EFFECTS OF MECHANICAL DEFORMATIONS ON THE ELECTRICAL PROPERTIES OF SINGLE AND MULTIWALL CARBON NANOTUBES

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Introduction

There is currently intense interest in the electrical properties of carbon nanotubes (CNTs). They can be metallic or narrow-gap or moderate-gap semiconductors depending simply on tube geometric characteristics, including diameter, chirality and distortions. Moreover conduction in defect-free CNTs is believed to be ballistic in nature, implying the absence of inelastic scattering and involving little energy dissipation. This peculiar electronic behavior, combined with high mechanical stiffness and strength as well as good thermal conductivity, make CNTs potential building blocks of a new, emerging carbon-based nano-electronic technology. To explore this exciting possibility, there has been a considerable amount of experimental and theoretical work. Progress in this field has been rapid, and already several prototypical devices have been constructed and demonstrated, including actuators, transistors and nano-switches. Most discussions of the electronic structure of CNTs assume perfect cylindrical symmetry, but this is somewhat of an oversimplification. High resolution images of CNTs often disclose structural deformations such as bent, twisted, or collapsed tubes. These deformations may develop during growth, deposition, and processing, or following an interaction with other CNTs, and with surfaces and surface features such as electrodes. These deformations break the tube symmetry, and a change in their electronic properties may result, depending on the distortions as well as the initial tube diameter and chirality. Despite the great interest in designing novel nano-structured devices, a sufficient understanding of the effects of mechanical deformations on the electrical properties of CNTs is far from being achieved.

In this work, we examine the electrical properties of mechanically deformed single-walled carbon nanotubes (SWNTs). A nonlinear structural mechanics based approach for modeling CNTs is used to determine the individual atom positions in the deformed configuration. The effect of mechanical deformation on the electrical transport properties of nanotubes is then studied using a tight-binding method. The success of

this modeling approach is verified by comparison with atomistic simulations of others available in the literature.

Modeling Procedures

An effective continuum/finite element approach (FE) is used for modeling the structure and the deformation of single and multi-wall carbon nanotubes CNTs [1, 2, 3]. Individual tubes are modeled using shell elements, where a specific pairing of elastic properties and mechanical thickness of the tube wall is identified to enable successful modeling with shell theory. An initial internal stress distribution through the thickness of the wall, due to the cylindrical nature of the tube, is incorporated. The effects of van der Waals interactions, crucial in tube/tube or tube/substrate interactions as well as in maintaining the interwall separation in MWNTs, are simulated by the construction of special interaction elements. This new CNT modeling approach was verified by comparison with MD simulations and high-resolution micrographs available in the literature [1, 2, 3]. Our technique has now been further enhanced to take into account the chirality of the CNT and to allow higher accuracy in modeling the deformation of small diameter SWNTs. Using quadrilateral shell elements, it is possible to create a FE mesh with hexagonal cells where the nodes correspond to individual atomic positions. The method allows the construction of FE models of CNTs of every type, including chiral ones. The atom positions in the deformed configuration are precisely determined using this approach, which then enables the effect of mechanical deformation on the electrical transport properties of nanotubes to be computed by a tight-binding (TB) method. The TB programs developed by Nardelli [4] and Nardelli and Bernholc [5] are used to perform density of state and quantum conductance calculations when given the coordinates of the atoms. The TB codes are based on the surface Green's function matching technique and the Landauer formula for coherent conductance. Infinitely long conductors or finite conductors spanning the distance between two leads can be investigated with a full sp^3, four-orbital, orthogonal TB model or a non-orthogonal TB model. For details on the quantum conductance calculations, the reader is referred to [4, 5].

Results and Discussion

Laterally Squeezed (8,8) SWNT

In Lu et al. [6], TB molecular dynamics and the Green's function method, are used to demonstrate that lateral squeezing of an armchair SWNT can be used to induce a metal-to-semiconductor transition (MST). They employed the four-orbital TB approach for investigations of both the mechanical analyses and the electronic transport properties. Here, we utilize our electro-mechanical approach to reproduce the Lu, et al. simulations of the effect of squeezing on the electrical properties of an (8,8) armchair SWNT. A schematic of the geometry and loading configuration is provided in Figure 1; for details on the simulations, the reader is referred to [6].

