Study may expand applied benefits of super-hard ceramics

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A discovery reported in the August 5 issue of Science could speed the design of materials that approach the hardness of diamond yet remain supple enough to be worked like metal.

In a massive computer simulation involving 128 computer processors and nearly 19 million atoms, materials scientist Izabela Szlufarska of UW-Madison and colleagues at University of Southern California demonstrated the precise atomic mechanisms that explain why "nanostructured" ceramic materials-some of the hardest substances known-also exhibit unusual pliability.

Unlike other exceptionally hard materials, these advanced ceramics tend to bend rather than break, meaning they could be shaped into extremely long-lasting yet lightweight parts for everything from automobile engines and high-speed machining tools to medical implants in the body.

But they are also notoriously difficult to engineer, because as their name implies they possess a grain structure that falls into the nano-size range of molecules and atoms.

"How to optimize their design is an open question," says Szlufarska, who is also a professor of engineering physics. "People have used a trial and error approach to make these materials harder. But there is still much to be understood as to why they are harder."

Simulations can help to answer this by providing a level of detail unavailable to experiments. Using atomic-scale simulations, the team observed for the first time how atoms moved and interacted as a super-hard ceramic deformed under stress. The advance has not only provided unprecedented insight into the properties of these materials, but also a tool that researchers can use to systematically nano-engineer them.

"This study is just the first step," says Szlufarska. "The goal is to design the strongest material possible."

The particular nanostructured ceramic Szlufarska focuses on, called nanocrystalline silicon carbide, is also exceptionally resistant to high temperature and radiation, which has NASA eyeing it as a coating for the space shuttle. Another important application is micro-electro mechanical systems (MEMS), tiny machines that are currently made of silicon.

"Today's MEMS can't have two surfaces rubbing against one another because the silicon is brittle and tends to break," says Szlufarska. "If we could instead make MEMS out of silicon carbide, the sky would be the limit in terms of applications."

Normal ceramics, like clays, become brittle when fired. But when ceramic is made from particles spanning mere atoms in diameter, the material exhibits dramatically improved ductility after bonding at high temperature and pressure.

This unusual combination of strength and suppleness is derived from the material's two-phase nature. In nanocrystalline silicon carbide, says Szlufarska, highly ordered, crystalline grains are surrounded by a more disordered, or amorphous, matrix of grain boundaries-much like tiny stones cemented by a semi-fluid mortar. And the volume of grain boundaries exceeds that in other nanostructured materials such as metals.

To understand, at the atomic scale, how nanocrystalline silicon carbide deforms under force, the team performed a simulation in which they pressed a tiny, virtual probe, called an indenter, into the material's surface and watched how the atoms moved in response. Initially, the grains deformed and then sprang back as a unit, an illustration of the material's hardness.

"At this point, the grains all moved together because the grain boundaries held them together

like glue," says Szlufarska.

But as the probe pressed deeper and exerted greater pressure, the researchers witnessed a surprising shift in the material's response. At a specific indentation depth, the grain boundaries began to yield, allowing individual grains to rotate and glide independently under the probe's force.

"Because the grain boundaries are flowing, the material is more ductile than normal ceramic would be," says Szlufarska. "And the grain boundaries initially take part of the deformation, so in essence they protect the grains from breaking."

In contrast, nano-structured metals go through no such phase; instead their grains take the brunt of the force, immediately developing defects, like tiny cracks, when the material begins to yield.

"Once defects occur in the system, the system is just weaker and it's going to break," says Szlufarska.

This crossover in response-from cooperative grain movement and hardness, to individual movement and ductility-is unique to nano-structured ceramics, she says. The researchers next want to learn how to control the crossover point so as to engineer greater hardness into nano-crystalline silicon carbide without compromising pliability. For example, they could vary the volume of the grain boundaries or the size of the grains. Impurities, or dopants, might also be added to the grain boundaries to make the material stronger.

Key to it all is the enormous computing power that allows scientists to simulate the material's atomic details.

"The experiments and devices have become smaller and smaller, while the simulations have grown larger and larger," says Szlufarska. "This is a unique time when the leading edge of materials design is exactly at the same length scale where fully atomic simulations are possible."

Source: University of Wisconsin