Physicists develop new insight into how disordered solids deform

August 31 2011

In solid materials with regular atomic structures, figuring out weak points where the material will break under stress is relatively easy. But for disordered solids, like glass or sand, their disordered nature makes such predictions much more daunting tasks.

Now, a collaboration combining a theoretical model with a first-of-its kind experiment has demonstrated a novel method for identifying "soft spots" in such materials. The findings from University of Pennsylvania and Syracuse University physicists may lead to better understanding of the principles that govern materials responses ranging from failure of glasses to earthquakes and avalanches.

The experimental research was conducted by professors Arjun G. Yodh and Andrea J. Liu, along with post-doctoral associates Ke Chen, Wouter G. Ellenbroek and Zexin Zhang and graduate student Peter J. Yunker, all of the Department of Physics and Astronomy in Penn's School of Arts and Sciences. They collaborated with Lisa Manning of the Department of Physics at Syracuse. Liu and Manning described the theoretical model in a separate study.

Both studies appear in the journal Physical Review Letters.

For materials with well ordered, crystalline internal structures, such as diamonds or most metals, identifying soft spots is easy; weak, disordered sections stick out like a sore thumb.

"In perfect crystalline materials, atoms are in well-defined positions. If you give me the position of one atom, I can tell you the position of another with precision," Yodh said. "There's also a well defined theory about what's happening with defects in crystals when stresses are applied to them."

"There's no periodicity in glass, however," Chen said. "You can't look at it and say, 'This part looks different than the rest,' because there is no background pattern to compare it with."

With physical structure a dead end for identifying soft spots, the physicists turned to another property: vibrations. Though the word "solid" is synonymous with "unmoving," the particles that make up solid matter are constantly vibrating. And like the different tones of guitar strings, there are many different ways particles in a solid can vibrate. These are known as "vibration modes."

For crystalline materials, the regular patterns of atoms lead to uniform patterns of vibrations within the material; nearly all particles are involved in a typical vibration. In disordered materials, with their unevenly spaced particles, particles in different regions vibrate differently, producing some new and different vibration modes, particularly at low frequencies.

"We can determine the spatial patterns of the different vibrations in our experiment, and then we can find out whether some of them, particularly low frequency vibrations, are connected with rearrangements or failure of the material when it is stressed," Chen said.

Manning and Liu developed a simulation to test this kind of correlation under idealized conditions. They were able to show that certain regions highlighted by low frequency vibration modes acted like defects in disorganized materials and that these defects were good candidates for where the material would fail when stressed.

"We showed, for the first time, a correlation between the soft spot population and rearrangements under stress," Manning said. "This is something people have been looking for over the past 30 or 40 years."

Though the success of the simulation was an exciting result by itself, it was only a first step. Real-world systems have additional layers of complexity, notably temperature and related thermal fluctuations that can rapidly change the interactions between neighboring particles and thus the system's vibrational patterns.

"It was not at all obvious that the soft spots we found in the simulation would still exist in the presence of thermal fluctuations, which are unavoidable in the real world," Liu said. "Thermal fluctuations, for example, might have caused the soft spots to be wiped out too rapidly to be used for analysis."

To see if this was the case, Chen developed an experimental system with many features similar to the one in the simulation. At its core was a colloidal glass, an effectively two-dimensional material consisting of a single disordered layer of soft plastic particles tightly packed together.

By analyzing video of the particles' motion in the colloidal glass as observed under a microscope, Chen was able to calculate the vibration patterns and then use Manning and Liu's model to locate regions vulnerable to rearrangement once the glass was put under stress. He then compared these regions to the rearrangements that actually happened.

Just as in the simulation, the soft spots predicted candidates for rearrangement, as some of the identified soft spots remained intact while others deformed. The experiment thus provides a new basis — low frequency vibration modes — for analyzing real-world disordered solids.

"Low frequency vibrations correspond to areas with weak interaction between particles, and because of these weak interactions their structure is less stable. When they're perturbed there is less resistance from their neighbors." Chen said.

Disordered solids are much more common than ordered ones, so having a working theory of how, why and where they break has many potential applications.

"You can bend a metal spoon, but you can't bend one made out of glass without breaking it. If you can understand how disordered solids fail, you might be able to make them tougher," Yodh said.

Provided by University of Pennsylvania

Citation: Physicists develop new insight into how disordered solids deform (2011, August 31) retrieved 9 April 2024 from https://phys.org/news/2011-08-physicists-insight-disordered-solids-deform.html

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