Coherent Transport through Carbon Nanotubes with Finite Length

Materials Transactions, JIM, Vol. 41, No. 5 (2000) pp. 571 to 573
Papers from JIM Fall Meeting (1999)

Coherent Transport through Carbon Nanotubes with Finite Length*

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The coherent transmission properties of armchair SWNTs with finite length are studied with the help of real space Green's function method. In the linear conductance study, we find that SWNTs indeed act as genuine quantum wires: the conductance peak occurs in existence of resonant tunneling through a discrete electron level that is aligned with the Fermi energy E_f of the electrodes. The doubling of the conductance peaks observed in a recent experiment is numerically verified. We also find that there exist negative differential conductance region for larger bias voltage and similar transmission behavior for armchair SWNTs in the non-linear conductance study.

(Received December 22, 1999; In Final Form February 2, 2000)

Keywords: *electron transport, nanotube, green's function method*

1. Introduction

Carbon nanotubes as well-defined stable and rigid one-dimensional materials which have attracted significant interests recently. Because of their potential application as one-dimensional (1D) quantum wires in carbon nanostructure electronics, many theoretical predictions and experimental proofs have been made for their electronic structures.[1–3] A single-wall carbon nanotube (SWNT) can be imagined by rolling up a single sheet of graphite along one of its two dimensional (2D) lattice vectors $\boldsymbol{R} = m\boldsymbol{R}_1 + n\boldsymbol{R}_2$ to form an (m, n) nanotube with radius $r = |\boldsymbol{R}|/2\pi$, where $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ are primitive lattice vectors. Armchair nanotubes are defined by rollup vector along the (n, n) direction, while ziazag nanotubes are defined by rollup vector along the $(n, 0)$ direction. Armchair and zigzag nanotubes will possess reflection planes and be achiral, and all other SWNTs are chiral. The electrical properties of carbon nanotubes strongly depend on their diameter and the chiral angle of the atomic lattice: armchair tubes are predicted to be truly 1D metals, whereas zigzag or chiral nanotubes are expected to be semiconductors with either a substantial gap (~1 eV) or a very low gap (~meVs). The measurement of transmission properties of carbon nanotubes has been the most challenging subject due to the small diameter of the tubes. Only very recently have ones been able to attach probes directly to individual tubes to measure their transmission properties.[4–8] In the case of multi-wall nanotubes, where many tubes are arranged in a coaxial fashing, the transmission properties of tubes have been shown to vary strongly from tube to tube.[4] However, in the case of SWNTs, the situation is quite different. C. Dekker *et al.*[6–8] succeeded in depositing individual SWNT molecules on metal leads and investigating their two-probe or four-probe resistance versus length, temperature, and gate potential. They found that SWNTs indeed acted as genuine quantum wires, and the electrical conduction seemed to occur through well separated, discrete electron states that is aligned with the Fermi energy E_f of the electrodes. Moreover, for multiprobe transport experiments they alleged also that it was electrically broken up into a chain of weakly coupled 1D quantum wires separated by local barriers.

Though the transmission properties of SWNT have been studied extensively, few works consider the finite size effects carefully till now. It is the purpose of this paper to present a calculation of transmission properties of SWNT with finite length by the real space Green's function method. It will be shown that the theoretical calculated results are not only in good agreement with the experimental ones, but also give a deep insight on the transmission properties of carbon nanotubes. Because of the experimental interest, we focus on the armchair SWNT in this study.

2. Real Space Green's Function Method

Consider a Tight-Binding like Hamiltonian H given by

$$H = \sum_i (h_i + \hat{v}_{i,i-1} + \hat{v}_{i,i+1}), \tag{1}$$

where h_i describes the energy in isolated region i, and $\hat{v}_{i,i\pm1}$ corresponds to the hopping between region i and $i \pm 1$.

The Green's function $G(z)$ is defined as

$$G(z) \equiv (z - H)^{-1}, \tag{2}$$

where z is a complex variable with a small imaginary part. The Green's function G_i^0 in the isolated region i and G in the whole system are related by the Dyson's equation:

$$G = G_i^0 + G_i^0 \hat{V}_i G, \tag{3}$$

with

$$\begin{cases} G_i^0(z) \equiv (z - h_i)^{-1} \\ \hat{V}_i = H - h_i. \end{cases} \tag{4}$$

By taking matrix elements of eq. (3) in region i, one obtains:

$$G_{i,i} = (G_i^{0-1} - v_{i,i+1} G_{i+1}^R v_{i+1,i} - v_{i,i-1} G_{i-1}^L v_{i-1,i})^{-1}, \tag{5}$$

where the left (right) Green's function $G_{i_0}^L$ ($G_{i_0}^R$) is the Green's function for a system in which all sites $i > i_0$ ($i < i_0$) are

*This Paper was Presented at the Fall Meeting of the Japan Institute of Metals, held in Kanazawa, on November 22, 1999.

