Computer model predicts nanotube breaks

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In theory, carbon nanotubes are 100 times stronger than steel, but in practice, scientists have struggled make nanotubes that live up to those predictions, in part, because there are still many unanswered questions about how nanotubes break and under what conditions.

Because nanotubes are single molecules - about 80,000 times smaller than a human hair - finding out what makes them break involves the study of molecular bonds, atomic dynamics and complex quantum phenomena. The fact that there are hundreds of different kinds of nanotubes, sometimes with radically different properties, adds to the complexity.

A new computer modeling approach developed by materials scientists at Rice University and the University of Minnesota is allowing researchers to create a "strength map" that plots the likelihood or probability that a nanotube will break - and how it's likely to break - based on four key variables.

"Nanotubes break in one of two ways: the bonds either snap in a brittle fashion or they stretch and deform," said Boris Yakobson, professor of mechanical engineering and materials science and of chemistry. "We found that the underlying mechanisms that cause both types of breaks are each present at the same time. Even in a particular test, either type of break can occur, but we were able to map out a pattern - based on statistical probabilities - of what was likely to occur in a range of conditions for the whole catalog of nanotube species."

Yakobson's results appear in this week's online edition of the Proceedings of the National Adacemy of Sciences.

Carbon nanotubes are single molecules of pure carbon. They are long, narrow, hollow cylinders with walls just one atom thick. Scientists estimate SWNTs are about 100 times stronger than steel at one-sixth the weight. By comparison, Kevlar® -- the fiber used in most bulletproof body armor -- is about five times stronger than an equal weight of steel.

The precise diameter of a nanotube can vary from less than half of a nanometer - a billionth of a meter - to more than three nanometers. Nanotubes can also vary by the angle at which they are twisted. This is known as the chiral angle, and a useful analogy is a roll of gift-wrap paper. If the roll is rewound carefully, there is no overhang on either end. However, if the roll wound at an odd angle, excess paper hangs off at one end.

The chiral angle of nanotubes can vary from 0 degrees (no paper hanging off the roll) to 30 degrees, and tubes with different chiralities and diameters can have very different physical properties. Some are metals for instance and others are not.

In developing his computational model of nanotube breaking patterns, Yakobson consider four critical values: load level, load duration, temperature and chirality.

"The breaking mechanism for a particular nanotube depends to a great extent on its intrinsic twist called chirality," said co-author Traian Dumitrica, a former Rice postdoctoral researcher who is now assistant professor of mechanical engineering at the University of Minnesota. "Yet, temperature still influences the outcome. We were able to summarize the intricate dependence on parameters in a map , which stands as a striking example for the predictive power of simulations in materials science research."

Source: Rice University