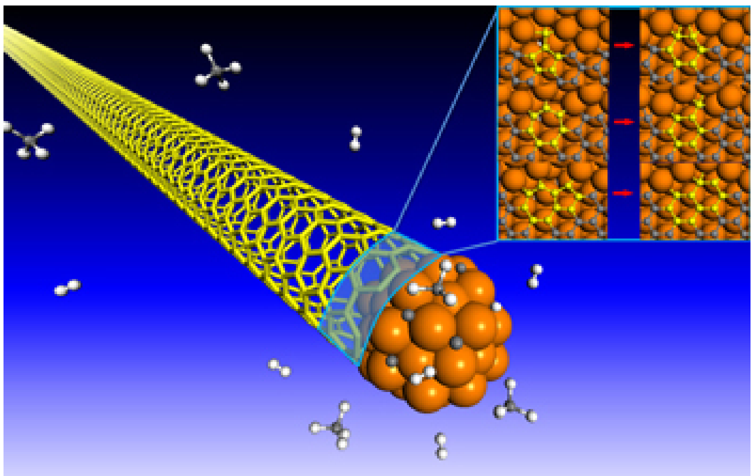
# In nanotube growth, errors are not an option

June 18 2012, BY MIKE WILLIAMS



Defects in nanotubes heal very quickly in a very small zone at or near the iron catalyst before they ever get into the tube wall, according to calculations by theoretical physicists at Rice University, Hong Kong Polytechnic University and Tsinghua University. Courtesy of Feng Ding/Rice/Hong Kong Polytechnic

(Phys.org) -- At the right temperature, with the right catalyst, there's no reason a perfect single-walled carbon nanotube 50,000 times thinner than a human hair can't be grown a meter long.

That calculation is one result of a study by collaborators at Rice, Hong Kong Polytechnic and Tsinghua universities who explored the self-healing mechanism that could make such extraordinary growth possible. That's important to scientists who see high-quality carbon nanotubes as critical to advanced materials and, if they can be woven into long cables, power distribution over the grid of the future.

The report published online by *Physical Review Letters* is by Rice theoretical physicist Boris Yakobson; Feng Ding, an adjunct assistant professor at Rice and an assistant professor at Hong Kong Polytechnic; lead author Qinghong Yuan, a postdoctoral researcher at Hong Kong Polytechnic; and Zhiping Xu, a professor of engineering mechanics at Tsinghua and former postdoctoral researcher at Rice.

They determined that iron is the best and quickest among common catalysts at healing topological defects – rings with too many or too few atoms – that inevitably bubble up during the formation of nanotubes and affect their valuable electronic and physical properties. The right combination of factors, primarily temperature, leads to kinetic healing in which carbon atoms gone astray are redirected to form the energetically favorable hexagons that make up nanotubes and their flat cousin, graphene. The team employed density functional theory to analyze the energies necessary for the transformation.

“It is surprising that the healing of all potential defects — pentagons, heptagons and their pairs — during carbon nanotube growth is quite easy,” said Ding, who was a research scientist in Yakobson’s Rice lab from 2005 to 2009. “Only less than one-10 billionth may survive an optimum condition of growth. The rate of defect healing is amazing. If we take hexagons as good guys and others as bad guys, there would be only one bad guy on Earth.”

The energies associated with each carbon atom determine how it finds its place in the chicken-wire-like form of a nanotube, said Yakobson, Rice’s Karl F. Hasselmann Chair in Engineering and a professor of materials science and mechanical engineering and of chemistry. But there has been a long debate among scientists over what actually happens at the interface between the catalyst and a growing tube.

"There have been two hypotheses," Yakobson said. "A popular one was that defects are being created quite frequently and get into the wall of the tube, but then later they anneal. There's some kind of fixing process. Another hypothesis is that they basically don't form at all, which sounds quite unreasonable.

"This was all just talk; there was no quantitative analysis. And that's where this work makes an important contribution. It evaluates quantitatively, based on state-of-the-art computations, specifically how fast this annealing can take place, depending on location," he said.

A nanotube grows in a furnace as carbon atoms are added, one by one, at the catalyst. It's like building the peak of a skyscraper first and adding bricks to the bottom. But because those bricks are being added at a furious rate – millions in a matter of minutes – mistakes can happen, altering the structure.

In theory, if one ring has five or seven atoms instead of six, it would skew the way all subsequent atoms in the chain orient themselves; an isolated pentagon would turn the nanotube into a cone, and a heptagon would turn it into a horn, Yakobson said.

But calculations also showed such isolated defects cannot exist in a nanotube wall; they would always appear in 5/7 pairs. That makes a quick fix easier: If one atom can be prompted to move from the heptagon to the pentagon, both rings come up sixes.

The researchers found that very transition happens best when carbon nanotubes are grown at temperatures around 930 kelvins (1,214 degrees Fahrenheit). That is the optimum for healing with an iron catalyst, which the researchers found has the lowest energy barrier and reaction energy among the three common catalysts considered, including nickel and cobalt.

Once a 5/7 forms at the interface between the catalyst and the growing nanotube, healing must happen very quickly. The further new atoms push the defect into the nanotube wall, the less likely it is to be healed, they determined; more than four atoms away from the catalyst, the defect is locked in.

Tight control of the conditions under which nanotubes grow can help them self-correct on the fly. Errors in atom placement are caught and fixed in a fraction of a millisecond, before they become part of the nanotube wall.

The researchers also determined through simulations that the slower the growth, the longer a perfect nanotube could be. A nanotube growing about 1 micrometer a second at 700 kelvins could potentially reach the meter milestone, they found.

**More information:** prl.aps.org/abstract/PRL/v108/i24/e245505

Provided by Rice University

Citation: In nanotube growth, errors are not an option (2012, June 18) retrieved 6 May 2024 from https://phys.org/news/2012-06-nanotube-growth-errors-option.html