NRL scientists study cracks in brittle materials

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The Naval Research Laboratory (NRL) is part of an international team of scientists that is learning more about how cracks form in brittle materials. The team used both computer modeling and experimentation to investigate how cracks grow at low speeds in silicon. This information has potential applications in the development of a variety of materials ranging from armor to machine parts. The research team published their findings in the October 30th edition of *Nature*.

Using the computer simulations, the scientists began by studying the motion of atoms that takes place when cracks occur in brittle materials. The instabilities that occur when the crack grows at high speeds are well-known, and scientists have already made significant advances in understanding the origin of these kinds of cracks. However, instabilities had not been observed and studied in cracks that grow at low speeds.

Until recently, scientists studied cracks primarily by continuum mechanics techniques, but now advances in computer power have made it possible to simulate materials by describing the motion of each atom, rather than making the approximation that matter is continuous. While most simulations of cracks ignore the quantum-mechanical nature of the bonds between the atoms, the research team overcame this limitation using a technique called "Learn-on-the-fly" (LOTF).

This method allowed them to use a quantum-mechanical description of bonding near the tip of the crack, where it is needed, coupled to a large (on the atomic scale) region described with a faster but non-quantum-mechanical method. This combined description was essential for correctly predicting the motion of the crack tip. The simulations showed that even in a brittle material like silicon, rearrangements of atoms usually associated with ductile materials like metals can occur, but they remain trapped near the crack tip. The team developed a model that showed how these rearrangements at the crack tip could lead to macroscopic changes in the path of the crack, leaving behind ridges on the crack surface.

The research team also carried out single-crystal fracture experiments in which this instability was observed for the first time at a range of low speeds. They conducted experimental studies of the cracks at low speeds using a novel technique for applying very small but steady and well-controlled tensile loads. The surfaces left behind by the crack showed ridge-shaped features, very similar to those seen in the computer models. In a different crack orientation, experiments and simulations showed qualitatively different behavior.

In experiment, the crack was never able to propagate in a straight line – it was immediately deflected in different directions. The simulations showed that the structure of the crack tip caused this deflection. At extremely low speeds the crack grew by breaking bonds directly ahead of it in an orderly manner. Very soon, however, the crack sped up and began to break bonds on different crystal planes, causing it to diverge from its initial direction. For both of these instabilities, the simulation results and experimental observations indicate that more is happening at crack tips in brittle materials than previously suspected. Preliminary results indicate that these processes also occur in other materials, such as diamond and silicon carbide.

"We discovered that even in apparently simple brittle materials, complicated things can happen at the crack tip, and these atomic scale features can have macroscopic implications," explains NRL's Dr. Noam

Bernstein. "We hope that we can take advantage of this complexity to affect the way cracks grow, to design tougher and more robust materials."

Source: Naval Research Laboratory

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