Simulation demonstrates how exposure to plasma makes carbon nanotubes grow

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At the U.S. Department of Energy's (DOE) Princeton Plasma Physics Laboratory (PPPL), research performed with collaborators from Princeton University and the Institute for Advanced Computational Science at the State University of New York at Stony Brook has shown how plasma causes exceptionally strong, microscopic structures known as carbon nanotubes to grow. Such tubes, measured in billionths of a meter, are found in everything from electrodes to dental implants and have many advantageous properties. In principle, they have a tensile strength, or resistance to breaking when stretched, 100 times greater than that of a same-sized length of steel wire.

The tubes are also used in transistors and might someday replace the copper in computer chips. But before manufacturers can produce such nanotubes reliably, scientists must understand in more detail how they form.

The new findings, reported in the journal *Carbon* in February, contributes to an ongoing project at PPPL's Laboratory for Plasma Nanosynthesis that focuses on the growth of nanoparticles in plasmas. Inaugurated in 2012, the laboratory combines PPPL expertise in plasma science with the materials science capabilities of Princeton University and other institutions and is part of the PPPL Plasma Science and Technology Department headed by physicist Philip Efthimion. Lead principal investigator is physicist Yevgeny Raitses; co-principal investigators are physicists Igor Kaganovich, deputy director of the Theory Department at PPPL, and Brentley Stratton, head of the diagnostics division at PPPL.

Scientists performed computer simulations at Stony Brook showing that the plasma, a soup of atoms and electrically charged particles, can give carbon nanotubes a negative electrical charge. The simulations indicated that a negatively charged nanotube would bind carbon atoms from the surrounding environment longer and more strongly to the surface of the tube. And the longer an atom spends attached to the nanotube, the more likely it is to move down to a cluster of atoms, known as a metal catalyst, causing the tube to grow.

"In our research we found a significant increase in the time the carbon atoms spent on the tubes," said Predrag Krstic, research professor at the Institute for Advanced Computational Science and a paper coauthor. "As a consequence, there is a significant increase in the migration rate of the carbon atoms towards the metal catalyst."

Increased availability of high-speed computers has recently made such research possible. "What has changed is that these days computers are so fast that we can accurately model phenomena like what happens to nanotubes when immersed in plasma," said Kaganovich, also a coauthor.

Going forward, researchers plan to develop a more detailed model of how both boron-nitride and carbon nanotubes grow in a real plasma environment. Advanced computational power makes the development of these new models possible.

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