What crystal-like glass under pressure can tell us about atomic ordering

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Topological ordering in a fishing net. Credit: Dr. Qingyang Hu

Glass was among the most expensive crafting materials before the invention of glassblowing techniques. An ancient recipe for making glass is as simple as annealing a molten mixture of silica sand and chemicals in the right proportion.

Made from crystals such as silica, the major difference between glass and crystal is the way the atoms pack together, which is called ordering. Quartz silica atoms are packed to occupy the corners of a honeycomb-like structure known as a hexagonal lattice by crystallographers. In general, atoms in crystals are packed using a unique ordering, while glass lacks such ordering.

This simple division between crystal and glass has seen many exceptions nowadays. By examining ordering, scientists have discovered new materials that exist between crystal and glass. The most famous one is probably the quasicrystal, which won the Nobel Prize in Chemistry in 2011. A quasicrystal has a crystal-like ordering in the short range, but such ordering is not periodic. Another good example is "pressure-to-make" glass. By compressing silica or silica-like materials like berlinite above 200,000 atmospheres, one can create materials that appear to be glass. This approach to making glass requires high pressure rather than heating.

"The pressure-to-make glass is not real glass, but a kind of material in between crystal and glass," said Sheng-cai Zhu, an associate professor of Sun-Yet Sen University and also an alumnus of the Center for High Pressure Science and Technology Advanced Research (HPSTAR).

"We compress a piece of berlinite to make glass. After removing pressure, it reverts to the crystal berlinite. This memory effect is triggered by the hidden topological ordering in berlinite," added Qingyang Hu, staff scientist at HPSTAR.

In fact, the memory effect of berlinite was observed by Kruger and Jeanloz in 1990, but its origin is still an arguable topic. The topological ordering is more resilient than crystal ordering. Similarly, you may fold, stretch or distort a fishing net such that it looks likes a muddle. But it is always possible to recover it through unfolding or withdrawing the force, unless you break up the net or cut a hole. The mesh of the fishing net is analogous to the topological ordering that maintains its shape.

"I've been studying pressure-to-make glass since my Ph.D., and till now we could describe it in detail. From quartz, coesite to quartz-alike berlinite, the topological ordering may exist in many known 'glassy' materials," said Qingyang. In fact, pressure-to-make glass is better regarded as imperfect crystal. Unlike perfect crystals, such ordering is propagated along specific directions. Observing from other directions may only reveal glass-like structural features.

"We employ a high-dimensional neuro-network energy potential to represent the structures of berlinite under pressure. The potential acquires enough accuracy from machine learning and is also computationally affordable. We've searched hundreds of thousands of structures to cover every possible structural change of berlinite under pressure," said Dr. Zhu. After collecting those structures, they constructed a full potential energy surface. It was then possible to trace the motion of atoms in berlinite through the established topological relation. The same technique can be introduced to a wide range of systems.

The findings, published in the *Journal of the American Chemical Society*, may raise some interesting perspectives in describing glass. Researchers have found hints of orderings in glass, but they are limited to relatively short length scales, e.g., the size of a cluster of atoms at the longest. The topological ordering can be regarded as long-range ordering, which extends to the bulk material. By identifying long-range ordering in glass, scientists may further reveal the enigma of glass formation and explain how atoms are bonded together in nature.

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