Graphene rips follow rules: Simulations show carbon sheets tear along energetically favorable lines

January 5 2012

Research from Rice University and the University of California at Berkeley may give science and industry a new way to manipulate graphene, the wonder material expected to play a role in advanced electronic, mechanical and thermal applications.

When graphene – a one-atom thick sheet of carbon – rips under stress, it does so in a unique way that puzzled scientists who first observed the phenomenon. Instead of tearing randomly like a piece of paper would, it seeks the path of least resistance and creates new edges that give the material desirable qualities.

Because graphene's edges determine its electrical properties, finding a way to control them will be significant, said Boris Yakobson, Rice's Karl F. Hasselmann Professor of Mechanical Engineering and Materials Science and professor of chemistry.

It's rare that Yakobson's work as a theoretical physicist appears in the same paper with experimental evidence, but the recent submission in *Nano Letters* titled "Ripping Graphene: Preferred Directions" is a notable exception, he said.

Yakobson and Vasilii Artyukhov, a postdoctoral researcher at Rice, recreated in computer simulations the kind of ripping observed through an electron microscope by researchers at Berkeley.

The California team noticed that cracks in flakes of graphene followed armchair or zigzag configurations, terms that refer to the shape of the edges created. It seemed that molecular forces were dictating how graphene handles stress.

Those forces are robust. Carbon-carbon bonds are the strongest known to man. But the importance of this research, Yakobson said, lies in the nature of the edge that results from the rip. The edge of a sheet of graphene gives it particular qualities, especially in the way it handles electric current. Graphene is so conductive that current flows straight through without impediment – until it reaches the edge. What the current finds there makes a big difference, he said, in whether it stops in its tracks or flows to an electrode or another sheet of graphene.

"Edge energy" in graphene and carbon nanotubes has long been of interest to Yakobson, who issued a paper last year with a formula to define the energy of a piece of graphene cut at any angle. In molecular carbon, armchair and zigzag edges are the most desirable because atoms along the edge are spaced at regular intervals and their electrical properties are well-known: Zigzag graphene is metallic, and armchair graphene is semiconducting. Figuring out how to rip graphene for nanoribbons with edges that are all one type or the other would be a breakthrough for manufacturers.

Yakobson and his team determined that graphene seeks the most energy-efficient path. The Berkeley team noticed that multiple cracks in a flake of graphene flowed strictly along lines that were at (or at multiples of) 30 degrees apart from each other.

"Graphene prefers to tear by expending the least amount of energy," Yakobson said. He noted the 30-degree separation between the angles that differentiate zigzag and armchair in a hexagonal graphene lattice.

To prove it, Artyukhov spent two months building molecular simulations that pulled virtual scraps of graphene apart in various ways. Depending on the force applied, a flake would rip along a straight line or fork in two directions. But the edges produced would always be along 30-degree lines and would be either zigzag or armchair.

"Basically, the direction of the crack in classical fracture theory is determined by the path it could take with the minimal cost in energy," Artyukhov said. "My simulations showed that under some conditions, this could be the case with graphene. It provided a pretty reasonable and clear and solid explanation for this unusual experimental thing."

Artyukhov found that pulling too hard on virtual graphene would shatter it. "Our main effort was to pull on it delicately enough that it has time to pick the direction it would prefer, rather than have a complete failure." He noted the simulations were much faster than rips that would happen in real-world circumstances.

Also surprising was the discovery that rips in graphene across grain boundaries follow the same rules. Tears do not follow the boundary, which would create energetically unfavorable edges, but pass through and switch to the most favorable direction in the new grain.

"The Berkeley folks didn't do controllable tears, but their work opens technological possibilities for the future," Yakobson said. "For electronics, you want ribbons that go in a particular direction, and this research suggests that this is possible. It would be a big deal.

"Think of graphene like a sheet of postage stamps: You apply a load, and you can tear the sheet in a well-defined direction. That's basically what this experiment reveals for graphene," he said. "There are invisible directions prepared for you."

More information: Read the abstract at pubs.acs.org/doi/abs/10.1021/nl203547z

Provided by Rice University