Researchers Improve Understanding of Mechanical Properties of Carbon Nanotubes

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Carbon nanotubes are tiny garden-hose-like hollow tubes that have considerable promise for future applications such as nano-sized plumbing and nanolithography, and for the creation of numerous tiny devices such as mass sensors and actuators. Such applications require improved understanding of the mechanical properties of carbon nanotubes. Previous studies pointed out that carbon nanotubes behave like macroscopic elastic hoses similar to garden hoses made of rubber.

Now, researchers at the California Institute of Technology have discovered through computer simulations that the bending of carbon nanotubes occurs differently from that of their macroscopic counterparts in significant ways. Rather than buckling immediately and squashing the hollow inner channel, the results show, the cross-section can be gradually flattened--a finding that could lead to applications in controlling the flow of fluids through real carbon nanotubes. The results are published in the current issue of the journal *Physical Review Letters*.

According to Konstantinos Giapis, an associate professor of chemical engineering at Caltech and lead author of the paper, the size of nanotubes that he and postdoctoral scholar Oleksandr Kutana used for the simulation are between two and seven nanometers. Previous studies had focused on smaller nanotubes.

When the slightly larger nanotubes are "bent" sufficiently in the simulation, Giapis explains, the walls meet when the two sides are brought close enough together, and an atomic attraction known as the van der Waals force causes the atoms of each side of the wall to stick together. This effectively clamps off the nanotube, stopping any flow of material within it until the tube is re-straightened.

"The results show that there is an intermediate regime where you can adjust the nanotube cross-section to your liking," Giapis says. "This intermediate bending regime is important for nanofluidics."

Unlike a garden hose, however, nanotubes are tiny enough to feel forces that are inconsequential in the macroscopic world. Whereas the van der Waals force is much too weak to cause the walls of a garden hose to stick together, the force should be sufficient at the microscopic level to act as a "glue" to hold the walls of nanotubes together even after the load has been partially removed.

The end result, Giapis explains, is a new understanding of how it may be possible to control microflow in the emerging world of nanotechnology. "The initial study was to understand how nanotubes bend and how their bending differs from that of macroscopic objects, but there are also practical applications.

"For future microfluidic devices, you're going to need valves," he says. These devices could include everything from pharmaceutical-delivery systems to nano-inkjet printers.

The article is available on-line at link.aps.org/abstract/PRL/v97/e245501

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