Simulations reveal formation of some glassy materials like the setting of a bowl of gelatin

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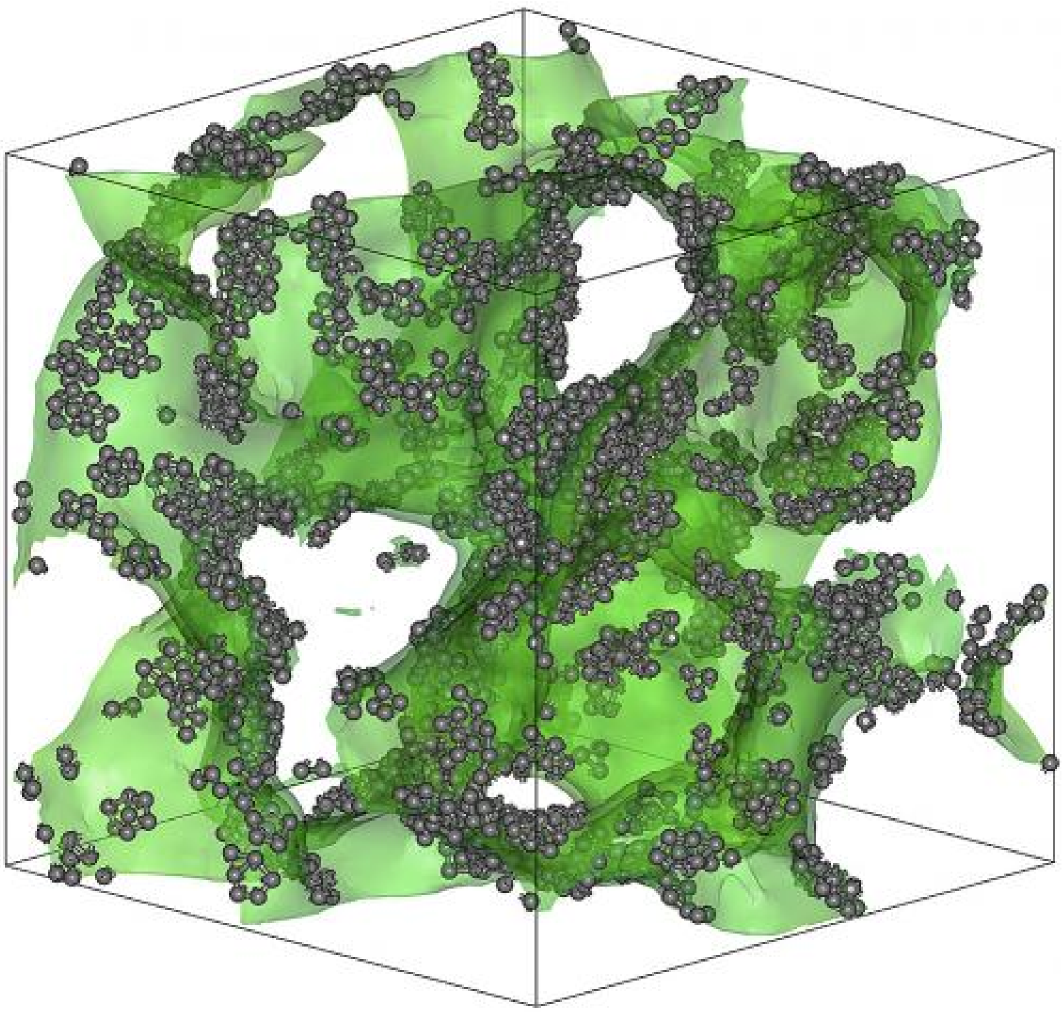

In a 50/50 mix of copper and niobium, regions that are richer in copper separate from regions that are richer in niobium. The interface between these two kinds of regions forms an irregular sponge-like surface, shown in this visualization in green. While most of the material is disordered (making it a glass), small collections of atoms at the boundary zone (shown in gray) form a stiff interconnected network, giving the material greater strength. Credit: Researchers

Gelatin sets by forming a solid matrix full of random, liquid-filled pores—much like a saturated sponge. It turns out that a similar process also happens in some metallic glasses, substances whose molecular behavior has now been clarified by new MIT research detailing the "setting" of these metal alloys.

The research is published this week in the journal *Physical Review Letters*, in a paper co-authored by assistant professor of materials science and engineering Michael Demkowicz and graduate student Richard Baumer. It addresses one of the "grand challenges" in physics, Demkowicz says: understanding what happens during what is known as the "glass transition" in materials, when their molecular structure settles into a disordered, yet solid, state.

"It was a serendipitous discovery," Demkowicz says, after Baumer "started out working on something completely different, studying the radiation response of amorphous metallic alloys." But in the course of that research, while conducting simulations of the behavior of these alloys, Baumer found something unexpected: a series of brief events in which tiny pockets of the alloyed metals melted and then solidified again.

Certain metallic alloys are known to form glasses—materials in which the atoms are distributed in a disordered way (unlike crystalline metals, which form perfectly regular arrays). While the alloy Baumer was studying was not of this type, its behavior provided hints that it might be capable of forming glasses.

The alloy, a 50/50 blend of copper and niobium, is "unlike other glass-formers," Demkowicz says: Normally its two constituents are like oil and water, and don't mix. (Typically, alloys that form glasses are composites of materials with a strong affinity for one another.)

But as the copper-niobium blend is quenched—that is, cooled quickly to below its melting point—a brief phase-separation occurs, then suddenly stops. But instead of separating out into adjacent, pure crystals of the two components, the alloy's structure remains disordered. "There are regions enriched in copper, and regions enriched in niobium, and interfaces between them," Demkowicz says. The regions themselves are too small to allow for the formation of a crystalline structure: "You can't make a perfect repeating structure out of any of them."

The boundary between the copper-rich and niobium-rich zones turns out to be crucial. This zone is similar to the spongelike structure that gives gelatin its stiffness, even though gelatin is mostly liquid. In this case, the pockets between the boundary regions are initially also liquid, but gain strength from the framework around them.

This "gelation" process, Demkowicz says, "may be more common than people think." As a result, this work could lead to reevaluation of a variety of metal alloys not previously considered good candidates for glass formation.

While the work is so far theoretical, Demkowicz says that this better understanding of the formation process may improve the mechanical properties of glasses—such as by creating new glass materials whose brittleness is minimized. "This may be a new way of controlling the distribution of components" within glass, he says.

Evan Ma, a professor of materials science and engineering at Johns Hopkins University who was not involved in this research, says, "Their findings in this metallic system are remarkably similar to gelation processes in polymeric and colloidal gels, and thus point to significant common features that bridge different kinds of amorphous materials and glasses." Yunfeng Shi, an assistant professor of materials science and engineering at Rensselaer Polytechnic Institute, adds that the work could lead to "understanding of the commonality in glass transition among all glass-formers."

More information: Glass Transition by Gelation in a Phase Separating Binary Alloy, *Physical Review Letters*.
prl.aps.org/abstract/PRL/v110/i14/e145502

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