An Analysis of Electronic Propagating Waves in Carbon Nanotubes

Toshihito Umegaki, Matsuto Ogawa, Yasuyuki Makino, and Tanroku Miyoshi
Graduate School of Science and Technology, Kobe University

Corresponding author e-mail address: umegaki@lerl.eedept.kobe-u.ac.jp

1. Introduction

In order to realize carbon nanotube (CNT) based devices, we have to analyze the electron transport characteristics in the CNTs. In particular, it is important to study the controllability of the conductance and the current density distribution in CNTs by means of their chirality. We have studied the basic conductive characteristics and the interaction with electromagnetic waves to apply CNTs to nanometer-size electrodes in high-frequency devices.

So far, it has been difficult to control the dimensions of metal electrode within 100 nm scale. On the other hand, the diameters of CNTs can be fabricated as small as several nanometers. In addition, the diameter control by means of self-organization and ballistic conductivity due to the ballistic carrier transport are of great advantages to CNTs.

In this paper, we study the basic conductive characteristics in view of the quantum transport of electronic waves in CNTs. In the next section, the models of CNTs are described and the band structures of CNTs are analyzed based upon the linear combination of atomic orbital (LCAO) expansion method. In Sec. 3, we discuss numerical results of the electron transport properties in the CNTs based upon the transfer matrix (TM) method. The results of the calculated *I-V* characteristics are also discussed in this section. Finally we summarize our conclusion.

2. Band Structures of CNTs

We have analyzed dispersion curves of electronic propagating waves as well as evanescent ones in CNTs based upon the linear combination of atomic orbital (LCAO) expansion method [1]. Substituting the wave function into the Schrödinger equation, we can easily obtain the $E-\mathbf{k}$ dispersion relations of the graphite sheet:

$$E(\mathbf{k}) = \varepsilon_0 \pm \gamma\sqrt{1+4\cos^2\frac{k^x a}{2}+4\cos\frac{k^x a}{2}\cos\frac{\sqrt{3}k^y a}{2}}\,, \qquad (1)$$

where ε_0 is the on-site energy on a carbon atom, γ is the hopping energy between nearest neighbors, a is the lattice constant and minus sign (-) and plus sign (+) denote the bonding and antibonding energy band, respectively. The schematic model is shown in Fig. 1. The CUCs are unit cells in the CNT, and GUCs are the unit cells of the graphite sheet. Potentials due to the bias voltage V_0 are assumed to be constant in each GUC. Black triangles in GUCs indicate lattice points of carbon atoms.

The dispersion relation of a CNT with (n, m) chirality can be obtained by imposing the periodic boundary conditions in the circumferential direction. From this boundary condition, we obtain *quantized* wave vectors in x direction as

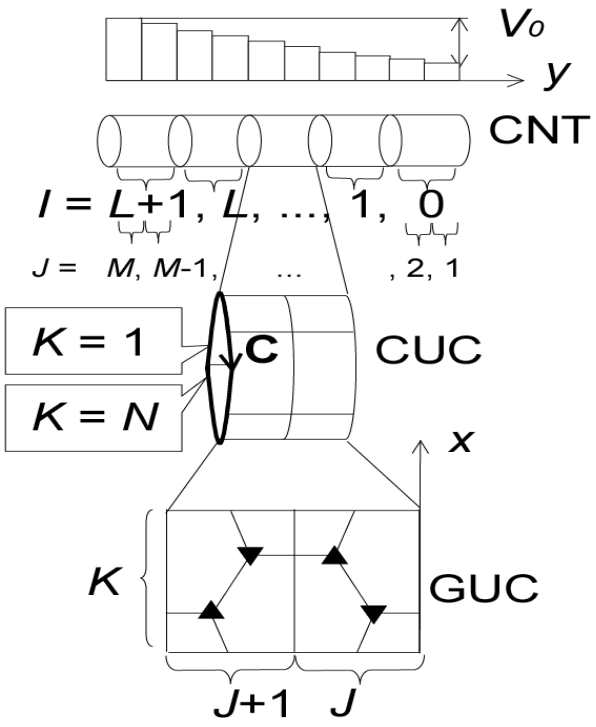

Figure 1. The schematic model of a CNT.

$$k^x = \frac{2\pi\, i^x}{\sqrt{n^2 + nm + m^2}\, a},\ (i^x = 0, \pm 1, \pm 2, \ldots) \quad (2)$$

From Equations (1) and (2), we obtain the eigenvalue equation of the *chiral* type CNT. We have evaluated the complex dispersion curves whose real bands correspond to the propagating and complex bands correspond to the evanescent waves. It is shown that the CNTs become metals or semiconductors depending on their chirality. CNTs with chirality of (n, m) become metals when $n - m$ is 3 times integer. In other cases, they become semiconductors. When m is 0 or n, CNTs are categorized into *zigzag* types or *armchair* ones, respectively. In either case, the mode number i^x given in equation (2) is restricted within $-(n-1)$, $-(n-2)$, … , 0, 1, 2, …, n due to the graphite sheet band-structure. Figure 2 shows the complex dispersion curves of the *zigzag* type CNT with the chirality of (19, 0). The real bands are shown in the right-hand side, whereas imaginary parts of the complex bands in the left, which correspond to the evanescent modes. We have plotted only branches with the positive group velocities. This is because it is convenient to classify the branches into the ones with positive group velocity and the others with negative when we calculate the electronic current propagating in the CNTs.

