

# **Argonne theorist gains new insight into the nature of nanodiamond**

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The newest promising material for advanced technology applications is diamond nanotubes, and research at the U.S. Department of Energy's Argonne National Laboratory is giving new insight into the nature of nanodiamond.

Argonne researcher Amanda Barnard, theorist in the Center for Nanoscale Materials, is working with colleagues at two Italian universities who produced innovative diamond-coated nanotubes.

The diamond-coated tubes resemble a stick of rock candy, holding a layer of diamond 20 to 100 nm thick. A nanometer is one millionth of a millimeter. The period at the end of this sentence is about one million nanometers long. The technology in its fledgling state has already caught the eye of the electronics industry for the promise of ultra thin televisions with cathode ray tube-like quality picture at a fraction of today's current flat panel television costs.

Diamond offers an amazing array of medical and technological possibilities. Wire molecules can be attached to it and diamond has superior light emission properties. While diamond is an insulating material, the surface is highly electronegative. A nanodiamond coating consists of pure surface diamond. This gives a diamond coated nanowire conductance from the nanotubes and the superior conduction from the diamond. Add to this superior light emission properties and very low voltage requirements, and the possibility exists for very flat, low energy displays.

"By using a more efficient conductor, nanotubes, with a more efficient field emitter, in this case nanodiamonds, you get more efficient devices," said Barnard. "A lot of groups are looking for something better to make electronic displays out of, and this is just another candidate that looks very promising."

Researchers from the University La Sapienza and the University Tor Vergata discovered the ability for a nanotube to grow nanodiamond under certain conditions in 2004, but did not know the specifics of how the diamond grew. To better understand the conditions that brought them their discovery, researchers from the group brought their discovery to Barnard.

Barnard, a postdoc from the Royal Melbourne Institute of Technology University, published her original results on the modeling of diamond nanowires in the October 2003 issue of Nano Letters. Her theories earned her the recognition of the Italian group and she was approached in March of 2004 to help with calculations on their discovery.

"They could make them, but they couldn't understand exactly what was happening or how they were forming," said Barnard. "They knew what it was, they could characterize it, but they didn't know how the growth progressed."

Barnard calculated that during the process of etching – the term for the degradation of nanotubes – atomic hydrogen can change the hybridization of chemical bonds between carbon atoms of a nanotube.

"Traditionally in a hydrogen environment carbon nanotubes would fall apart and disintegrate, but something different was happening. We actually established that if the amount of hydrogen present [is in correct proportion], the defects that form will nucleate into diamond before there is a chance to etch."

These imperfections that form uniformly across the nanotube's surface allow for the bonding of diamond molecules, which then begin to grow the length of the tube. An added bonus property is that the end of the nanotube is coated with a thicker bulb of nanodiamond and upon formation the structures stand upright without manipulation.

Barnard is now on a fellowship at Oxford University, but is continuing to conduct research at the Center for Nanoscale Materials, now under construction. Barnard has great expectations for the opportunities the new center will open up for nanoscale research.

"I hope that the CNM will give me more opportunity to collaborate with experimental groups," said Barnard. "I am a great advocate of doing experimentally relevant theory, and the CNM will be a great place for doing that."

The Center for Nanoscale Materials at Argonne is being built with funding from the Department of Energy Office of Science and the State of Illinois, each of which is contributing \$35 million to construction and instrumentation of the facility.

Source: Argonne National Laboratory

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