Metallic Glass Yields Secrets Under Pressure

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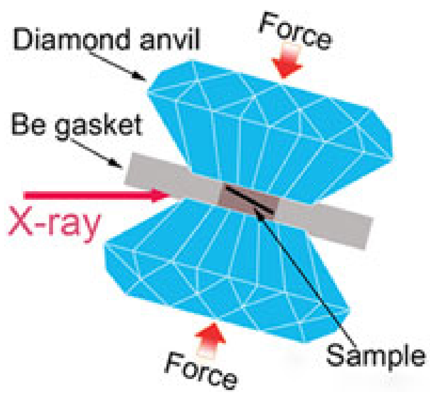

Diamond anvil cell used for high-pressure experiments.

(PhysOrg.com) -- Metallic glasses are emerging as potentially useful materials at the frontier of materials science research. They combine the advantages and avoid many of the problems of normal metals and glasses, two classes of materials with a very wide range of applications. For example, metallic glasses are less brittle than ordinary glasses and more resilient than conventional metals. Metallic glasses also have unique electronic behavior that scientists are just beginning to understand.

In a new study, scientists at the Carnegie Institution used high pressure techniques to probe the connection between the density and electronic structure of a cerium-aluminum metallic glass, opening up new possibilities for developing metallic glasses for specific purposes.

"High pressure is an extremely powerful tool for understanding these materials," says Ho-kwang Mao of Carnegie's Geophysical Laboratory, a co-author of the study published in Physical Review Letters. "Pressure can cause changes in their properties, such as their volume or electronic behavior, which in turn tells us about their structure at the atomic scale. The more we know about the structure, the better we can predict their properties and more quickly we can develop new materials."

Unlike ordinary metallic materials, which have an ordered, crystalline structure, metallic glasses are disordered at the atomic scale. This disorder can actually improve some properties of the material, because boundaries between crystal grains are often sites of weakness, leading to breakage or corrosion. Metallic glasses can therefore have superior strength and durability as compared to other metals. The disordered structure also makes metallic glasses highly efficient magnets because it lacks the kinds of defects found in crystalline metals.

Density is a property that can be altered by subjecting a material such as glass to high pressure. But unlike other glasses, which reduce their volume under pressure by rearranging their atoms to take up less space, metallic glasses have a structure in which the atoms are already closely packed. For this reason, researchers previously thought that metallic glasses could not be converted into denser phases. But in 2007 two teams made the surprising discovery that cerium-rich metallic glasses did in fact become denser at high pressure. Theorists suggested that the volume collapse happens through changes in the electronic structure of the cerium atoms in which electrons bound to specific atoms under low pressure become "delocalized" (that is, free to move among the atoms) under high pressure. This causes the bond between atoms to shrink, allowing them to pack even more closely. Until now, however, there has been no direct experimental evidence for this transformation.

The research team, led by predoctoral fellow Qiaoshi Zeng of Carnegie's

HPSynC (also a graduate student at Zhejiang University, China) with other co-workers from the Geophysical Laboratory, Zhejiang University, Stanford University and SLAC used a combination of in-situ high pressure synchrotron x-ray absorption spectroscopy and diffraction techniques to observe the electronic transformation in a cerium-aluminum metallic glass ($Ce_{75}Al_{25}$). The researchers used this glass because its high cerium content made the electronic transformation easier to detect. The experiments showed that at high pressures (between 1.5 and 5 gigapascals, equivalent to 100 to 360 tons per square inch) the volume of the glass decreased by close to 9%. At the same time, x-ray absorption spectra revealed that electrons in the cerium atoms known as 4f electrons did become delocalized, as predicted.

"This result confirms that the volume reduction is due to changes in electronic properties, and shows the key role cerium plays in the phase change." says Mao. "We may find similar transformations in other densely packed metallic glasses that contain cerium or similar rare earth metals. This is important because with the phase change the glass becomes a new material with new properties. It opens up possibilities for optimizing these materials and for fine-tuning their physical and electronic properties for a variety of applications."

Provided by Carnegie Institution