An Atomic Look at Why Thing

BY CHARLES XIE

Most children learn early that things break, whether it's a stick, a favorite toy, or Humpty Dumpty himself. Although the nursery rhyme may be culturally specific, the phenomenon is universal. But it turns out that what is so common in our daily experience contains a lot of profound science that even scientists do not fully understand today.

Molecular literacy

The question about why things break has to be answered from a microscopic perspective. Ultimately, things break because atoms and molecules are pulled apart. Such a bottom-up approach of explaining things based on an atomic-scale picture is called *molecular literacy.* Like language literacy, students need experience and opportunities for learning in order to acquire molecular literacy. The Molecular Workbench (MW) software developed by the Concord Consortium is a powerful tool that can greatly help students develop their molecular literacy.

In this Monday's Lesson, your students can use MW simulations to answer the questions about why and how things break.

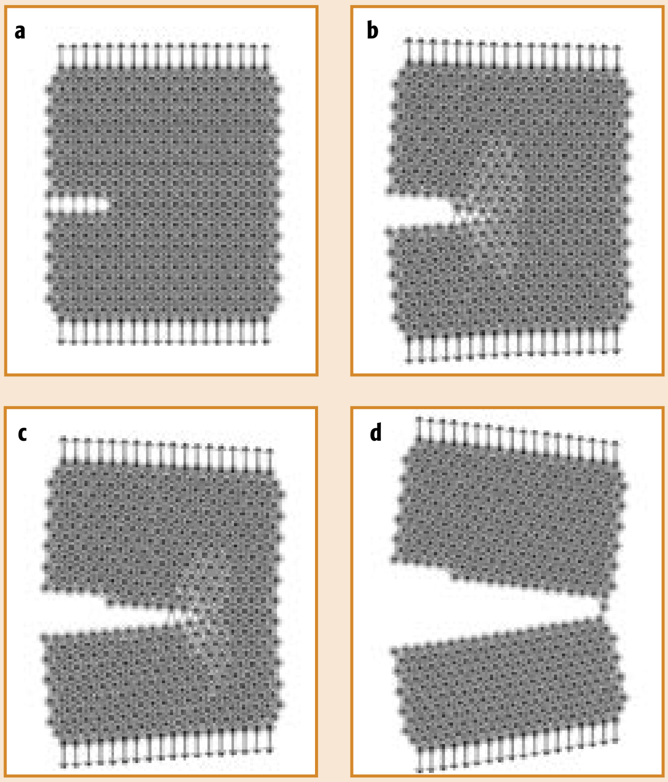

Figure 1 An MW model showing crack propagation, initiated from a cut in a perfect crystal.

System requirements

You must have Java Version 5 or higher in order to run MW. Go to *http://java.com* to get the latest Java software.

Crack propagation

A break often starts from a microscopic crack, which may be an imperfection in the material when it was made, or created by an impact or repeated flexing "fatigue." A crack can grow longer and larger when a force is applied. Think of cracking an egg on the side of a frying pan. This is called crack propagation, and it's useful to understand for physics, engineering, and geosciences, not to mention making breakfast.

A crack is a wonderful example of a micro-macro connection, that is, where events at the molecular level affect phenomenon at the macroscopic or visible realm. Regardless of its size, a crack has a tip where the atoms are just coming unzipped. What happens at the tip is the most important thing during the growth of a crack and, therefore, the entire process of breaking.

Go to: *http://mw.concord.org/modeler1.3/mirror/materials/fracture.html*

Click "Launch the models." Then "Trust" the certificate.

The model depicts a lattice of atoms, representing a crystal. External forces are applied to the top and bottom layers of atoms, represented by the arrows. The yellow bar serves as a marker to create an initial cut.

1. Click the "Cut" button to cut the lattice, and then run the simulation. Observe what happens.

ngs Break

2. Reset the model, then "Shift cut area to the right," cut, and run the model again.
3. Reset, shift the cut area two units, cut, and run a third time. What do you notice?

An astute student will observe during the simulation that the bonds at the tip break one at a time as the crack grows. Without that small fissure, the crystal would not have broken under the same stress. Students can run the simulation of the same crystal without a crack to verify this. Simply move the yellow bar to the left (off the crystal entirely) and run the model. The atoms wiggle in place due to the external forces, but nothing breaks!

