Engineers uncover strength, toughness of hexagonal boron nitride

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Mechanical engineering professor M. Zubaer Hossain recently uncovered new insights about the strength and toughness of the 2D material hexagonal boron nitride. Credit: University of Delaware

From smartphones that bend to solar panels that wrap around houses, flexible electronics could make consumers very happy. But first, someone has to figure out how to make them. One important question is which materials are tough enough to maintain their electronic properties under such harsh conditions?

The answer could lie in 2-D materials, emerging materials that are single layers of atoms. 2-D materials have unique electronic properties, and they are expected to be useful in future electronic devices, nanocomposites, medical devices, photovoltaics, thermoelectrics and more. However, 2-D materials are brittle, which has the potential to limit their use.

At the University of Delaware, M. Zubaer Hossain studies ways to control the toughness and strength of 2-D materials and understand how they behave under loading conditions, such as being stretched, dropped, or bent. In a paper recently published in the *Journal of Applied Physics*, Hossain, an assistant professor of mechanical engineering, described new insights about the strength and toughness of the 2-D material hexagonal boron nitride, which is being investigated for use in part because it is a very good insulator.

"We wanted to understand strength and toughness in this brittle material and try to understand the behavior, strength and toughness along different directions," he said. "And what we find in this work is that they depend a lot on the loading direction."

Imagine that you hold a piece of paper face down in front of you. If you pull the right and left sides straight out, the paper will not bend, said Hossain. However, if you pull those edges downward, the paper will bend. "This same piece of paper has different mechanical properties depending on which direction you load it, and the same idea can be applied to 2-D materials," he said. When properties depend on the direction of load, the material is anisotropic.

Hossain sought to determine whether hexagonal boron nitride is anisotropic in regard to strength and toughness, and found that it is. He also wanted to understand how anisotropy in this material affects its electronic properties. If the electronic properties change, the result could pose a problem, or in some cases, an opportunity—a brand new functionality researchers can utilize. Either way, the scientists need to understand what's happening in order to maximize the use of the material.

Hossain also examined the material up to the maximum stress point to determine whether the loading direction affects failure.

"This work shows that the strength or the loading at which a material begins to fail depends strongly on the loading direction," he said. They also determined where the material would start to crack and how to determine the path of the crack. The path is predicted by the loading direction just as other properties are.

Hossain examined the material at the atomic scale—after all, every material is just a collection of atoms bonded through electronic interactions.

"There is an atomistic basis behind this differential response," he said. "The arrangement of atoms is different in different directions."

The bonds between atoms change and overlap, and electrons redistribute. This redistribution of electrons depends on the loading direction.

The atomic activity also helps to explain what happens when the material cracks. When the crack first starts by breaking a bond at the atomic scale, the event may not be detectable from macroscopic measurements, due to time involved in propagation of the stress signal. A broken bond can self-heal so long as the stress leading the bond rupture process stops increasing its intensity.

"Defects can self-heal if the loading is just right, but if you go past that critical point, it may not be recoverable anymore," he said.

Hossain's expertise in mechanical engineering allows him to take a unique approach to this research.

"Usually material properties and mechanisms at the quantum scale are studied by physicists or materials scientists, mostly under equilibrium or undeformed conditions that are far from the mechanical condition where the fracture processes start nucleating or propagating," he said. "Our research is interdisciplinary. We look at strength and toughness, which are traditional subjects of mechanical engineering, but we try to understand the strength and toughness from a quantum mechanical perspective, which is not usually the case for mechanical engineers. We try to build and apply physics-based analysis and tools to reveal nanoscale mechanisms and to identify their role on the mechanical behavior that we see at longer length scales."

These are increasingly important skills as devices become increasingly fast and sophisticated and consumers demand more versatile products.

"Nowadays, we need to be able to engineer behavior at the electronic level," he said.

More information: Tousif Ahmed et al. Strength and toughness anisotropy in hexagonal boron nitride: An atomistic picture, *Journal of Applied Physics* (2018). DOI: 10.1063/1.5052500

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