Computer Simulations of Fracture at the Atomic Level

Ruth M. Lynden-Bell

At first, it may be surprising that computer experiments are useful for investigating a macroscopic process such as fracture. Many aspects of fracture involve changes in structure on a large scale and, even at the atomic level, the motion of dislocations over long distances is important (*1, 2*). Numerical experiments, where one takes a few hundred or even a few thousand atoms arranged in a crystal lattice and stretches the crystal, would seem to have little relevance given that the size of such a system is only about 100 Å or less in each direction. However, every large-scale process involved in fracture involves the motion of individual atoms on the nanometer scale, and numerical experiments can be used to investigate processes at this level.

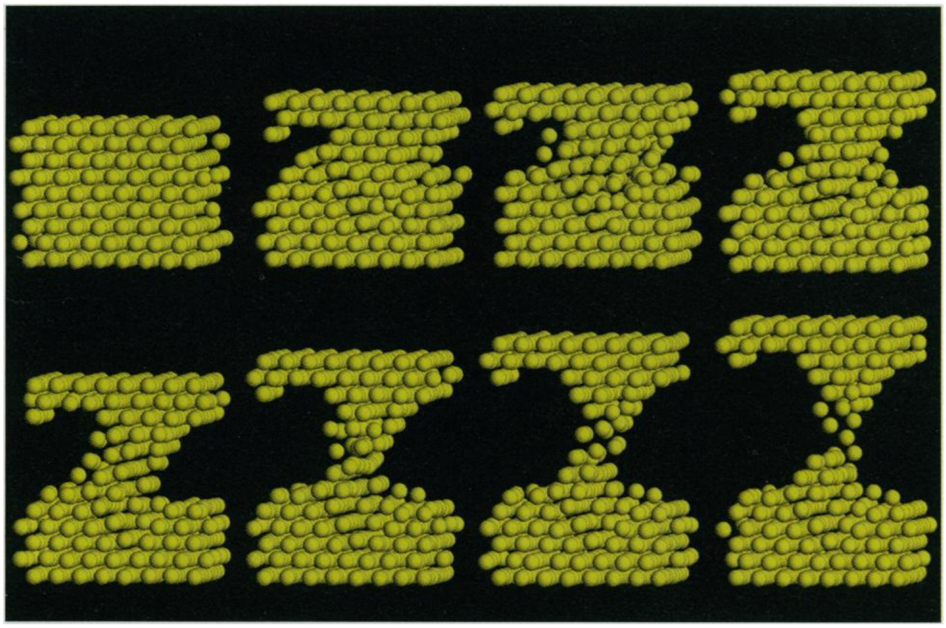

Fig. 1. Sequence of images showing position of rhodium atoms during a numerical experiment to explore fracture mechanisms. The material begins as a solid slab (upper left) with ideal crystal above and below (not shown). As the top and bottom are pulled apart, the rhodium atoms form a bridge, until the crystal finally fails (bottom right).

Most of the numerical experiments that have been done so far have started with a perfect defect-free crystal of some material and have investigated what happens when the crystal is stretched in one direction (*3*). Figure 1 shows a sequence of pictures during such an experiment on a crystal of rhodium at room temperature. In order to interpret these pictures one needs to know that the top and bottom atoms shown are fused to slabs of solid material (not shown) and the slabs are steadily pulled apart.

The technique used for these numerical experiments (or computer simulations) is known as molecular dynamics (*4*). The idea is simple. The motion of each atom is determined by the force on it through Newton's law of motion—acceleration equals force divided by mass. In order to use this, one needs a force law (or intermolecular potential) and a starting point, that is, an initial set of positions and velocities for all of the atoms. Provided the computer program runs for long enough, one then obtains the behavior of the material that is being modeled at some definite temperature. At higher temperatures the atoms move faster. So to change the temperatures one only needs to reset the velocities to a higher or lower value and run the computer program again.

The crystal of rhodium shown in Fig. 1 contains nine layers, each with 64 atoms. Above and below these layers of moving atoms are slabs of crystal of the same material in which the atoms are fixed in position, and these slabs are not allowed to move in the simulation. To avoid edge effects at the sides, the crystal is surrounded by replicas of itself on all sides.

