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Electronic Transport Properties of CNT Fibers

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INTRODUCTION

Carbon nanotube (CNT) fibers are promising in applications involving high strength and light weight conductors. Moreover, industrial-scale production of 30 m long fibers appears to be feasible [1]. The measured electrical resistivity of fibers are however considerably larger than that of individual CNTs. In fact, the fiber resistivity is $10^{-4}\Omega$cm, which is almost two orders of magnitude larger than that of copper. In this work we perform *first principles* calculations to determine the electronic and transport properties of defect free CNT fibers. This allows us to determine some underlying mechanism for such high resistivity and ways to decrease it so that CNT fibers compare better with copper.

METHODOLOGY

Our procedure to calculate transport properties of a CNT fiber consists of the following steps: *(i)* Determine the equilibrium distance between nanotubes in a bundle using density functional theory (DFT). *(ii)* The inter-tube distance obtained in *(i)* is used to construct junctions of two tubes as well as single fiber trajectories which consist of a number (N) of CNTs. *(iii)* We determine the inter-tube interaction Hamiltonian between two neighboring tubes by performing DFT calculations on a system of two adjacent tubes. *(iv)* The inter-tube Hamiltonian is treated as a perturbation to the ideal CNTs' Hamiltonians. *(v)* We calculate the conductance between two CNTs as a function of their overlap distance. *(vi)* We model transport through a single fiber trajectory in the phase decoherent limit by following reference [2]. *(vii)* We use the computed conductance in *(vi)* to derive the conductance through macroscopically large fibers and determine the limiting factors of fiber conductance.

RESULTS

Our calculations demonstrate that fibers are more stable compared to CNTs. In Fig. 1-a, we show the total energy (E_T) for an (8,8) CNT bundle as a function of inter-tube distance (d) and orientation angle (θ) between CNTs. The lowest energy configuration is obtained for $d = 3.07$ Å, with very weak rotational barrier. In Fig. 1-b, we also show the band-gap (E_g), which opens due to tube-tube interaction. At the equilibrium distance, $E_g \sim 50$ meV and its effect on transport is expected to be small at room temperature.

The inter-tube conductance oscillates as a function of overlap distance. When mirror symmetry is preserved and for tubes with similar chiralities, the conductance oscillates between 0 and $2G_o$. In Fig. 2, we present the (8,8)x(7,7) inter-tube conductance as a dotted line. If the tubes have different chiralities, Fermi wave vectors of the two tubes are different and this results in substantial conductance reduction. The inter-tube conductance between (8,8) and (12,0) CNTs is $\leq 0.01G_o$ as shown in Fig. 2. We also find that when mirror symmetry is broken, the conductance decreases. In Fig. 3, we show the inter-tube conductance between (8,8)x(8,8) CNTs, which undergoes damped oscillations. The zero-temperature conductance (transmission at E_F) is shown in Fig. 3 as a continuous line, which vanishes for large overlap distance. This is due to E_g formation and is demonstrated in the insets.

Our model for transport through a fiber trajectory is shown in Fig. 4-a. For a given number of CNTs, the conductance is independent of overlap length (L_{ov}) and bare CNT length (L_0), as shown in Fig. 4-b,c. However, the conductance is inversely proportional to the number of tubes. In the phase decoherent limit we determine inter-tube transmission coefficient, $T_a = \frac{(N-1)T}{1+0.5\times(N-2)T}$, where T is the total transmission coefficient through the trajectory. The calculated T_a values from all simulations are shown in Fig. 4-d and result in $T_a \sim 1.0$. Within this model, the fiber resistivity is estimated to be, $\rho \sim [\frac{1}{T_a} - 0.5] \times \frac{1}{l_0} \times 10^{-5}\,\Omega$cm, where l_0 is the average CNT length in μm. Using the computed value of $T_a \sim 1.0$ found in Fig. 4-d, we find that if the fiber is composed of short nanotubes (0.5μm) [1] the resistivity is $\rho \sim 10^{-5}\,\Omega$cm. This value is within the experimental range of Ref. [1]. However, if each CNT has a length of 10μm, we find that the conductivity of an the fiber can be comparable to that of copper.

References

[1] Lars M. Ericson, *et al.*, *Macroscopic, Neat, Single-Walled Carbon Nanotube Fibers*, Science, **305**, 1447-1450 (2004).

[2] Y. Gefen and G. Schön, *Effect of inelastic processes on localization in one dimension* Phys. Rev. B **30**, 7323 (1984).

