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Chris Patrick

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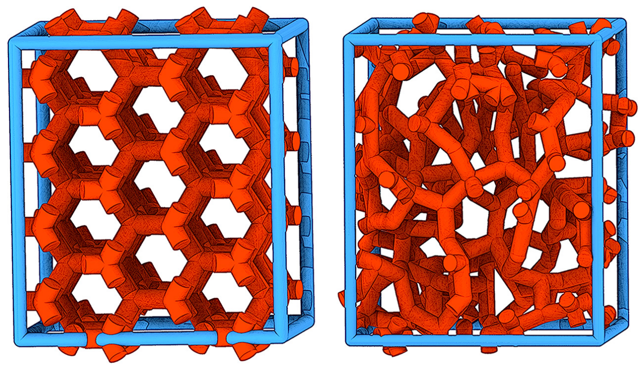
Computer simulations of supercooled liquid melts of binary alloys advance the characterization of amorphous materials.



Materials science struggles to connect the properties of amorphous materials, such as glass and many plastics, to their atomic structure, which lacks long-range order.

At low temperatures, most amorphous materials consist of a large number of diverse low energy local structures. However, Pedersen et al. identified a new class of exceptional amorphous materials. This potentially large group of metallic alloys exhibit a small number of stable local crystal-like arrangements at low temperatures, similar to crystalline materials.

“This result opens up the fascinating prospect of developing an intelligible account of amorphous structure, at least in this class of simple amorphous materials, based on structural motifs from well-studied crystal structures,” said author Peter Harrowell.

Using computer simulations of supercooled liquid melts of binary alloy, the authors determined that a significant portion of the liquid demonstrated a crystal-like structure, specifically a Laves structure.

Typically, even a tiny amount of added crystallinity rapidly crystallizes a supercooled liquid. The presence of crystal-like structure in the liquid alloy, however, did not induce such an instability. The authors determined that this was because the complexity of the Laves crystal structure permits the formation of stable partial unit cells without the formation of complete unit cells. This stability is what allowed the liquid to “borrow” crystal structure without fully crystallizing.

“With this new structural insight, we will better understand why some materials form amorphous solids when cooled while others crystallize, why some amorphous materials are brittle when strained while others are ductile, and how the distinction between liquid and crystal structures can be blurred by this borrowing of structure by liquids from crystals,” Harrowell said.

Source: “How a supercooled liquid borrows structure from the crystal,” by Ulf R. Pedersen, Ian Douglass, and Peter Harrowell, *Journal of Chemical Physics* (2021). The article can be accessed at https://doi.org/10.1063/5.0033206.