Compression of metallic glasses sheds light on phase transitions

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Scientists at the U.S. Department of Energy's Argonne National Laboratory have identified an unusual variation in the compressibility of an unusual class of metals in research that may shed light on the electrodynamics of amorphous materials.

Using high-energy X-rays produced by Argonne's Advanced Photon Source (APS), researchers from Argonne, the Carnegie Institution of Washington and the International Center for New-Structured Materials at Zhejiang University discovered an unusual change in the bulk modulus of lanthanum/cerium-based bulk metallic glasses at a pressure of about 14 GPa, more than 100,000 times the pressure of Earth's atmosphere.

The bulk modulus of an object denotes how much its volume shrinks as the surrounding pressure increases; at pressures above 14 GPa, the samples began to shrink at slower rates than they had at pressures below the break.

This sudden change in compressibility may indicate the occurrence of an "amorphous-to-amorphous" phase transition in these types of materials. Amorphous solids, of which metallic glasses are one example, have long confounded scientists who seek to characterize them. Unlike crystalline solids, which possess a regular long-range atomic order, amorphous materials consist of atoms arranged rather randomly with only short-range order, making their behavior much harder to predict, said Argonne physicist Yang Ren, who worked on the project.

"It's very difficult to get an amorphous form for metals – they love to crystallize," said Guoyin Shen , another physicist on the project. "Just being able to synthesize a metallic glass larger than 10 millimeters is an accomplishment."

While scientists have an easy time detecting amorphous-to-crystalline phase transitions, like water freezing into ice, the natural disorder of the atomic structure of metallic glasses had precluded them from seeing amorphous-to-amorphous transitions until very recently.

Even those physicists who believe that they have observed an amorphous-to-amorphous transition have not yet explained the mechanisms that underlie the transformation, Ren explained. "We know quite a bit about phase transitions in crystalline materials, but for amorphous material it gets quite complicated. You have to ask, 'just how do you define a phase?'"

In order to answer this question and to explain the bulk modulus discontinuity, the researchers looked for the cause on the atomic level. Even if they are not visible to the naked eye, pressure-induced phase transitions in amorphous materials at high pressure often produce a change in the number of atoms that surround the central atom, known as the atom's coordination number.

However, the experiments at the High-Pressure Collaborative Access Team (HPCAT) APS beamline showed that no coordination change had occurred, leaving the research team with one other plausible explanation: the pressure engendered a sudden reconfiguration of the electrons that surround each atom in the material. "For decades," Shen said, "people have been able to study the long-range order in materials at high pressures, but we have now begun to study short-range order as well."

"If this kink is caused by electron reconfiguration," he said, "we can come up with a recipe that makes use of that type of change in the next phase of the research. This discovery is significant because it provides us with important information about how to work with a poorly understood, but widely used, class of materials."

Applications of bulk metallic glasses include recording heads, sensors and transducers, motors, sports equipment and power transformer cores. In general, the superior fracture strength and toughness, the excellent corrosion and wear resistance, and improved plasticity of bulk metallic glasses may lead to more applications in structural materials, electronic products, medical, defense and security systems in the future. The lanthanum/cerium-based metallic glass, due to its superplastic behavior at low temperatures, could be used for stamps, Shen said.

Results of the research, which was funded by DOE Office of Basic Energy Sciences, were published in the August 21 issue of the *Proceedings of the National Academy of Sciences*.

Source: Argonne National Laboratory