deleted. Then, the matrix recursion formula can be obtained as

$$\begin{cases} G_i^L = (G_i^{0-1} - v_{i,i-1} G_{i-1}^L v_{i-1,i})^{-1} \\ G_i^R = (G_i^{0-1} - v_{i,i+1} G_{i+1}^R v_{i+1,i})^{-1}. \end{cases} \tag{6}$$

We can also obtain the non-diagonal block element of G from the Dyson's equation as follows:

$$\begin{cases} G_{i,i'} = G_{i,i} v_{i,i+1} G_{i+1}^R v_{i+1,i+2} \ldots v_{i'-1,i'} G_{i'}^R & \text{for } i' > i \\ G_{i,i'} = G_{i,i} v_{i,i-1} G_{i-1}^L v_{i-1,i-2} \ldots v_{i'+1,i'} G_{i'}^R & \text{for } i' < i. \end{cases} \tag{7}$$

From the above equations, it can be seen that, all the Green's function G for the whole system can be calculated through the determination of the left and right Green's functions, which are the inverses of matrices with dimensions much smaller than the system matrix H.

The recursive procedure given above is a useful method for most Green's function applications, especially for some calculations where only parts of the Green's function for the system is necessary.

We conclude this section by noting that, in many applications, it is not necessary to calculate all the elements of the Green's function, that will economize greatly both the storage space and the cpu time.

3. Results and Discussions

In this section, we study the transmission properties of SWNT. The primitive lattice vector of a SWNT is $a = 0.246$ nm and the distance between equivalent slices along the tube axis is written as c. For armchair SWNT, $c = a/2$, while for zigzag ones, $c = \sqrt{3}a/2$. The value of c for chiral ones are in between.

It is well known that the carbon system can be described well by the Tight-Binding (TB) parameters. Though the correlated interaction between electrons may be important in some cases, the non-interacting TB model is effective enough to express most of the main characters of the carbon systems. So, a simple TB representation of the electron states is used in our calculation. To study the transmission properties through this system, we attach two semi-infinite ideal leads to the SWNT from both sides. In order to make the representation simple, the on site energy E_{site} is taken as energy zero point, the hopping energy t between the neighbor carbon atoms is taken as energy unit, and the leads are taken to be 1D ones.[9] Then, the Green's function at the edge site of the semi-infinite ideal leads is given by[10]

$$G^0(E) = E/2 - [(E/2)^2 - 1]^{1/2}, \tag{8}$$

and the conductance g through the SWNT is calculated by the Landauer formula.[11]

Now, let us focus on the transmission properties in this system. As an example, the conductance-Fermi energy curves for a (9, 9) armchair SWNT are shown in Fig. 1, where the total number of slices in the calculations is 700, which corresponds to a 86 nm long tube. For a finite 1D tube of length L, the component of momentum along the axis will also be quantized, with an energy separation between levels of $\delta E \propto 1/L$.

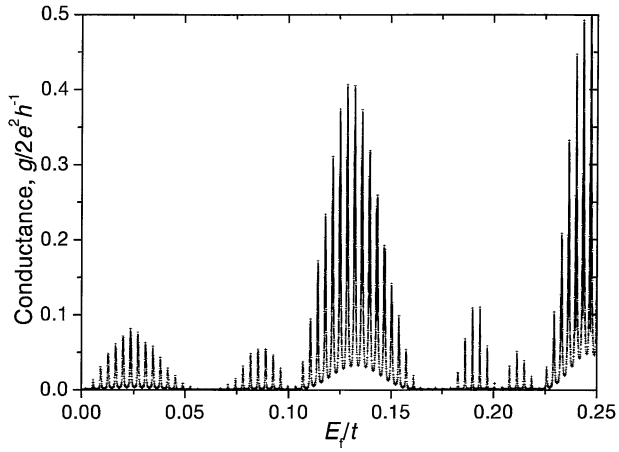

Fig. 1 Conductance g (in unit of $2e^2/h$) as a function of the Fermi energy E_f for a (9, 9) armchair SWNT with 700 slices. The marks give the calculated values of the conductance.

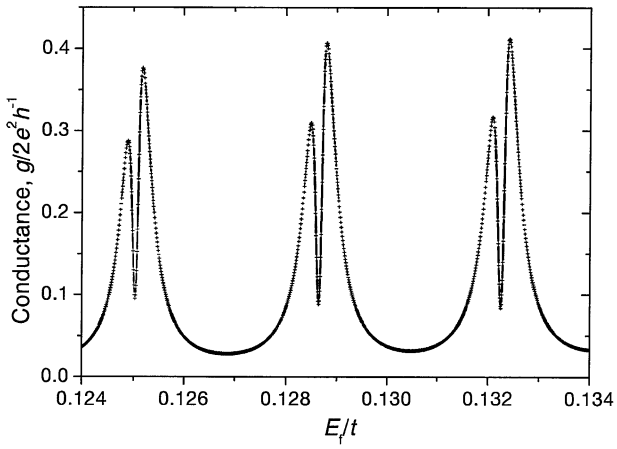

Fig. 2 Detailed structure of Fig. 1.

