COMPUTATIONAL MATERIAL SCIENCE

Roughing It

Michael Marder

Ideal solids—such as the tetrahedron, cube, and sphere—have long provided models of the natural world. Yet the more closely one looks at a natural object, such as a round stone, the more resolutely it differs from a sphere. Seen sufficiently close, most surfaces resemble mountainous landscapes, jagged and irregular (see figure, part A). Kalia *et al.* have found through their computer simulations (*1*) the ways in which roughness can arise spontaneously in the most primitive act of creating new surfaces, the process of fracture.

The subversive idea that natural forms are better described by irregular fractal shapes than by Euclid's five regular polyhedra is Mandelbrot's (*2*). Not only did he assemble the mathematics needed to describe primitive forms of irregularity and dictate the terminology of a new field, he also carried out detailed observations of natural phenomena in varied fields. One of these case studies (*3*) showed that the surface of shattered steel is self-affine; that is, seen from a distance, it may appear smooth, but viewed under a microscope at magnification M, the apparent roughness in the field of view grows as $M^{0.75}$. This simple law has continued to receive confirmation in experimental studies (*4*), but where does it come from? Why should surfaces be rough at all, and why should the jaggedness grow in such a predictable way under the microscope?

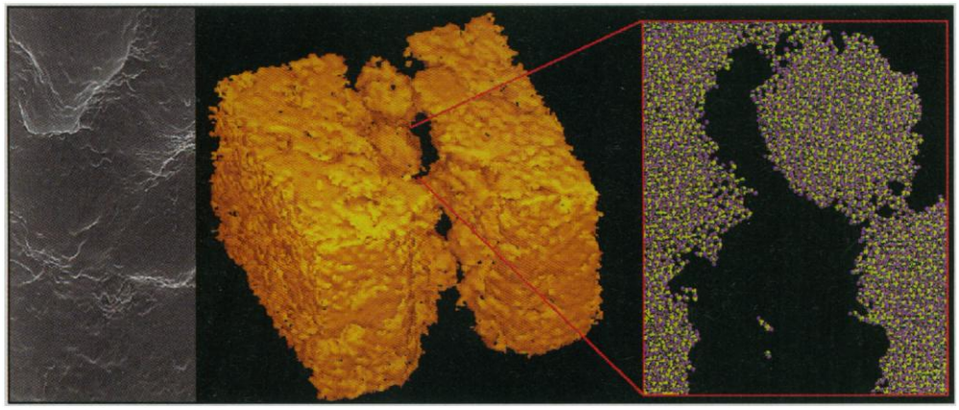
One possibility, strongly supported by the numerical simulations by Kalia *et al.*, is that such roughness arises naturally in the act of breaking two surfaces apart. Almost all means of exposing a new surface to the world are types of breaking, from the erosion of a tiny chip of stone from a cliff face to the dropping of a drinking glass. Breaking up is hard to do in anything but a rough and messy way because crack tips go unstable.

Think of a crack tip racing through a solid, cutting its atoms apart. Experiments have long shown (*5*) that when the tip becomes too energetic, the material rips rather than dividing cleanly. The simulations by Kalia and co-workers (*1*) are now showing that this mechanism leads in large-scale computer simulations to fractal fracture surfaces with quantitative resemblance to those in experiments.

Their simulations take place in a variety of virtual materials, including graphite and silicon nitride. The computations typically involve more than a million atoms, and because it is out of the question for the programmers to specify the initial positions of all of these atoms individually, the descriptions of how the simulations were prepared have a peculiar ring of real-world experiments. To create noncrystalline silicon nitride, the researchers cut small spherical clusters out of a perfect crystal, ram them together under pressure, heat them to 2000 K, wait for them slowly to become more dense, and finally cool the resulting solid down to room temperature. To study breakage, the computer saws a small notch into one side of the block, grabs two opposite sides in imaginary jaws, and pulls them apart until the block snaps in two (see figure, part B).

Without fractal geometry, there would be no language to describe the results, except to say that they look like a mess. As the crack jumps ahead, its head splits repeatedly into multiple cracks, most of which proceed a short distance sideways into the solid and then die. Between searching for weak spots in the solid and fending off powerful acoustic waves racing around inside the sample at high speeds, it is hardly surprising that the main crack path is quite irregular on the atomic scale, although it is overall a straight line. Viewed through Mandelbrot's microscope, the increase of roughness with increasing magnification appears to occur in an orderly fashion, as $M^{0.75}$. There is a variety of different ways to measure roughness, some of which give different answers at small and large scales, and the computer captures these variations as well, although it cannot encompass the large span of magnification scales accessible to experiment.

The simulations represent a considerable technical achievement. Calculations of such a size are possible only with a parallel computer in which large numbers of separate processing units work simultaneously. All such machines are still a bit experimental, but this group is roughing it even more than most, having built its own supercomputer by hooking together the innards of 40 workstations. They set a high standard for the realism built into the atomic interactions, which are derived as thoroughly as possible from other types of computation and from experimental data. Such large-scale computations are still too new to say whether the results are realistic and compare well with experiment on a detailed level. The necessary experiments have not even been formulated, much less performed. Some experimental aspects of silicon nitride, such as highly elongated crystallites, have not yet been incorporated into the simulation. Still, this first rough cut at replicating reality in the computer looks promising. It is messy, and in the right way.



Fractal fracture. (**left**) Scanning electron micrograph of the surface of a broken silicon crystal, about 1.3 μm across. [Courtesy of U. Purbach, J. Hauch, and A. De Lozanne] (**middle** and **right**) Computer simulation of the fracture surface of a broken piece of silicon nitride. [Courtesy of P. Vashishta and R. Kalia]

The author is in the Department of Physics and Center for Nonlinear Dynamics, The University of Texas at Austin, Austin, TX 78712, USA. E-mail: marder@chaos.ph.utexas.edu

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