Pure nanotube-type growth edges toward the possible

6 December 2010

New research at Rice University could ultimately show scientists the way to make batches of nanotubes of a single type.

A paper in the online journal Physical Review Letters unveils an elegant formula by Rice University physicist Boris Yakobson and his colleagues that defines the energy of a piece of graphene cut at any angle.

Yakobson, a professor in mechanical engineering and materials science and of chemistry, said this alone is significant because the way graphene handles energy depends upon the angle -- or chirality -- of its edge, and solving that process for odd angles has been extremely challenging. But, he wrote, the research has "profound implications in the context of nanotube growth, offering rational ways to control their chiral symmetry, a tantalizing yet so far elusive goal."

Graphene is the single-atom-thick form of carbon that has become of tremendous interest for its potential to revolutionize electronics, optics, sensing and mechanical devices. Getting a handle on how this chicken-wire-shaped sheet of carbon atoms transports electricity has been the focus of intense study.

A sheet of graphene with zigzag or armchair edges squares up nicely. Zigzags are metallic, armchairs are semiconductors, and their atoms march in rank, evenly spaced, along the edges. A full 30 degrees of rotation separates one from the other.

But if the hexagons that make up a sheet are offset less than 30 degrees, atoms along a straight edge are unevenly spaced. "That makes analysis of the energy very complicated, because it's a large irregular structure. It's like noise," Yakobson said. "We've found a way to calculate the energies in these arbitrary angles," he said.

Yakobson and his co-authors, Yuanyue Liu, a graduate student in his lab, and Alex Dobrinsky, a former graduate student and now a postdoctoral researcher at Brown University, soon wondered how these findings applied to carbon nanotubes.

"There are as many ways to roll graphene into a nanotube as there are ways to roll a newspaper," Yakobson said. "The text can be aligned circumferentially or run straight along the axis or spiral at an angle."

While rolling a newspaper makes it hard to read, rolling carbon into a nanotube makes it relatively easy to "read" its type -- whether armchair or zigzag or some variation in between. What's impossible is controlling how the tube will roll. The process tends to be willy-nilly, leaving researchers the task of separating the nanotubes they need from the bulk through ultracentrifugation or other expensive procedures.

Yakobson said it would be a real game-changer if they could, for instance, grow batches of pure armchair nanotubes for use in such projects as armchair quantum nanowire (AQW). As imagined by Rice's late Nobel Laureate Richard Smalley, AQW could revolutionize the nation's power grid by carrying 10 times the amount of electricity as copper at only one-sixth the weight.

Yakobson's work may open a path to do so. A nanotube's chirality is determined by the combination of energies at play in its nucleation. "When it just emerges from the 'primordial soup' of carbon, the edge of the tube is essentially the same as the edge of graphene," he said.

"At first, it's just a cap. There's no stem yet. You're frying these caps on a skillet, and they're bubbling," he said. "The probability for different bubbles to emerge is controlled by energy around the edge."

The chirality of the nascent nanotube is set when atoms in the cap self-assemble a sixth pentagon (necessary to mold the hexagons into a dome). "That's where we can, I think for the first time, make some quantitative judgment about how different chiral structures emerge," Yakobson said.

It may be worth chemists' efforts to look more closely at the energy between the catalyst and carbon structure. "This has some promise," he said. "If you can tweak this preference, if you can change energy from the catalyst side, you change the preference of the chirality. And then you can tell these self-assembling carbons, 'Please dance this way; don't dance that way.'"

Yakobson hopes the new work helps solve the long-standing problem of nanotube chirality. "For almost two decades, we didn't have a good understanding of this process," he said. "Actually, we didn't have a clue. I'm not saying this is a full solution, but this is the first time we've seen a quantitative approach, an order in the seeming chaos. It just feels satisfying.

"The bottom line is simple. We figured out the graphene edge and bridged it to the holy grail of nanotubes, which is chirality control."

More information: Read the abstract at: prl.aps.org/abstract/PRL/v105/i23/e235502

Provided by Rice University