Students discover that crack propagation is the key that causes things to break. It provides a mechanism for conveying a large force to the atoms at the tip and ripping apart bonds between them one at a time as the crack travels.

Testing "what if?" conditions

If a crack is not deep enough, it cannot propagate (figure 3a). But if there are microcavities nearby, it can "hop" to them and the material breaks apart along a path that connects these defects, as illustrated by figure 2.

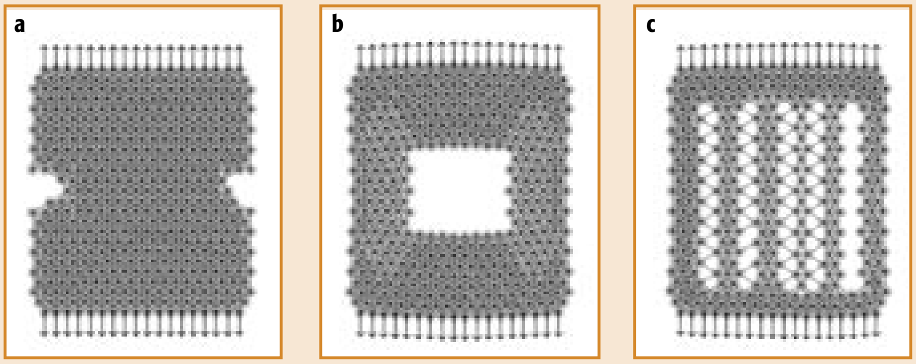

Figure 3 Some structures that do not break under the same stress.

LINKS *Monday's Lesson*

The Molecular Workbench
http://mw.concord.org/modeler

A fascinating aspect of a computational model is that it allows students to test many different "what if?" conditions quickly.

For example, have your students use the scissors tool on the tool bar above the model to cut out a big cavity in the middle of the material (figure 3b), or create a structure that looks like a bundle of fibers (figure 3c). They will soon discover that these structures can withstand a surprising amount of tension. Such experimentation may help them dispel the idea that heavy pieces are stronger than lighter ones.

Finally, you can assign a challenge to your students and have them document their success. For example, what's the smallest initial crack that will cause a crack propagation? Or, what's the largest design of microcavities that will not break?

Have students take and annotate snapshots and print or submit a report.

Conclusion

Fracture is one of the most important factors that affects our safety. We rely on each piece in the backbone structures of the buildings we live in, the planes we travel on, and the bridges we cross not to break. Preventing fracture is a hot research topic; fracture in real materials under real conditions is still not well understood.

Nevertheless, as we can see, a better understanding of fracture can be built upon the very simple essence of the atomic-scale mechanics without formal treatment or complicated mathematics. By applying the basic ideas that a material is composed of interacting atoms and the interactions among them govern the material's behavior under different conditions, students can develop concepts and intuitions through a pathway that may be less difficult. The innovative Molecular Workbench software provides many technical capabilities that have made such a new treatment much easier to implement.

Unfortunately, not even MW can put Humpty Dumpty—or that favorite toy—together again!

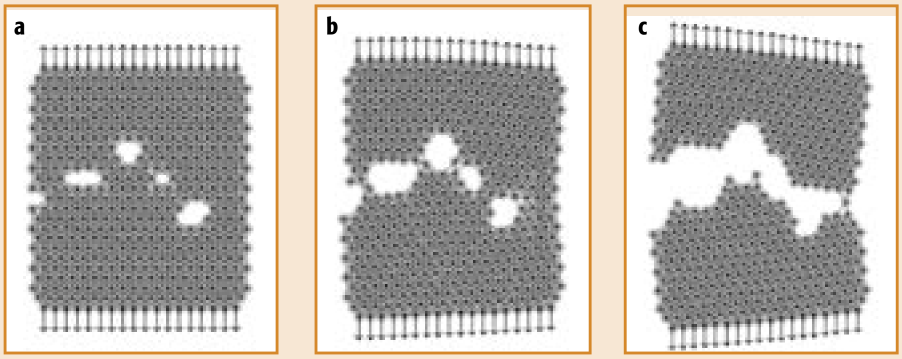

Figure 2 Crack propagation in the presence of microcavities.

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