This sequence of pictures shows what happens when the crystal is put under tension. We also need to look at a graph of the force that has to be applied to the slabs to maintain a given value of the extension (Fig. 2). When the crystal is not extended, no force need be applied, and that is where we start. As the extension increases, at first the force increases linearly, but then begins to curve over. In the initial linear region, the material is behaving elastically according to Hooke's law (restoring force is proportional to extension). The steadily increasing deviation from Hooke's law at higher extensions is dramatically interrupted by a sudden decrease in the force as the crystal fails. After this, there are a couple more smaller downward steps in the force curve, which then gradually declines to zero.

In the initial region before the failure, the crystal does not change its appearance. It is still ordered and all that seems to happen is that the layers get further apart. The first step in the force curve occurs between the first and second pictures. A void has formed in the material. Once the void forms, the atoms quickly rearrange themselves into a new structure with a bridge connecting the two halves of the crystal. The presence of the unchanged slabs of crystal above and below the moving atoms does not allow the dimensions of the crystal perpendicular to the direction of pull to alter.

Because the density of the crystal is inevitably decreased as the crystal is pulled under these conditions, it is not surprising that failure occurs by means of the formation of a void. We have done many similar numerical experiments on a number of different materials. In many ways, the behavior shown in this sequence of pictures is typical of metals and atomic solids at temperatures well below their bulk melting points. It is characteristic of these materials at low temperature that as the void grows, the material remains highly ordered and the bridge lengthens by increasing the number of layers of atoms in it in a stepwise process. Each such step leads to a decrease in the number of atoms in each layer, and the bridge thins until it breaks. One can also see in some of the pictures that a volume of the crystal above and beneath the bridge is distorted by the tension. Dislocations are formed and move through the material particularly in the region where the bridge joins the crystal surface.

What happens at higher temperatures? Nearer the bulk melting point, one finds rather different behavior, as it is easier for the material to become disordered and

---

The author is at the University Chemical Laboratory, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, United Kingdom.

even liquid-like than it was at lower temperatures. The force curve is qualitatively similar, rising to a maximum value and then suddenly decreasing as voids are initiated. There is little evidence of any further steps in the force-extension curve at higher temperatures. Pictures of atom configurations show that the material behaves rather differently from what we have seen already. Near the maximum force, one sees a good deal of disorder in the crystal. Again, failure occurs when a void is initiated, but the bridge of material joining the upper and lower parts of the broken crystal is disordered. This allows the crystals themselves to remain more ordered and not to develop the kinds of defects seen in the pictures. Essentially, we can say the bridge is liquid-like at these higher temperatures, although it is difficult to make a clear distinction between a solid and a liquid bridge because, even in well-ordered bridges, the atoms are quite mobile.

Although Fig. 1 shows pictures from an experiment on rhodium, perhaps this would be better described as "rhodium." The material in a numerical experiment is defined by its force law, but we do not know the exact force law for rhodium. The one used gives a good approximation for many of the properties of the metal and also describes those of silver at half the temperature. One of the points of interest in this work is to compare the properties of different types of materials; but in order to do so, we need to know the intermolecular force laws. The modeling of force laws is an area of considerable research activity, but there are no definitive answers. However, it is sufficient if one has force laws that describe the physics of the process being investigated, even if the exact details are not quite correct.

One can distinguish four main types of materials: molecular and atomic crystals, metals, ionic crystals, and covalently bonded materials such as silica or diamond. The types of bond that have to be broken when these materials are fractured is different. Atomic and molecular crystals are held together with van der Waals' forces, which are well understood and can be modeled without difficulty.

Metallic bonding is caused by delocalized electrons. When a crystal of a metal breaks, the new surfaces have a lower energy than they would in a molecular crystal with the same bulk energy. This may be an important factor in the fracture process. Even more important is the fact that the atoms in a metal can slide past each other more easily than in a molecular crystal, and this is more pronounced for some metals, such as platinum and gold, than it is for others, such as rhodium or silver. It is necessary to describe these properties reasonably well.

The forces in an ionic crystal are understood but have the problem that they are much longer ranged than other intermolecular forces. Covalent forces on the other hand are specific and directional. The consequences of these different types of binding are well known at the macroscopic level. Ceramics, in which the forces are mainly ionic, tend to fracture in a brittle way, making a clean break with little change in the local structure of the two half crystals. Metals, on the other hand, usually show ductile fracture in which parts of the crystal slide past each other, and dislocations and defects play an important role.

