Atomic trigger shatters mystery of how glass deforms

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Throw a rock through a window made of silica glass, and the brittle, insulating oxide pane shatters. But whack a golf ball with a club made of metallic glass—a resilient conductor that looks like metal—and the glass not only stays intact but also may drive the ball farther than conventional clubs. In light of this contrast, the nature of glass seems anything but clear.

A new study at the Department of Energy's Oak Ridge National Laboratory, published Sept. 24 in *Nature Communications*, has cracked one mystery of glass to shed light on the mechanism that triggers its deformation before shattering. The study improves understanding of glassy deformation and may accelerate broader application of metallic glass, a moldable, wear-resistant, magnetically exploitable material that is thrice as strong as the mightiest steel and ten times as springy.

Whereas metals are usually crystalline, metallic glasses are amorphous in atomic structure. Amorphous metals, studied since the 1950s, have a tendency to crystallize when heated, which makes them extremely brittle. Metallic glass alloys that did not crystallize so easily were discovered at Tohoku University and Caltech in 1991 and introduced commercially in golf clubs in 2001.

Glass hangs in a metastable state in which the energy of the system is higher than the lowest-energy state the system could assume, a crystalline state. But its state is stable enough at room temperature to last a human lifetime.

"Exactly speaking, a metastable state cannot last; it evolves," said project leader Takeshi Egami, a distinguished scientist/professor at ORNL and the University of Tennessee–Knoxville who directs the Joint Institute for Neutron Sciences (JINS), a partnership of ORNL and UT. "For instance, diamond is only metastable. Graphite is a stable state. Hollywood says 'Diamonds Are Forever.' Scientifically that is completely incorrect."

Due to its relative stability, metallic glass can be melted and precision-cast into molds without going back to its most stable, crystalline state. The resulting parts do not need to be machined, which saves money. That said, metallic glass is pricey. (A club made of it can set a golfer back $800.) Regardless, it has been used in biocompatible bone implants, rust-resistant razors and scalpel blades, resilient coatings for refinery pipes, transformers with half the energy loss, Andre Agassi's tennis racquet and the scratch-resistant logo of Apple's iPhone 6.

It may gain wider application if dabbed on computer chips to reduce electromagnetic noise that produces heat. Wider deployment may drive down costs of metallic-glass watches, rings, skis and baseball bats. The material may be used in vehicle bodies and casings for smartphones and computers as well. But for metallic glass to achieve its promise, it must first overcome a long-standing problem.

"Metallic glasses are too brittle, meaning the materials easily break without significant ductile deformation," said Yue Fan, a Wigner Fellow at ORNL and the study's lead author. "It is extremely important to understand the origin of deformation in metallic glasses to engineer solutions that would increase their usefulness." Case in point: Initial prototypes shattered after as few as 40 hits. To improve ductility, which is a material's ability to be deformed without fracture, manufacturers had to resort to a composite including crystalline material. While metallic glass golf clubs remain in demand today, manufacturers stopped making them 10 years ago because they are costly.

Universal trigger

Fan and Egami, with JINS postdoctoral researcher Takuya Iwashita, found through a computer simulation study that before glass shatters, one mechanism is in play during early deformation: Patches of only five or so atoms exchange atomic bonds with each other (see video). Prior to the discovery, scientists thought the number of atoms triggering deformation ranged from 20 to 600.

"This trigger was the same for stable and unstable glass," Fan said (see technical highlight). "The only difference was how triggers organized themselves. The individual triggers were identical. Until now people didn't believe a universal trigger existed and thought every case was different. But now we see some kind of universality."

The organization of universal triggers correlates with a material's ductility. This ability to deform under external stress will have to improve for metallic glasses to achieve mass-market viability.

"Our simulation study on the deformation of metallic glasses can shed light on controlling ductility," Fan said. The study compared metallic glasses that were heated to reach a liquid state at 2,000 kelvins and then cooled, either slowly or quickly, to near absolute zero kelvin, a temperature so cold that atoms barely move. In the quickly cooled glass, more of the five-atom deformation triggers, or regions of atomic bond switching, developed than in the slowly cooled glass. The greater density of triggers created more pathways by which energy could dissipate, creating a glass with greater ductility, Fan explained.

