Cracks: More Than Just a Clean Break

NEWS

The complexity of materials has long thwarted efforts to understand their failure, but researchers now believe defects may be the key

Fracture is ubiquitous in our daily lives: Cups break, handles snap off, windows shatter. It is also one of the most important causes of economic loss in industrialized society, as bridges fail, ships break up, and buildings collapse—all because of cracks. According to a 1983 study by the U.S. Department of Commerce, materials failure costs Americans roughly 4% of the gross national product. But despite the scale of the problem, what makes some cracks remain small and benign while others rip through a material at high speed is still a puzzle. James Langer of the University of California, Santa Barbara, who has studied cracks for the last 10 years, says that he once thought he understood how they work. "I am now pretty sure I don't," he notes.

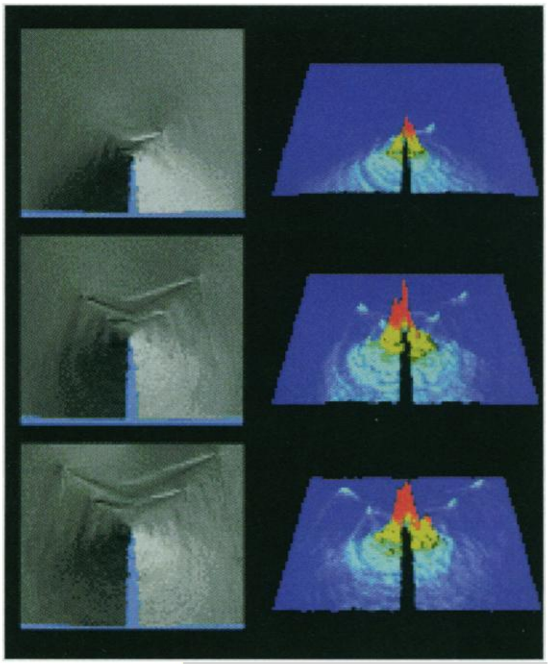
Crack research is finally on the move, however. The catalyst for this change is a more realistic view of the materials that cracks propagate through. Far from being the fault-free, regular crystals beloved by computer modelers, they are full of defects—microscopic impurities and dislocations in their crystal structure—that play a key role in the evolution of cracks. Scientists have found that defects are not only pivotal to the path and speed of the propagating crack, but that the crack tip itself transforms the material by creating a cloud of microcracks and dislocations around itself.

Computer modelers have been having trouble keeping up with this new trend. Simulating a crack that spawns a complex, three-dimensional network of defects around itself requires them to model hundreds of millions of interacting atoms, many more than are necessary for a crack that cleaves a material cleanly, and so they are limited by available computer power. Experimentalists, on the other hand, are racing ahead and probing the role of defects with advanced microscopy and other new experimental techniques. Although many researchers who spoke with *Science* believe it will take years to understand cracks well enough to predict where and when they will occur, they hope that the two branches of the field will converge and produce a better understanding of the basics of crack behavior. "We have learned a lot about the interaction of the defects," says Peter Gumbsch of the Max Planck Institute for Metals Research in Stuttgart, Germany.

Wolfgang Knauss of the California Institute of Technology (Caltech) in Pasadena says that scientists began studying cracks in earnest during the 1940s and '50s. They were prompted by a number of perplexing catastrophes, such as the failures of the wartime Liberty freighters, the first all-welded ships—of the 4700 ships built, more than 200 developed catastrophic fractures, some simply splitting in two while in port—and the loss of two Comet airliners, the pioneering, British-designed commercial jets. Early studies focused on why some materials behave in a ductile fashion, blunting cracks and stopping them easily, while others are brittle, allowing cracks to propagate in a flash over great distances. Researchers also hoped to understand why materials that are ductile in some conditions are brittle in others, like the steel hull of the *Titanic*. Ductile at room temperature, in the freezing waters of the North Atlantic and under heavy impact, it responded as a perfectly brittle material, instantly splitting open after the ship struck the iceberg.

Models lag. The experimental and modeling branches of crack research have always worked side by side. Following the disasters 4 and 5 decades ago, engineers started testing materials by stretching and bending them to breaking point under controlled conditions. Theorists fed these data into macroscopic mathematical models that generally simulated materials as perfectly homogeneous substances characterized by general properties, such as elastic constants. Such models are still far from producing reliable predictions of the failure of materials, says Ladislas Kubin of ONERA, France's national aerospace research center in Châtillon, near Paris: "If the model works for one material, you have no certainty it will work for another one."