The SWNT is laterally squeezed between two identical rigid tips, each with a width of 0.580 nm, initially separated by 1.087 nm (the initial diameter of the SWNT). It

is well known that a perfect armchair (8,8) SWNT exhibits metallic behavior, as also found in the TB calculations of Figure 2 (a). When the separation between the two tips is reduced to 0.700 nm, there is a very small change in the conductance, Figure 2 (b).

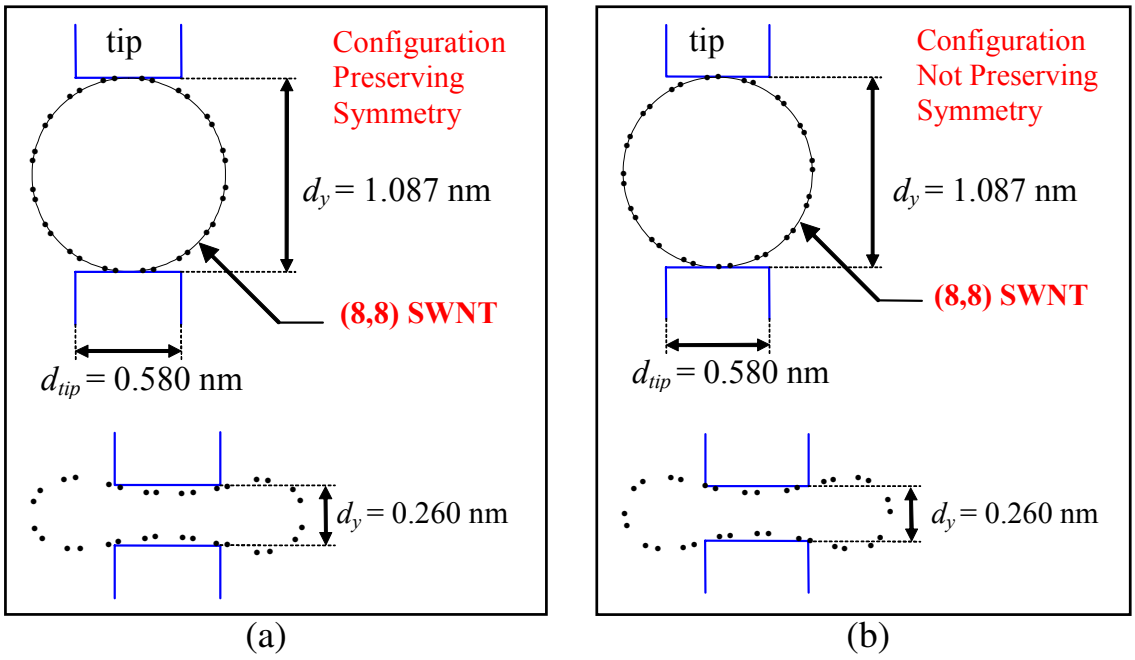
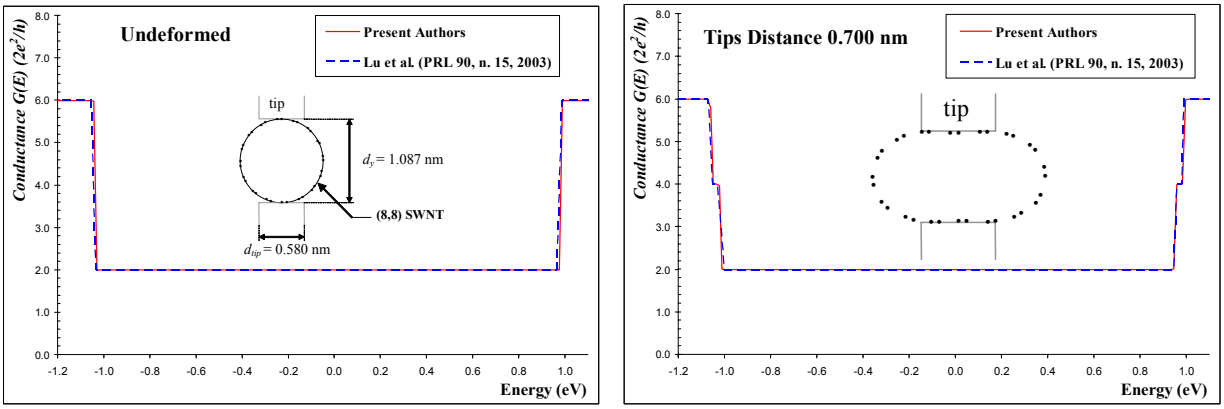


