Researchers find “a touch of glass” in metal

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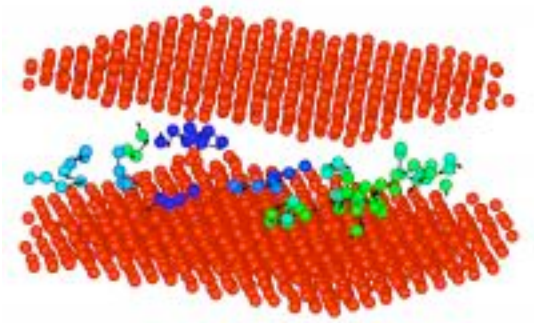
Metals and ceramics have more in common with glass than has been previously recognized, a new study indicates.



The findings could lead to better predictions of how many industrially valuable materials behave under stress, according to the scientists who carried out the research, from the U.S. National Institute of Standards and Technology.

Most metals and ceramics used in manufacturing are known as polycrystals. The steel in a bridge girder, for instance, is formed from countless tiny metal crystals that grew together in a patchwork as the molten steel cooled and solidified. Each crystal, or “grain,” is very orderly on the inside, but in the thin boundaries it shares with the grains around it, the molecules are disorderly.

Because these grain boundaries profoundly affect the mechanical and electrical properties of polycrystalline materials, engineers would like a better understanding of grain boundaries' formation and behavior. Unfortunately, grain boundary formation in most technically useful metals has eluded efforts to observe it for a century.

“You'd like to have simple engineering rules regarding how a material's going to break,” said materials scientist Jack Douglas at the institute. “For example, corrosion typically travels along grain boundaries, so polycrystals usually fracture along them. But metals melt and deform at very high temperatures, so observing them under those conditions is a challenge.”

While some scientists had speculated that the molecules in grain boundaries behave similarly to the way molecules do in glass-forming liquids, whose properties are well understood, none had found conclusive evidence to back up such a claim.

That started to change when theorist James Warren at the institute saw a conference presentation by the University of Alberta's Hao Zhang concerning some odd “strings” of atoms in his simulation of grain boundary motion using a simulation technique. The collective atomic behavior observed in grain boundaries reminded the team of prior findings about glass-forming liquids, whose atoms also form strings.

The team later found that the strings of atoms arising in grain boundaries are strikingly similar in form, distribution and temperature dependence to the string-like collective atomic motions generally found in glass-forming liquids—and that properties for both types of substances change with temperature in virtually the same way.

“All the important qualities relating to atomic motion in both of these types of materials—the development of these string-like atomic motions, or the amplitude [size of the vibrations] at which their atoms rattle—are strikingly similar,” Douglas said. “For all intents and purposes, grain boundaries are a type of glass.”

He added that the findings could permit progress in predicting the failure of many materials important in construction and manufacturing and could improve our understanding of how crystals form boundaries with one another.

Image: Between a polycrystalline material's grains (saffron layers) exist disorderly areas called grain bound aries, the behavior of which has been difficult tounderstand. The green and blue objects in the boundary are string-like collec tions of atoms that scientists have found behave like *glass-forming liquids, a similarity that should help scientists analyze a wide range of materials. (Credit: NIST)*