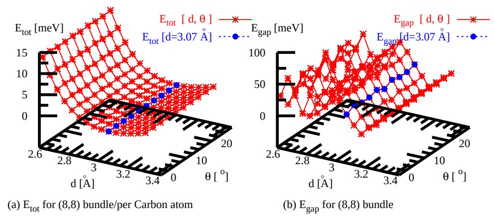

Fig. 1. (a) Total electronic energy (E_T) per atom, and (b) band gap (E_g) for an (8,8) CNT bundle as a function of inter-tube separation distance d, and orientation angle θ between tubes. Lines represented with • correspond to the results with the lowest E_T. Similar results have been obtained for other metallic tubes, (10,4) and (12,0) CNTs.

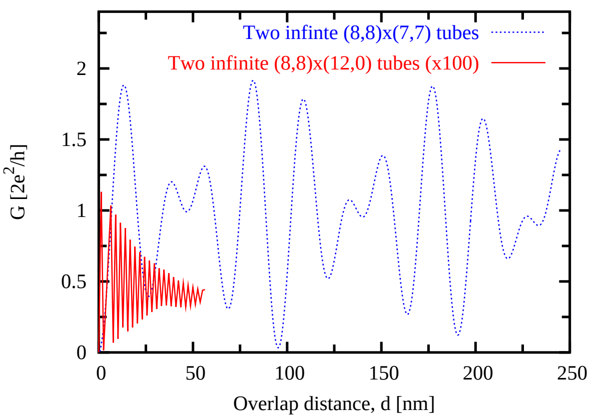

Fig. 2. Inter-tube conductance at $T = 300K$ as a function of overlap distance between two CNTs. Results for (8,8)x(7,7) CNTs where mirror symmetry is preserved, are shown as a dotted line; and those of (8,8)x(12,0) CNTS are shown as a continuous line and multiplied by 100 for clarity.

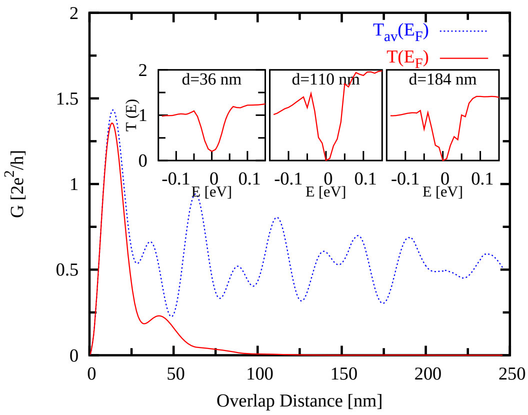

Fig. 3. Inter-tube conductance between (8,8)x(8,8) CNTs where mirror symmetry is broken by 5^o. Dotted and continuous lines correspond to conductance at $T = 300K$ and $T = 0K$, respectively. Insets represent inter-tube transmission coefficient in the vicinity of E_F, and indicate that $T(E_F) = 0$ for $d \geq 110$ nm. Atomic positions of the CNTs are also displayed.

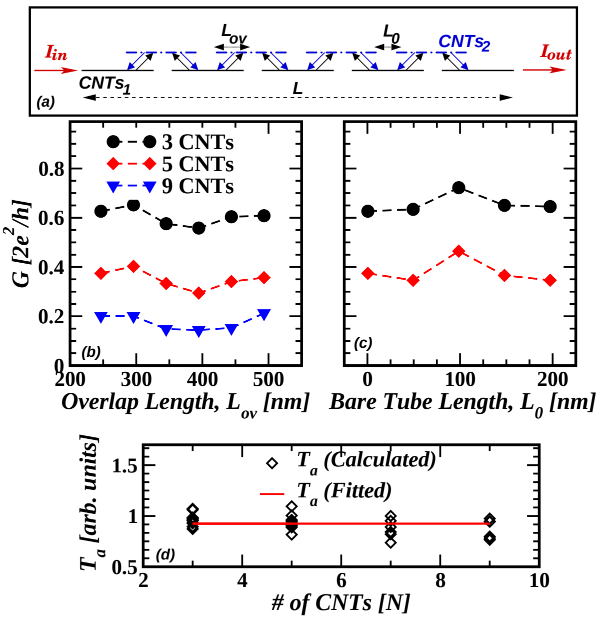

Fig. 4. (a) Single trajectory model through a fiber of length L with N tubes so that $L_{av} = 2 \times L/N$ is the average length of each CNT. L_0 and L_{ov} are the bare CNT length and overlap distance between the CNTs, respectively. We consider CNTs$_1$ and CNTs$_2$ as (8,8) CNTs with mirror symmetry broken by 5^o. (b) Conductance as a function of L_{ov}, with $L_0 \sim 5$ Å and the number of CNTs in the trajectory are $3, 5$, and 9. (c) Conductance as a function of L_0, with $L_{ov} \sim 250$ Å and the number of CNTs in the trajectory are 3 and 5. (d) Inter-tube transmission T_a (shown as open diamonds) for various configurations considered. Continuous line is an average fit of the computed T_a values and the results correspond to $T_a = 0.924 \pm 0.095$.