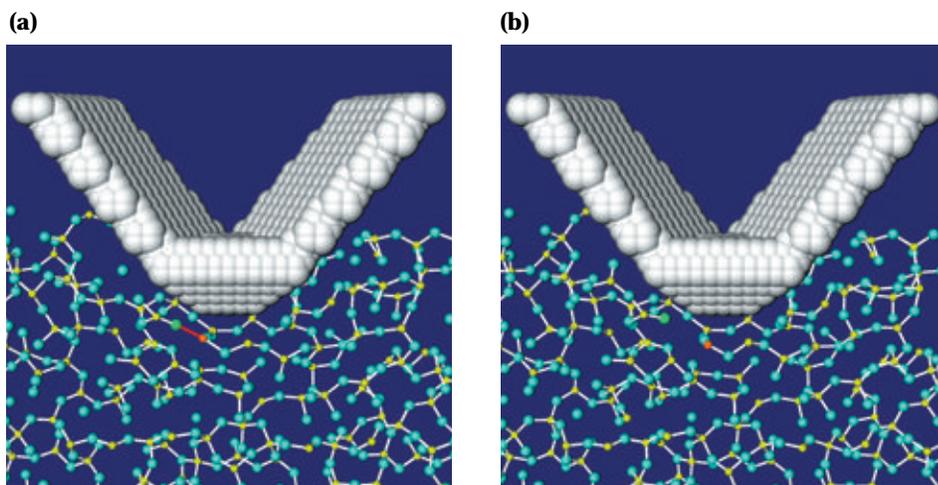
For example, in designing a car or bridge, it is obviously not practical to simulate the motion of every atom in the structure. Instead, a practicing engineer treats a car or bridge as a continuous material. The behavior of a car crashing into a wall is simulated

by calculating the response of every small volume that makes up the car, in the same way that we calculate the response of every atom in an MD simulation. These small volumes are assumed to be so large that they contain a vast number of atoms—far too many to simulate individually. The quantities we use to describe the small volumes, for example density and temperature, are the same as those we use to describe our everyday macroscopic world. These quantities represent, in an average way, what the atoms inside the volume are doing.

The way such a continuum mechanics simulation represents materials with widely different behaviors, such as metals and glasses, is to tabulate the particular behavior of interest for that particular material. For instance, when a thin wire is pulled with a certain force, it stretches. However, the precise amount of stretch depends on whether the material is plastic or metal or glass; that is, it depends on the atomic structure of the material. Such a tabulation of material behavior is known as a “constitutive relation,” and, in practice, a separate relation must be specified for every behavior that might arise in a simulation.

Continuum mechanics simulations are extremely useful when the amount

Figure 8. A cross-sectional plot through the center of the diamond tool for the simulation shown in Figure 7 immediately before (a) and immediately after (b) the onset of plasticity when the material yields. The bond shaded in red in (a) is one of the bonds that breaks when the silica network rearranges.



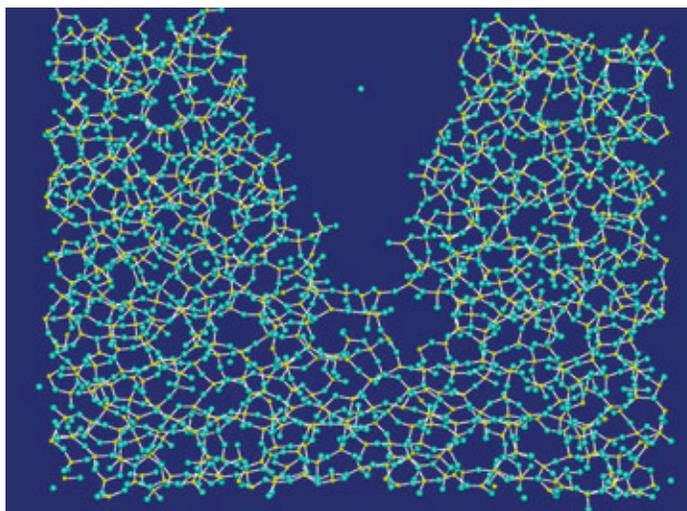


Figure 9. Large-scale, or macroscopic, plasticity in silica is dominated by the propagation of cracks. We simulated the mechanism of crack propagation by creating a notch on a silica surface and pulling the material apart at a constant velocity. Our calculated critical stress (the stress required to move the crack tip) agrees well with experiments. We also observed a novel stick-slip phenomenon. As the crack tip enters a large void, such as the one just below and to the right of center, the tip momentarily halts as the stress is lowered, then the crack continues to propagate again.

