A new approach to finding and removing defects in graphene (w/ Video)

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Engineering professor Vivek Shenoy (right) and graduate student Akbar Bagri have explored the atomic configuration of graphene oxide, showing how defects in graphene sheets can be located and treated. Credit: Mike Cohea, Brown University

Graphene, a carbon sheet that is one-atom thick, may be at the center of the next revolution in material science. These ultrathin sheets hold great potential for a variety of applications from replacing silicon in solar cells to cooling computer chips.

Despite its vast promise, graphene and its derivatives "are materials people understand little about," said Vivek Shenoy, professor of engineering at Brown University. "The more we can understand their properties, the more (technological) possibilities that will be opened to us."

Shenoy and a team of U.S. researchers have gained new insights into these mysterious materials. The team, in a paper in *Nature Chemistry*, pinpoints the atomic configurations of noncarbon atoms that create defects when graphene is produced through a technique called graphene-oxide reduction. Building from that discovery, the researchers propose how to make that technique more efficient by outlining precisely how to apply hydrogen — rather than heat — to remove impurities in the sheets.

The sheets produced by graphene-oxide reduction are two-dimensional, honeycomb-looking planes of carbon. Most of the atoms in the lattice are carbon, which is what scientists want. But interwoven in the structure are also oxygen and hydrogen atoms, which disrupt the uniformity of the sheet. Apply enough heat to the lattice, and some of those oxygen atoms bond with hydrogen atoms, which can be removed as water. But some oxygen atoms are more stubborn.

Shenoy, joined by Brown graduate student Akbar Bagri and colleagues from Rutgers University and the University of Texas-Dallas, used molecular dynamic simulations to observe the atomic configuration of the graphene lattice and figure out why the remaining oxygen atoms remained in the structure. They found that the holdout oxygen atoms had formed double bonds with carbon atoms, a very stable arrangement that produces irregular holes in the lattice.

The oxygen atoms that form double bonds with carbon "have very low energy," Shenoy said. "They're unreactive. It's hard to get them out."

Now that they understand the configuration of the resistant oxygen atoms in the graphene, the researchers say adding hydrogen atoms in prescribed amounts and at defined locations is the best way to further reduce the graphene oxide. One promising technique, they write in the paper, is to introduce hydrogen where the oxygen atoms have bonded with the carbon atoms and formed the larger holes. The oxygen and hydrogen should pair up (as hydroxyls) and leave the lattice, in essence "healing the hole," Shenoy said.

Another approach is to remove the oxygen impurities by focusing on the areas where carbonyls — carbon atoms that are double-bonded to oxygen atoms — have formed. By adding hydrogen, the researchers theorize, the oxygen atoms can be peeled away in the form of water.

The researchers next plan to experiment with the hydrogen treatment techniques as well as to investigate the properties of graphene oxide "in its own right," Shenoy said.

Provided by Brown University

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