

Fast molecular rearrangements hold key to plastic's toughness

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Polycarbonate, a type of polymer glass, can be bent (sheet), mashed (cylinder), or twisted (rod) without breaking. UW-Madison chemistry professor Mark Ediger studies the fundamental properties of polymer glasses that allow them to bend rather than break when put under stress. In a paper appearing in Science Express on Nov. 28, 2008, Ediger reported that a pulling force speeds up the movements of individual molecules within a polymer glass by more than a factor of 1,000. These fast molecular rearrangement allow the material to be shaped without cracking. Photo by: Hau-Nan Lee, UW-Madison dept of chemistry

(PhysOrg.com) -- Plastics are everywhere in our modern world, largely due to properties that render the materials tough and durable, but lightweight and easily workable. One of their most useful qualities, however - the ability to bend rather than break when put under stress - is also one of the most puzzling.

This property, described as "plastic flow", allows many plastics to change shape to absorb energy rather than breaking apart, says



University of Wisconsin-Madison chemistry professor Mark Ediger. For example, one type of bulletproof glass stops a bullet by flowing around it without breaking. Regular window glass, unable to flow in this way, would simply shatter.

"This is an odd combination of properties... These materials shouldn't be able to flow because they're rigid solids, but some of them can," he says. "How does that happen?"

Ediger's research team, led by graduate student Hau-Nan Lee, has now described a fundamental mechanism underlying this stiff-but-malleable quality. In a study appearing Nov. 28 in Science Express, they report that subjecting a common plastic to physical stress - which causes the plastic to flow - also dramatically increases the motion of the material's constituent molecules, with molecular rearrangements occurring up to 1,000 times faster than without the stress.

These fast rearrangements are likely critical for allowing the material to adapt to different conditions without immediately cracking.

Plastics are a type of material known to chemists and engineers as polymer glasses. Unlike a crystal, in which molecules are locked together in a perfectly ordered array, a glass is molecularly jumbled, with its constituent chemical building blocks trapped in whatever helter-skelter arrangement they fell into as the material cooled and solidified.

While this atomic disorder means that glasses are less stable than crystals, it also provides molecules in the glass with some wiggle room to move around without breaking apart.

"Polymer glasses are used in many, many different applications," including polycarbonate, which is found in popular reusable water bottles, Ediger says. Aircraft windows are also often made of



polycarbonate. "One of the reasons polymer glasses are used is that they don't break when you drop them or fly into a bird at 600 miles per hour."

However, their properties can change dramatically under different physical conditions such as pressure, temperature, and humidity. For example, many polymer glasses become brittle at low temperatures, as anyone knows who has ever dropped a plastic container from the freezer or tried to work on vinyl house siding in cold weather.

As plastics become more and more prevalent in everything from electronics to airplanes, scientists and engineers face questions about the fundamental properties and long-term stability of these materials over a range of conditions.

For example, next-generation commercial aircraft are trending toward including less metal in favor of higher proportions of lightweight polymer materials - roughly 50 percent in the new Boeing 787 compared to only 10 percent in the Boeing 777 - and engineers need to know how these materials will respond to different stresses: a hard landing, strong winds, or changes in temperature or humidity.

"How is it going to respond 20 years from now when it gets twisted, or stretched, or compressed? Is it going to respond by absorbing that energy and staying intact, or is it going to respond by breaking bonds and flying apart into pieces?" asks Ediger.

The Wisconsin team examined the mechanics of a common plastic called polymethylmethacrylate - also known as Plexiglas or acrylic - and found that a pulling force had a pronounced effect on the molecules within the material, speeding up their individual movements by more than a factor of 1,000. The team observed internal molecular rearrangements within 50 seconds that would have taken a full day without the force applied. They believe this increased motion allows the



material to flow without breaking.

"When you pull on it, you increase the mobility in the material," Ediger says. "The act of pulling on it actually transforms the glass into a liquid that can then flow. Then when you stop pulling on it, it transforms back to a glass."

The work has benefited from collaboration between chemists and engineers in a Nanoscale Interdisciplinary Research Team (NIRT) supported by the National Science Foundation (NSF), which includes UW-Madison chemical and biological engineering professor Juan de Pablo and groups at the University of Illinois and Purdue University.

"From the most fundamental perspective, we're trying to understand why pulling on a glass allows it to flow," Ediger says. "The answer to that question will help us to better model the behavior of real materials in real applications."

In addition to Ediger and Lee, the paper is authored by Keewook Paeng and Stephen Swallen. The work was funded by NSF.

Provided by University of Wisconsin

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