Science and Engineering. “We wanted to study the material under conditions that prevail at the tip of the crack, the point at which the crack pulls open the glass. We wanted to see the steps that develop as the material splits at that location. That’s where dramatic things happen: atoms are pulled apart, bonds are broken.”

At the site where this breakup begins, a vacant space—a bubble—is left behind. Falk’s research group discovered that cavitation—spontaneous formation of tiny bubbles under high negative pressures—plays a key role in the failure, or breakdown, of metallic glasses.

Falk said, “Once it appears, it releases energy as it grows bigger, and it may eventually become big enough for us to see it under a microscope. But by the time we could see them, the process through which they had formed would be long over.”

Therefore, to study the bubble’s nucleation, Falk’s team used a computer model of a cube of a metallic glass made of copper and zirconium, measuring only about 30 atoms on each side. By definition, a bubble appears as a cavity in the digital block of metallic glass, with no atoms present within that open space.

The simulations revealed that these bubbles emerge in a way that is well-predicted by classical theories, but that the bubble formation also competes with attempts by the glass to reshuffle its atoms to release the stress applied to a particular location. That second process is known as shear transformation. As the glass responds to pressure, the researchers found which of the two processes has the upper hand—bubble formation or shear transformation—varies. They determined that bubbles dominate in the presence of high tensile loads. But when the pulling forces were small, the atom reshuffling process prevailed.

Falk and his colleagues hope their findings can help scientists developing new metallic glass alloys that can take advantage of the material’s high strength and elasticity, along with its tendency not to shrink when it is molded to a particular shape. These characteristics are important for applications, for example, in cell phones and computers.

“Our aim is to incorporate our findings into predictive models of failure for these materials,” Falk said, “so that they can be optimized and used in applications that require materials that are both strong and fracture-resistant.”

A series of polar magneto-optical Kerr effect microscopy maps showing expansion of a magnetic domain (blue) under an applied magnetic field of 170 Oe with increasing time (from left to right). Row (a) shows the material in its virgin state, without electric-field poling. In this case the domain propagates unperturbed. Row (b) shows the material after poling the dashed region, which then acts to pin the propagating domain. Reproduced with permission from Nature Nanotech. (2013), DOI: 10.1038/NNANO.2013.86. © 2013 Macmillan Publishers Ltd.
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