In the calculations, it is clear shown that with longer length L, the energy separations become smaller. With long enough length L, the details of the curves are dominated by the δE, where the conductance peaks are caused by the sub-energy-levels of the tube, while the envelope reflects the structure indices (m, n) of the tube. Because the zero-bias conductance peaks occur only when an electron level is shifted to the Fermi energy by the gate voltage, this curve also demonstrates the energy spectum of the tube. Moreover, it is interesting to note that we find there always exists a valley at each conductance peak. For example, the detailed structure of the curve shown in Fig. 1 is enlarged as shown in Fig. 2. It seems that we should take them as "double peaks" rather than simple sequent peaks. It is just the phenomenon, the doubling of the conductance peaks, observed in a recent experiment.[6] Because of the finite size effects, the energy bands split to well-sperated energy levels. While the existence of two sublattices in nanotubes, may lead to quasi-degenerate energy levels. Though it is conjected that it may be the result of switching offset charges,[6] we believe that it is the quasi-degenerate energy levels which result in the doubling of the conductance peaks. Meanwhile, the non-degenerate energy level which may be caused by the defects, on the contrary,

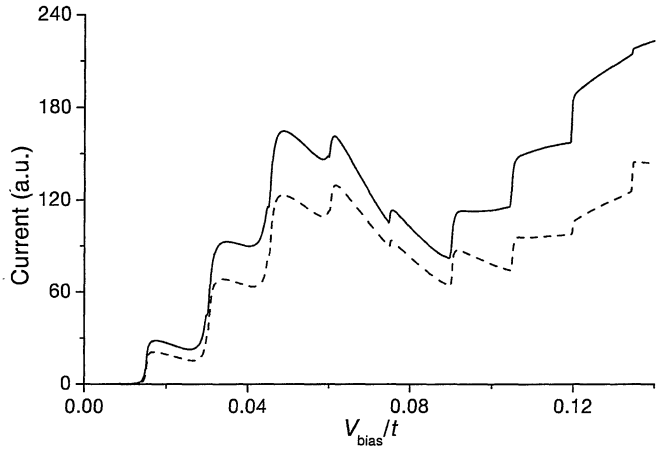

Fig. 3 Current as a function of applied bias voltage for armchair nanotubes with 120 slices. The solid/dashed curve is for a (7, 7)/(10, 10) tube.

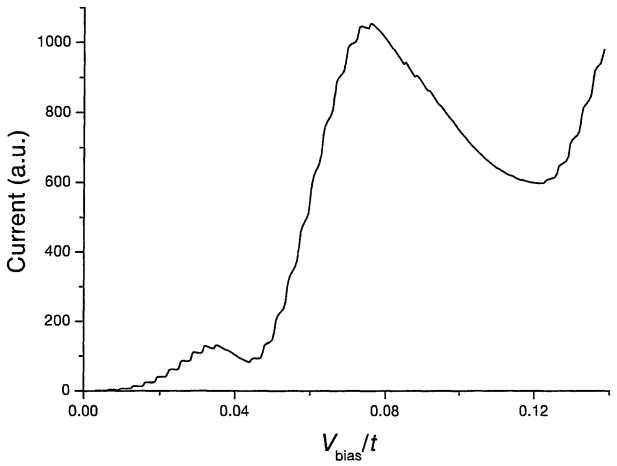

Fig. 4 Current as a function of applied bias voltage for a (7, 7) armchair nanotube with 570 slices.

will result in only single conductance peak.

The typical non-linear transmission properties through armchair SWNTs are shown in Fig. 3. These calculations are done on armchair SWNTs with 120 slices. It is obvious that the current steps under small bias voltage are caused by the resonant tunneling through the tube. With increasing bias voltage, more and more energy levels of the tube fall into the energy window by the bias voltage, and result in a sharp increase of the current. While, what is more interesting is that we do find the negative differential conductance under larger bias voltage, which is attributed by the energy levels dismatch caused by the energy drop within the tubes. This behavior is more distinct for longer tubes, as shown in Fig. 4. Though this phenomena has not been reported experimentally, it may be observed under larger bias voltage (as mentioned above). And it was also theoretically predicted for some doped tubes.[12] It is also interesting to note that we find very similar transmission behaviors for armchair tubes, with larger diameter of the tube corresponding to smaller conductance, as shown in Fig. 3.

4. Summary

In conclusion, the coherent transmission properties of armchair SWNTs with finite length are studied with the help of real space Green's function method. It is found that SWNTs indeed act as genuine quantum wires. The linear conductance peak occurs in existence of resonant tunneling through a discrete electron level that is aligned with the Fermi energy E_f of the electrodes. The doubling of the conductance peaks observed in a recent experiment[6] is numerically verified. We also find that there exist negative differential conductance region for larger bias voltage and similar transmission behavior for armchair SWNTs in the non-linear study.

Acknowledgement

The authors would like to express sincere thanks to the Information Science Group of the Institute for Materials Research, Tohoku University for their continuous support of the HITAC S-3800/380 supercomputing system.

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