Grand challenge

In crystals, atoms regularly pack into identical unit cells of well-ordered lattices. In glass, however, they sit at random distances from each other, an arrangement that infinitely increases the number of possible configurations. The same atomic chaos is true of a liquid. In fact, atomically, solid glass is a "frozen" liquid and flows, albeit over centuries.

Physics Nobel Prize winner Philip Anderson called glass "the deepest and most interesting unsolved problem in solid-state theory" due to its disordered atomic packing.

"In the 20th century we developed solid-state physics of the crystalline state," said Egami. "In crystals one unit cell is repeated many, many, many, many times, so if you understand one [cell], you understand everything. This periodicity was a major key in advancing the theory of solids. Glasses and liquids do not have this periodicity."

Atoms in the repeating cells of a crystal are like citizens under a dictatorship—individuality is not tolerated and interactions are regimented, according to Egami. But atoms in glassy and liquid states are like democracies—atoms and their environments are diverse. "It's the many-body problem in physics," Egami explained. "That means you can solve one or two [atomic interactions], but three already is a many-body problem that cannot be solved rigorously. It's a tremendous mathematical problem."

That makes glass a grand challenge not only in materials science but also in condensed matter physics.

"There's a huge vacuum in what we know about the science of liquid and glasses simply because it's a difficult challenge and not much has been done," Egami said. "A large portion of materials in the world are simply not understood."

Hiking the potential energy landscape

Strength varies even in materials of the same ilk. One crystalline material may be a thousand times stronger than another, whereas the strongest glass may be only three times as sturdy as the weakest. "It's surprising that strength is not that dependent on composition," Egami said.

Studying defects that weaken glass requires a different approach than investigating flaws that cripple crystal. When crystal is subjected to stress, imperfections in the lattice can dislocate rows of atoms. Glass, in contrast, does not have a lattice. It does, however, have defects—so many that scientists cannot even define "defects" in glass. That makes the mechanism of deformation in amorphous materials like metallic glass controversial. "There are many, many ideas about how it happens, but still it is not really understood," Egami said.

The evolution of a system, such as an oxide glass or a metallic glass, is governed by its energy configuration, or underlying potential energy landscape (PEL).

Prior researchers had focused on initial and final states of systems during the deformation process. Instead, Fan, Egami and Iwashita focused on "saddle points"—points of highest energy during an atom's movement in a system—between neighboring minima. If minima are like valleys, saddle points are ridges that must be traversed to get to a neighboring valley. "There are many local minima on the PEL, and the system's deformation consists of the hoppings between neighboring minima," Fan said.

In glasses, the findings indicate, deformation happens when only five hikers/atoms have enough energy to climb the mountain together and cross the saddle point. Other hikers may strain themselves to do the same but lack the energy to succeed, so they return to their tents in the valley to rest.

In an unstable system, atoms can get to saddle points more easily than they can in a stable system. In a stable system, atoms have to scale taller mountains and expend more energy before they can rest in adjacent valleys.

Snowball to shattering

For the simulation study, the researchers calculated how atoms move on a personal computer. To describe deformation at the atomic level, they sampled a large number of paths along which a system can evolve. Analyzing the ensuing ensemble, they arrived at the statistically likely scenario.

"We unraveled the mystery of this deformation mechanism in not only the metallic glass system but also the general amorphous system," Fan said. "It's a challenging randomness problem, but from this huge model statistical result, we find [these two systems] are surprisingly governed by the same mechanism."

Next the researchers will explore what happens between deformation and shattering. "As a consequence of deformation, next comes the stage where 20 atoms are affected," Egami said. "Sometimes they start an avalanche. Then hundreds of atoms are involved. At the end, all atoms in the system are involved—billions of atoms. So shattering is first started by five and then snowballs into big action."

The researchers' improved fundamental understanding of metallic glasses creates new knowledge of a material class about which little is known. Such advances may contribute to the federal government's Materials Genome Initiative, launched in 2011 to accelerate discovery, manufacture and deployment of advanced materials for the global marketplace.

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