Basic researchers similarly began to investigate how materials fail. Although they could not at that time examine samples at the atomic level, they knew that their models would have to describe how individual atoms or molecules interact with each other around the propagating crack tip. But the models had a similar lack of success in predicting how real materials behave. These microscopic models generated "purely mathematically sharp cracks that existed in ideally brittle materials," says Knauss, adding: "The answers don't help you really understand what goes on in the laboratory." For example, such models invariably yielded a maximum propagation speed for the crack equal to the speed of sound over the surface of the material—known as the Rayleigh speed. But in experiments, such high speeds have never been encountered. "It is typically one-third," says Knauss. "If you get half of it, you are doing very well."



Hot tip. Velocity (left) and temperature signatures of a crack and its V-shaped dislocations.

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In many cases, a simple lack of number-crunching power has hampered simulation efforts. Many rely on a technique called molecular modeling, in which an artificial array of atoms is created and the forces between them specified. Because of the complexity of accounting for all the forces between atoms, current simulations run on supercomputers can handle a maximum of about 100 million atoms or molecules. Although this sounds like a lot, it still represents a very tiny bit of material. "Even if they can deal with 1 billion atoms, you still only have a micron cube. This is not enough; a real plastic zone [formed at the tip of a crack] extends over millimeters," says Gumbsch.

Over the past few years, however, several groups have reported computer simulations that come closer to mimicking physical reality. Brad Lee Holian at the Los Alamos National Laboratory in New Mexico says that his group and others have done molecular dynamics simulations that show a "range of behaviors, ranging from brittle to ductile behavior." Holian thinks a good choice of parameters describing the forces between atoms and defects, and a simulation large enough to encompass several tens of millions of atoms, are the key to success. Farid Abraham of the IBM Almaden Research Center in

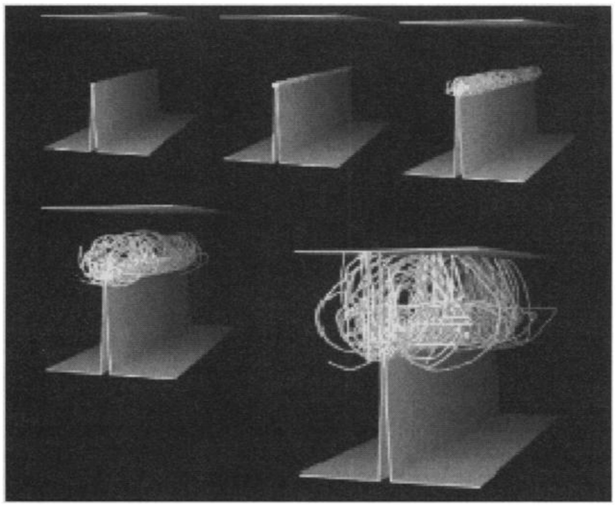
San Jose, California, says his team has improved on its simulation results by combining macroscopic continuum models with atomistic ones. "We now see a general convergence of the numerical methods, where all of the computational disciplines for the various size scales, the macroscopic to the microscopic, are coupled," he says.

Nevertheless, modelers are still struggling to keep up with the phenomenon that experimental studies suggest may be the key to crack behavior: the microcracks and dislocations that are formed around the crack tip. "That is something the modelers, including us, are still working on," says Gumbsch. There have been a few attempts at simulating dislocations near the crack tip in three dimensions, Gumbsch says, but modelers usually try to simulate just one dislocation at a time, looking at how it nucleates from a step in the crack front. "We still don't have reliable simulations," says Gumbsch.

Get to the point. With computer models still falling well short of a realistic depiction of cracking, researchers have been devising new kinds of experiments to study fracture in real materials. The key numbers describing crack formation are the speed of the crack tip and its path. Although cracks travel at less than the speed of surface waves on a material, their pace is still daunting. Typically, cracks in silicon crystals can travel at speeds of 4 to 5 kilometers per second.

