

## PREDICTING PROPERTIES OF MATERIALS AND COMPOSITES: NANOTUBES

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Advances in theory, together with the availability of powerful computers, have made possible the prediction of the existence and the understanding of new materials from first principles. We report here the application of these methods to the study of a new class of nanostructure materials, the nanotubes.

Nanotubes are tubule structures which are typically several nanometers in diameter and hundreds of micrometers in length. In addition to the multi-wall tubes first discovered in the soot in the arc-discharge productions of fullerenes, single-wall tubes and ropes of close-packed single-wall tubes have been synthesized. These quasi-one-dimensional objects have highly unusual electronic properties (some are conductors, others are semiconductors or insulators). It is also possible to fill the nanotube with foreign materials, and to collapse the tubes into flat, flexible nanoribbons. In this talk, we present theoretical calculations on the structures and properties of the carbon nanotubes, and those of a new class of tubes made out of various combinations of B, C, and N atoms such as BN, BC<sub>3</sub> and BC<sub>2</sub>N. Because of their nanometer dimensions, these systems are predicted to have novel properties and yield unusual scientific phenomena. Calculations have been carried out to determine their stability, electronic properties, and the occurrence of chiral currents. The possibilities of making nanoscale devices with nanotube junctions have also been explored.

Carbon nanotubes, which are just rolled up graphite sheets geometrically, have generated intense experimental and theoretical interest since their discovery in 1991 [1]. Theoretical work has predicted that their properties would be variable; for example, that they would be metallic or semiconducting, depending sensitively on tube diameter and chirality. We show that different half-tubes may be joined with 5-member ring/7-member ring pair defects to form junctions [2]. Such a structure allows the formation of a metal-semiconductor Schottky barrier. The electronic density of states as a function of position shows

that this kind of junction is very similar to standard metal-semiconductor interfaces and, in this sense, is an atomic or molecular level device.

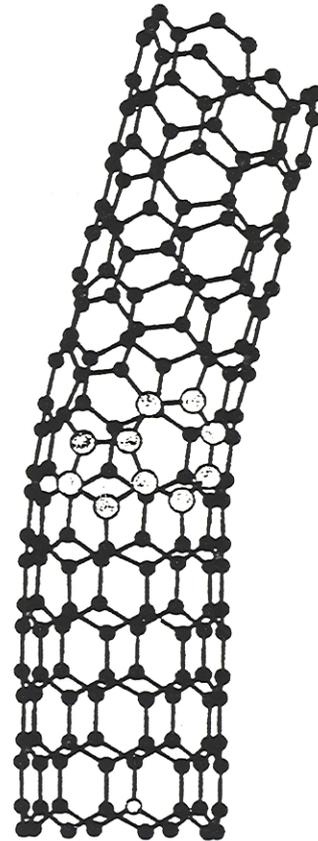


Fig. 1. Atomic structure of a metal-semiconductor nanotube junction.

Figure 1 illustrates a carbon nanotube junction with functionally different ends forming a metal-semiconductor Schottky barrier. One end of the tube has the carbon hexagons aligned in bands, and is therefore semiconducting, while the other end has a spiral structure which causes it to be metallic. In such a structure, higher energy electrons from the semiconductor half can flow "downhill" into the metallic half, but they cannot travel the other way, making it a atomic-scale diode.

Similarly, incorporating 7- and 5-member ring defect pairs into other carbon nanotubes are predicted to produce semiconductor-semiconductor and metal-metal junctions [2,3]. In the case of metal-metal nanotube junctions [3], theory predicts a new and unusual phenomenon which does not have an analog in bulk metal-metal contacts. Owing to the limited number of channels for electron conduction (because of the nanoscale dimensions) and the rotational symmetries of the tubes, symmetrically matched straight junctions often will not conduct because of the mismatch of the symmetry of the electron states. On the other hand, asymmetrically matched (or bent) junctions will conduct. This novel effect leads to the possibility of using this kind of junctions as nanoswitches or strain gauges [3].

Moreover, our theoretical calculations have shown that nanotubes may be made from boron nitride and other compounds such as  $BC_2N$  and  $BC_3$ , which are isoelectronic with graphite and also have similar hexagonal layered structures [4]. Unlike the carbon nanotubes, the boron nitride nanotubes are found to be widegap semiconductors, regardless of tube diameter and structural chirality. The  $BC_2N$  and  $BC_3$  nanotubes are also predicted to be semiconducting and could be doped with carriers. Following these predictions, Zettl's group at Berkeley [5] and several other groups around the world have succeeded in synthesizing this new class of nanotubes.

Because of their consistent semiconducting behavior, boron nitride nanotubes have great potential for nanodevice applications. Other novel predicted properties include the existence of chiral currents in the  $BC_2N$  nanotubes which would make them the world's smallest coils, or nanocoils [6].

Calculations and measurements have shown that carbon and BN nanotubes possess the world's highest Young's moduli among fibers. These materials thus may be useful as elements in composites.

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