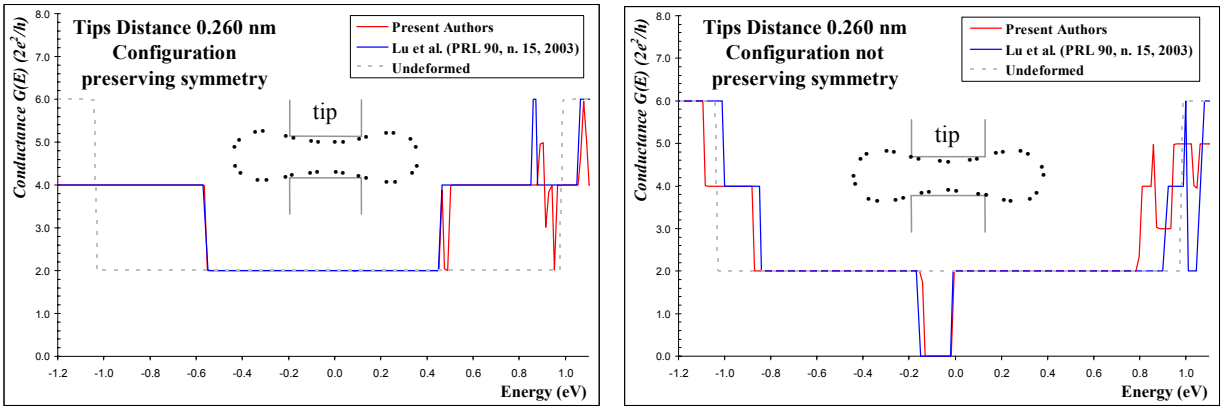
Figure 1. Initial and deformed configurations of an armchair (8,8) SWNT squeezed between two tips: a) configuration preserving vertical mirror symmetry; b) configuration not preserving vertical mirror symmetry.

But when the separation is further reduced to 0.260 nm, in addition to the strong change in the curvature of the walls, the orbitals on the opposite diameter start to overlap. At this level of deformation, an initial configuration that preserved the mirror symmetry with respect to the compression axis is found to exhibit an electronic behavior different than one where initial mirror symmetry of atomic positions was not prescribed. To show this dependence on initial configuration, two cases are investigated: one where atomic positions exhibit mirror symmetry about the tip centerline (the compression axis), and one where symmetry is broken by a rotation of the SWNT by 7.75 degrees, corresponding to Lu, et al. [5, figures 1 (c) and (e), respectively]. The effect on the conductance is notable as shown in Figures 3 (a) and (b): for a configuration preserving mirror symmetry, Figure 3(a), the CNT retains its metallic behavior, whereas in the configuration breaking symmetry, Figure 3 (b), a band gap is determined. The charge density plots reported in Lu, et al. [6, Figure 2] further emphasize these differences. It should be underlined that, with further squeezing, both tubes become semiconducting. Also, good agreement between our calculations and those from Lu et al. [6] is shown in Figure 3.



(a) (b)

Figure 2. Conductance of an armchair (8,8) SWNT squeezed between two tips in the: (a) undeformed configuration, and (b) when the two tips have a distance of 0.700 nm.



(a) (b)

Figure 3. Conductance of a squeezed armchair (8,8) SWNT when the two tips have a distance of 0.260 nm and: (a) the initial configuration preserves the mirror symmetry with respect to the direction of compression, (b) the initial configuration does not preserve mirror symmetry.

Conclusions

In summary, a previously established methodology for constructing FE-based nonlinear structural mechanics models of carbon nanotubes has been modified to take into account the chirality of the CNT and to allow higher accuracy in modeling the deformation of small diameter SWNTs. The technique enables providing individual atomic positions of deformed CNTs as input to an advanced and flexible tight-binding code in order to determine the electrical behavior in the distorted geometries. The accuracy of this modeling approach was verified by comparison with atomistic simulations available in the literature on the electrical transport properties of armchair SWNTs subjected to lateral squeezing.

Acknowledgements: This research was funded in part by the Cambridge-MIT Institute Project on Carbon Nanotube Enabled Materials, and in part by the AFOSR DURINT on Microstructure, Processing and Mechanical Performance of Polymer Nanocomposites Contract No. F49620-01-1-0477.

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