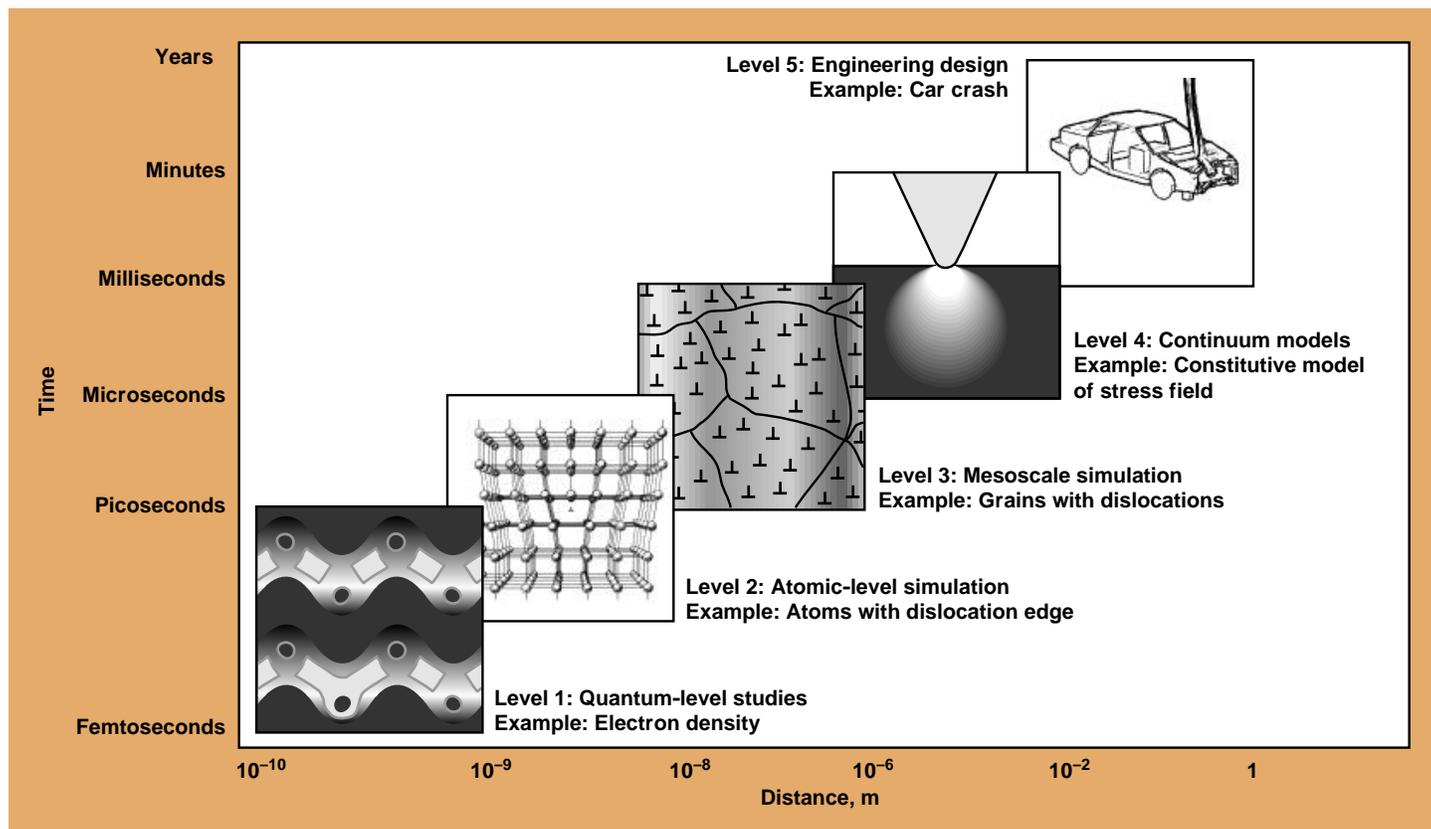


Figure 10. Multiscale modeling. This schematic shows the different types of studies and models needed to simulate various materials problems. At the shortest length and time scale, quantum studies (Level 1) look at electronic structure, such as electron density. Level 2 simulations take into account that the world is composed of atoms. This is the type of simulation we have applied in our studies of nanotribology. Level 3, referred to as mesoscale simulation, is concerned with objects that define microstructure, such as grains with dislocations. Level 4 is concerned with continuum models, such as stress-strain relationships. Continuum models are, in turn, extremely useful for solving practical, Level 5 engineering problems, such as a car crashing into a wall. Our new work will focus on Level 3 and 4 modeling to bridge what we are learning from atomic-scale studies to real-world engineering problems. (This illustration was adapted from W. A. Goddard et al.⁵)

of deformation is small. Unfortunately, a serious problem arises when the deformation we want to study is severe. In such cases, the local material microstructure (grain size, dislocation density, and so forth) changes, and the constitutive models used prior to the severe deformation are no longer valid. Furthermore, we have no way to predict which new constitutive model to use without knowing the new microstructure of the material.

To address this challenging problem, we are developing a methodology known as multiscale modeling. To illustrate this approach, **Figure 10** shows a hierarchy of different types of models that are used to simulate various problems. At the macroscopic level, continuum models (shown as Level 4) take into account regions of stress and strain. They are extremely useful for solving practical engineering problems (Level 5), such as a car crashing into a wall. However, continuum models, by themselves, do not account for the fact that the world is composed of atoms (Level 2) and that interatomic

interactions are determined by electronic structure (Level 1).

To bridge the gap from the microscopic, atomistic level to the macroscopic, engineering level, we will use large-scale MD simulations to study the atomic-scale origins of microstructure interactions and to develop models for mesoscale studies (Level 3) of microstructure evolution. In mesoscale simulations, the objects we study are those that define the microstructure—that is, dislocations and grain boundaries. In such simulations, the atoms do not appear explicitly, as they do in MD modeling. Next, we will calculate material constitutive relations (Level 4) from our new mesoscale simulations to understand the connection with microstructure. This type of approach will allow us to predict the evolution of microstructure when an object is subjected to a macroscopic stress or strain, and hence predict the new constitutive model to use at the continuum mechanics level.

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