Researchers gain new insight into strength of crystalline industrial materials

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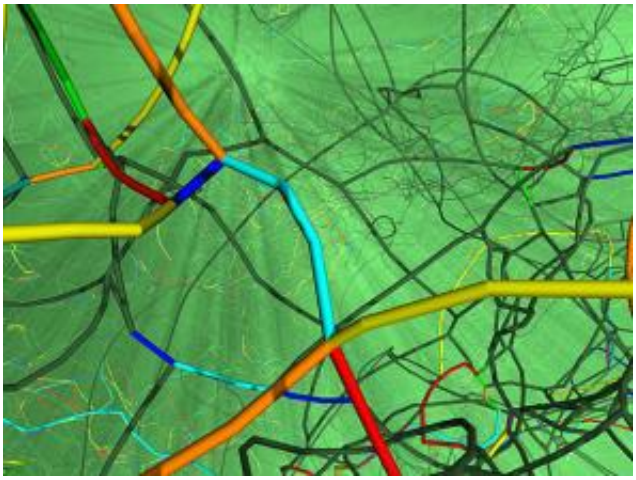

A computer graphic shows defect lines in a crystal. In the foreground, four different types of lines join together to form a "multi-junction," a previously unrecognized microstructure imparting strength to materials

A team of 11 researchers, including 10 at Lawrence Livermore National Laboratory and one at Stanford University, has gained a fundamental new insight into the physical strength of crystalline materials, which perhaps surprisingly include the industrial mainstays of aluminum, iron, gold and silicon. Findings of the study, which was led by Lawrence Livermore researcher Vasily V. Bulatov, appear in the April 27 issue of the journal *Nature*.

This is very fundamental research," says Stanford mechanical

engineering Assistant Professor Wei Cai, who developed computer simulations of crystals at the atomic scale that helped confirm the study's counterintuitive finding that crystals gain strength from a complex intersection of dislocations in their structure. While many solids do not look like the crystals of everyday experience (for example, table salt), most solids are in fact crystalline in that their atoms are arranged in a regular lattice.

A useful, if imperfect, analogy that explains the new research is traffic gridlock. Think of two intersecting streets as intersecting planes in a crystal. When the cars on those two streets become gridlocked, it's bad enough, but imagine now a third street (or plane of the crystal) cutting through the intersection on a diagonal. The more streets leading into the intersection, the more tangled traffic can become. Similarly, more intersecting dislocations on more planes mean a stronger tangle within the crystal.

Accurate simulations are especially important in the tiny realms of nanotechnology and microelectromechanical systems, where direct experiments to gauge material strength are difficult to perform. "Ultimately, as we gain further understanding along these lines, this [knowledge] could be used to make stronger materials," Cai says.

An ideal crystal, which is a stack of planes of atoms, would be as orderly as a lattice made out of Tinkertoys. But all real crystals have defects, which are borders between areas in the planes of the crystal that shift around in different directions as a result of some outside pressure or stress. These shifting borders manifest themselves as lines that wind through the crystal like veins through marble. Since the 1930s, scientists have suspected that at least simple intersections between two defect borderlines influence material strength, but they did not know much about how.

"There is this fundamental connection between defects and strength, but no one had really made that quantitative," Cai says. "That [connection] has been really a triumph of ours over the last few years. Through computer simulation, we have seen how this defect network evolves."

Through not only such simulations but also direct physical observations in a real crystal of molybdenum, Bulatov's team has shown that previously unnoticed intersections of several defect lines, called multi-junctions, give crystals much greater strength than intersections of just two lines. The reason why more complex intersections give crystals greater strength is that they are a product of more planes getting in each other's way, hindering further shifting within the planes. Also, the formation of multi-junctions is a process that removes energy, which helps the local borders of these areas settle.

Understanding nanoscale materials

An obvious goal of this research is to be able to predict the strength of materials. Another, longer-term goal is to devise entirely new materials with desirable properties. At the macroscale of bridges and car parts, engineers have long used experiments and empirical measurements to assess material strength, Cai says. At everyday scales, a fundamental explanation down to the atomic level hasn't been necessary to assess materials or to make them useful for a variety of purposes.

But scientists and entrepreneurs are increasingly interested in creating devices and structures at scales of millionths to billionths of meters—the so-called "nanoscale." There, very little is known about material strength. In fact, much of the wonder regarding nanotechnology derives from the fact that at those dimensions, most materials behave very differently than they do at macro scales.

The greatest applicability of the Bulatov team's discovery, Cai says, will

be in giving engineers more systematic, predictive insight into the strength of nanoscale materials. The study does not give them all the tools they need, but it is an important advance.

"We are simplifying the situation by simulating a pure single crystal," he acknowledges. "But this is a first step."

Source: Stanford University, by David Orenstein