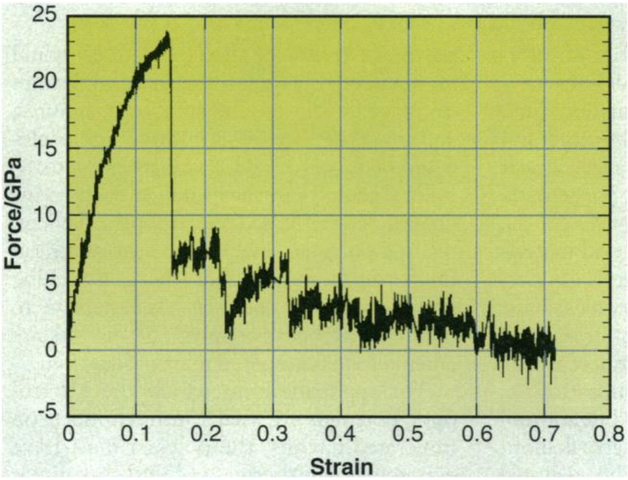

Fig. 2. Calculated force required to pull the rhodium apart in the numerical experiment (at temperature $T = 300$ K).

Because the number of moving atoms in these numerical experiments is restricted and because the crystal is surrounded by exact replicas of itself, large-scale slipping cannot be seen. For example, a real rhodium crystal when pulled might slip along the (111) plane, but this is forbidden in the experiment described. The presence of such artificial constraints can be put to advantage as they can be removed selectively so that particular processes can be investigated. In the numerical experiment on rhodium described above, no lateral relaxation was permitted, but in other experiments, it has been allowed.

Particularly interesting results were obtained on some numerical experiments on platinum crystals (5). When these were stretched with no lateral constraints, a surprising result was obtained at low temperatures. As the stretching force was increased, at first the extension increased steadily as expected. Then we saw a sudden jump to a longer extension, after which the crystal continued to stretch steadily until it broke. One advantage of a numerical experiment is that one can look at the atomic positions and how they change during an unexpected process such as this. When we did this, we found that the crystal had undergone a phase change as a result of the stress. Initially, it was being stretched in the (100) direction, and each layer of atoms perpendicular to this direction was square in shape and had its 64 atoms arranged with square symmetry. Although the crystal is close packed, this plane of atoms was not close packed. After the phase change, the atoms in each layer had moved closer together to form a close-packed array with hexagonal symmetry. At the same time, the overall shape of the layer had changed to being trapezoidal. What had happened was that the new structure was related to the old structure by a rotation so that the crystal was naturally longer in the stretched direction. This allowed it to relieve the imposed stress to some extent.

Numerical experiments of various kinds have been used to study condensed matter for the past few decades. As computers become faster and more powerful and better intermolecular force laws are developed, one can anticipate an increasing impact of numerical experiments in the field of materials science (6). More accurate force laws will allow one to study the quantitative behavior of particular materials under extreme conditions with confidence, whereas at present, we are at the stage of using numerical experiments to understand the basic physics of processes rather than to predict accurate numerical values. In the particular example of fracture, one will expect to see numerical experiments in which defects of different kinds are introduced and the way in which they change and move under stress studied, thus providing a link between theory and experiment for real (rather than ideal) materials. The future use of much larger systems (say larger by a factor of 10^6 or even 10^9) could bridge the gap between current numerical experiments on the nanometer scale and experiments in which real materials are observed in a microscope.

References and Notes

1. R. W. K. Honeycombe, *The Plastic Deformation of Metals* (Arnold, London, ed. 2, 1984).
2. A. Kelly and N. H. Macmillan, *Strong Solids* (Oxford Univ. Press, Oxford, ed. 3, 1986).
3. R. M. Lynden-Bell, *J. Phys. Condens. Matter* **4**, 2127 (1992).
4. M. P. Allen and D. J. Tildesley, *The Computer Simulation of Liquids* (Oxford Univ. Press, Oxford, 1987)
5. R. L. B. Selinger, R. M. Lynden-Bell, W. M. Gelbart, *J. Chem. Phys.* **90**, 9808 (1993).
6. See, for example, recent issues of the journal *Molecular Simulation*.