# Glass has potential to be stronger, researchers say

September 21 2012, by Mike Williams

(Phys.org)—Glass is strong enough for so much: windshields, buildings and many other things that need to handle high stress without breaking. But scientists who look at the structure of glass strictly by the numbers believe some of the latest methods from the microelectronics and nanotechnology industry could produce glass that's about twice as strong as the best available today.

Rice University chemist Peter Wolynes is one of them. Wolynes and Rice graduate student Apiwat Wisitsorasak determined in a new study that a process called chemical vapor deposition, which is used industrially to make thin films, could yield a glass that withstands tremendous stress without breaking.

Wolynes, a senior scientist with the Center for Theoretical Biological Physics at Rice's BioScience Research Collaborative, and Wisitsorasak reported their results this week in the Proceedings of the National Academy of Sciences. Their calculations were based on a modified version of a groundbreaking mathematical model that Wolynes first created to answer a decades-old conundrum about how glass forms. With the modifications, Wolynes' theory can now predict the ultimate strength of any glass, including the common varieties made from silica and more exotic types made of polymers and metals.

If metal glass sounds odd, blame it on the molecules inside. Glass is unique because of its molecular structure. It freezes into a rigid form when cooled. But unlike ice, in which water molecules take on regular crystalline patterns—think of snowflakes—the molecules in glass are suspended randomly, just as they were as a liquid, with no particular pattern. The strong bonds that form between these randomly-arrayed individual molecules are what hold the glass together and ultimately determine its strength.

All glasses share the ability to handle a great deal of strain before giving way, sometimes explosively. Exactly how much strain a glass can handle is determined by how much energy it can absorb before its intrinsic elastic qualities reach their limitations. And that seems to be as much a property of the way the glass is manufactured as the material it's made of.

Materials scientists have long debated the physics of what occurs when glass hardens and cools. In fact, the transition is one of their last great puzzles of the field. Cooling temperatures for particular kinds of glass are well defined by centuries of experience, but Wolynes argues it may be possible to use this information to improve upon glass's ultimate strength.

The elastic properties of the finished product and the configurational energy (the positive and negative forces between the molecules) held in stasis by the "freezing" process determine how close a glass gets to the theoretical ideal—the most stable glass possible, he said.

"The usual impression of glass is that, relative to other materials in your life, it seems easy to break," said Wolynes, Rice's Bullard-Welch Foundation Professor of Science and a professor of chemistry. "The reality is that when it's freshly made and not scratched, glass is very strong."

Wolynes, who specializes in how molecular systems move across microscopic "energy landscapes,"particularly as they relate to protein folding in biology, has an interest in glass that goes back many years. His random first-order transition theory of glasses, which quantifies the molecules' kinetic properties as they cool, helped set the stage for decades of debate among theorists over how glass actually forms.

But the theory, based on work by Wolynes and collaborators that goes back to 1989, did not consider the strength of glass.

"You can come up with a theory of something and ignore one of the most practical implications because you just don't think about it," Wolynes explained.

A chance encounter with a metallurgist last year made Wolynes think again about just how strong glass could be. "We had never worked on that kind of property, and the problem struck me as intriguing – and relatively simple in the framework of the theory we already had. We just hadn't thought to calculate it," he said.

Traditional glass is so ubiquitous that people rarely think about it (until it breaks). "Even though we now have Gorilla Glass and other tempering developments, they've been developed in a somewhat Edisonian fashion," he said, noting that such hardened glasses commonly used in cell phones have a self-healing surface treatment that protects the glass itself from scratching. "Our paper is about what determines the limits on the strength of the glass, if there is no surface problem."

Wolynes noted the strength of materials has been studied since the 1920s, when Russian scientist Yakov Frenkel "calculated how strong something could be if we just take into account the direct forces between atoms. He made a simple calculation: If you have a row of atoms and pull it over another row of atoms, when would it go from one way of aligning to the next?" Wolynes said that determines a material's elastic modulus—"how springy the material is"—an easy concept to understand in metals that bend before they break.

"The elastic modulus is related to the thermal vibrations in the material," he said. "Basically, if you have a material that has a very high melting point, its elastic modulus is also very high. According to Frenkel, the strength should also be very high.

"That overall trend is true. That's why fighter jets are made of titanium, one the highest-melting metals, and low-melting aluminum, which is not as strong but lighter, is used for other things."

The theory didn't seem to relate to glasses, however. "In the early days, when people first measured the properties of glasses, they found they were easily breakable. Silica glass is very high-melting, so you'd expect it to be strong," Wolynes said. "Then they did finally figure out this was because cracks at the surface were propagating in. If they could eliminate the cracks, they would get much higher strengths."

Current metallic glasses like the Liquidmetal famously licensed by Apple for consumer electronics "come to be about a quarter of this theoretical Frenkel strength," Wolynes said. "So what is it that limits their strength? We ask whether the collective motions that go on in liquids as they're becoming glasses are the same motions that are being catalyzed when we stress the material.

"Basically, we applied our theory for what determines how the liquid rearranges as it's becoming glass. Add to that the extra driving force when you apply stress, and see what that predicts for the limit of how much it can be pushed before the atoms roll over each other" and the glass breaks, he said.

He noted the theoretical results closely match experimental ones for most materials. "The good news is, according to this theory, if you could make a material that is much closer to ideal glass – the glass you would get if you could make it infinitely slowly – then you would be able to increase its strength." That may not be possible through traditional cooling of silica, metal and polymer glasses, which Wolynes' and Wisitsorasak's calculations indicate are approaching their limits.

But it might be possible through vapor deposition of atoms, akin to the chemical vapor deposition process used in microelectronics and nanotechnology to make thin films. "It would require tuning the deposition rate to the liquid/glass transition properties," he said.

"Our theory says the best you can do with this is get about halfway to ideal glass," which he said some experimentalists have demonstrated. "It's possible there's some loophole we don't yet see that will let us get even closer to the ideal," Wolynes said. "But at least, at this point, we can get halfway there. That means it would be possible, in principle, to get glass with at least twice the intrinsic strength of current glasses."

Wolynes' theory comes with a caveat, though. Glass hardened even to the point of near indestructibility can still be destroyed, and with dramatic effect. "If you could have something infinitely strong, then you'd never need to worry about it," he said. "But there's a little bit of a problem if you make something that's very strong but can eventually break. It contains a huge amount of energy, so when it breaks, it fails catastrophically."

**More information:** www.pnas.org/content/early/201 … /1214130109.abstract

Provided by Rice University

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