To measure such speeds, scientists first resorted to high-speed photography, applying stress to materials and snapping up to 2 million frames per second to follow the evolution of cracks. But a method developed in 1992 by a team led by Michael Marder of the University of Texas, Austin, called the "potential drop" experiment, now gives the most accurate results. Researchers first coat a Plexiglas or glass sample with a thin layer of aluminum, then put the sample under stress and pass an electric current through the aluminum. As the crack forms, the aluminum layer is ruptured and the researchers measure the current drop to determine the speed of the crack with an accuracy of 20 meters per second.

These experiments raised the puzzle that researchers are now starting to solve: the lower-than-expected speed of cracks. Although speed does increase with increasing load on the material, it levels off far short of the Rayleigh speed. No matter how hard you pull apart a sample of Plexiglas, a crack will not travel faster than about 800 meters per second. Researchers are now starting to understand this discrepancy, as they realize that cracks are far more complex phenomena than previously thought.



Model failure. One-hundred-million-atom simulation of a crack and its dislocation "cloud."

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The source of the speed limit seems to be the "cloud" of tiny cracks that forms around the crack tip. These microcracks, ignored in early models, are caused by dislocations spreading out from the crack tip, says Holian. At each point the crack tip has to "choose" which particular microcrack to follow. This explains why the direction of a crack can change suddenly. "It is possible that the crack will follow the dislocation along a [plane of atoms] that is at an angle to the crack tip," Holian says. The surface left by a fracture records what happened during crack propagation, including the dislocations and microcracks generated by the crack tip, and researchers have tried to characterize fracture surfaces mathematically. The surface exhibits a roughness that can be described as a fractal surface—similar shapes can be found over a wide range of different size scales, says Kubin of ONERA, from nanometers to hundreds of micrometers: "There is something universal in the geometry of the crack surface."

Researchers now believe that the processes responsible for this fractal geometry—the constant creation of microcracks and the shifts of direction—are also what slow the crack down. "This process takes a substantial amount of time away from the idealized crack propagation process," says Caltech's Knauss. He and his colleagues tested this hypothesis by artificially creating very weak joints in materials, which prevent microcracks from forming. In such materials, they observed crack speeds of up to 95% of the Rayleigh wave speed. "If you get rid of this multiple flaw generation, you deal with idealized materials, and the idealized high-speed crack model is applicable," he says.

As well as simply slowing down the crack, the creation of defects ahead of the tip actually changes the mechanical properties of some materials locally, in a process called brittle-to-ductile transition. "At a certain temperature and certain strain rate, the crack starts emitting dislocations" that make the material ductile, says Kubin. Dislocations are shifts of layers of atoms in the crystal lattice, and because dislocations can move through the material, it becomes ductile. This transition can bring the crack to a halt in some materials.

Studying the brittle-to-ductile transition is very difficult in anything but the simplest of materials, says Steve Roberts of Oxford University. Recent, as-yet-unpublished research with tungsten samples has convinced Gumbsch and his colleagues that what determines whether the transition takes place is the ability of the dislocations to spread out from the crack tip rapidly, making the area around it ductile. "If dislocations can be generated from the crack, that is, injected into the matrix [of the material], and can move away, the material responds in a ductile way. If the dislocations cannot move away from the crack fast enough, then it responds in a brittle way," says Gumbsch.

Gumbsch and his colleagues have recently performed experiments in which they investigated tungsten "post-mortem" with scanning electron microscopes to see the details of how a ductile response can slow down or stop a crack. The microscopic observation of dislocations created at different temperatures in the samples shows that a dislocation moving away from a crack "intercepts" part of the external force field. "It prevents the crack from seeing the outside load," says Gumbsch. If the crack tip creates enough dislocations, they will shield the crack entirely and it will slow down or even stop. "If you can create sufficiently many dislocations, and they move away fast enough, then the crack tip will deform and the material response will be ductile," he adds.

These brittle-to-ductile transitions occur in a range of materials, such as silicon and metals with a crystal structure known as body-centered cubic, but the temperatures at which the transition takes place are sometimes difficult to pin down because there is no precise way of identifying ductile behavior. It is a "gray area," says Holian, but he adds that the transition is more likely to occur at higher temperatures.

Although researchers are learning a huge amount through experimental studies of cracks, Kubin is convinced that computer modelers will have to incorporate this new knowledge if crack researchers are going to achieve a true understanding of material failure. "In this domain, you can make experiments and experiments and experiments, but it will not advance your understanding. We should not look at complicated situations and materials; we should try to understand basic things."

–ALEXANDER HELLEMANS

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