Transport through mechanically deformed nanotubes

A. A. Farajian[1], B. I. Yakobson[2, 3], H. Mizuseki[1], and Y. Kawazoe[1]

[1]Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

[2]Mechanical Engineering and Materials Science Department, Rice University, Houston, Texas 77005-1892

[3]Center for Nanoscale Science and Technology, Rice University, Houston, Texas 77005-1892

The electronic/transport properties of carbon nanotubes, as well as their response to mechanical deformation, have been the subject of both theoretical and experimental studies recently. The results have shown promising features, which could be useful in nano-device applications. Our study focuses on the relationship between mechanical deformation and transport characteristics of carbon nanotubes. This has the potential of nano-electromecanical applications, in particular in nano-sensors.

We use a tight-binding model, with four orbital per atom, both to obtain the optimized structures of the nanotubes under deforming forces, and to calculate their transport properties. Three basic nanotubes configurations, i.e., metal, semiconductor and metal/semiconductor junction, with a diameter of about 8 angstroms and a rather long length of about 100 angstroms are used in our study. This reveals the dependence of the results on the electronic properties of the undeformed nanotubes.

Starting with the undeformed nanotubes/junctions, we first obtain the relaxed structures when the nanotubes are bent, with various bending angles. We check how the presence of intrinsic defects, such as pentagon-heptagon defects, affects subsequent deformations of the nanotubes, especially for larger bending angles.

The optimized structures are then used in calculating the electronic transmission coefficients corresponding to the electrons passing across the deformed region. This is done via the Green's function approach, in which the surface Green's functions of two semi-infinite undeformed nanotubes are attached to the Green's function of the deformed region. The Green's function of the whole system projected onto the deformed region is thus obtained, from which the transmission coefficient (and conductance) at any energy is derived. Next, a potential difference is applied to the deformed region, and the current-voltage characteristics are obtained. The I-V curves are then used to establish a correspondence between mechanical deformations and electronic transport of the nanotubes/junctions under consideration.

It is observed that there is indeed a correspondence between the bending angle and the current that is passing through the deformed tube. For example, the current passing through a (6,6) metallic tube with a bending angle of 180° at 2.0 V bias shows ~ 30% reduction as compared to the same tube at a bending angle of 120°.
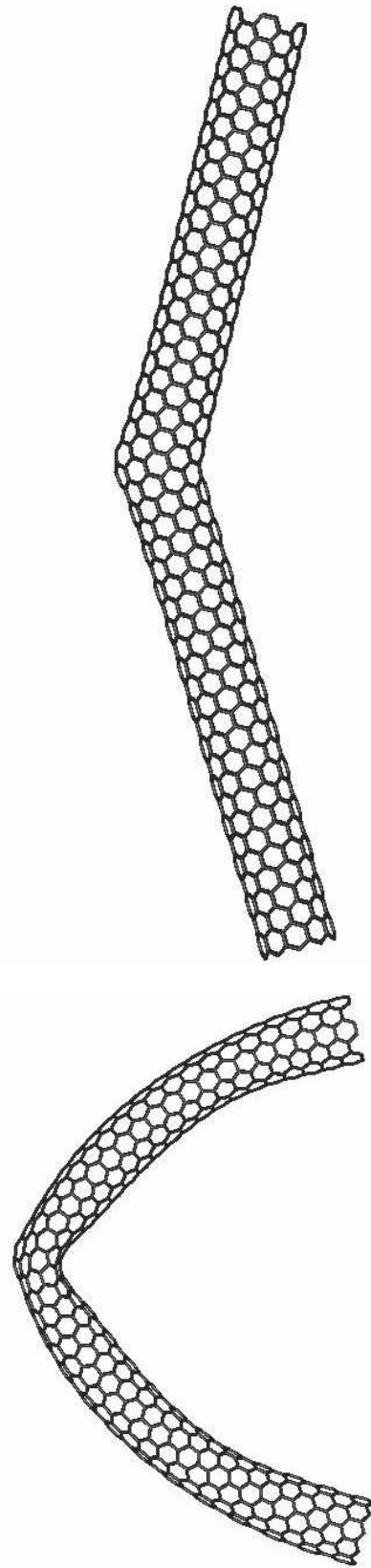

Fig. 1: Junction between a semiconducting (10,0) tube and a metallic (6,6) tube, with the intrinsic bending angle 30° (top) and the imposed bending angle 150° (bottom). The fully optimized structures are used in establishing a relationship between the mechanical deformations (e.g., bending angles) and the I-V characteristics of the junction.