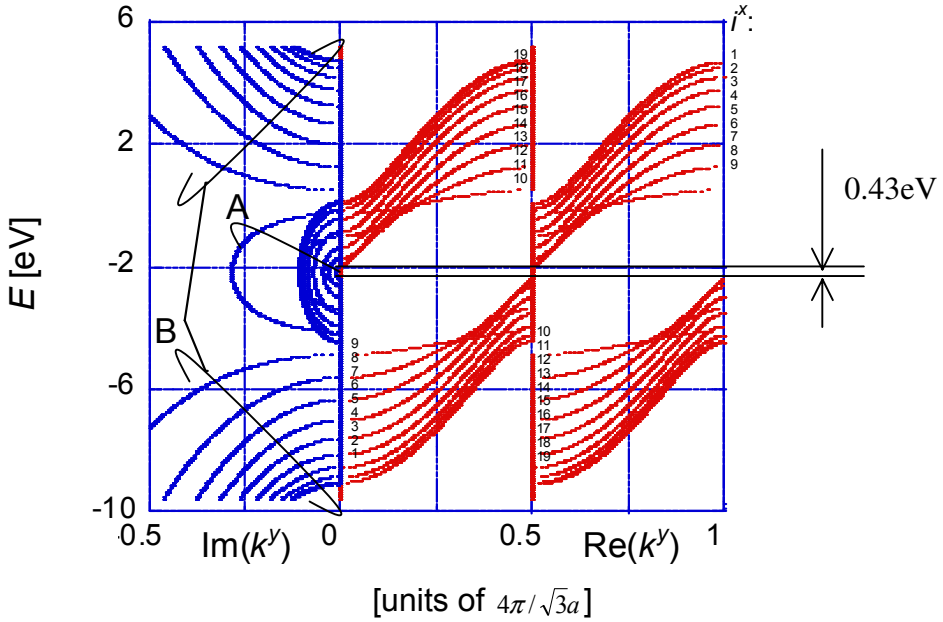

Figure 2. Complex dispersion curves of the *zigzag* type CNT with chirality (19, 0).

The branches with negative group velocities can be simply obtained by taking mirror-reflection of the positive branches at the center of the Brillouin zones due to the symmetric properties of the graphite sheet band-structure. When the CNT becomes semiconductor, imaginary parts of the complex bands appear in the band gaps (A) and the band edges (B).

3. Current in CNTs

We have studied the current-voltage (*I-V)* characteristics and the current density distributions around the circumference of the CNTs by using the transfer matrix (TM) method [2] [3]. Figures 3 and 4 show *I-V* characteristics without and with evanescent modes, respectively. The current increases with the length of the CNT *L.* This reason is that the electronic waves are reflected by the discontinuity between the rectangular potentials in neighboring CUCs and they decay when *L* becomes larger. The *I-V* characteristics with evanescent modes at the voltage smaller than 0.43V are almost same as those without evanescent ones. The current with evanescent modes, however, increases under the bias voltage larger than 0.43V when *L* is less than 20. The increase in the current is due to the additional current paths by way of the evanescent modes in the middle of the CNT as shown in Fig. 2 (A). The electronic waves propagate in the real mode at the input terminal, then couple with the evanescent modes in the middle, and finally couple again with the real modes at the output terminal. As shown in Fig. 2, the narrowest band gap is 0.43eV. It corresponds to the voltage where this current increase appears in Fig. 4. The current in the CNTs with *L* larger than 50 does not show such abrupt increase, since the length of the CNTs are so long that the amplitudes of the existing evanescent modes can fully vanish. Therefore, these evanescent modes should be taken into account when we analyze transport characteristics of the CNTs with *L* less than 20 CUCs.

4. Conclusions

We have studied the transport properties of the CNTs as coaxially rolled 2D graphite sheets based upon the LCAO and the TM methods. We have evaluated the complex dispersion curves and the *I-V* curves without and with evanescent modes. It is found the evanescent modes play an important role in the transport of electrons in the CNTs especially when the length is shorter than 20 CUCs.

Acknowledgement

One of the authors (T.U.) wishes to acknowledge the supports of the “Foundation Advanced Technology Institute” and the “Hyogo Science and Technology Association”.

References

[1] P. R. Wallece, “The Band Theory of Graphite,” Phys. Rev., **71**-9, 622/634 (1947).
[2] R. Tsu and L. Esaki, “Tunneling in a Finite Superlattice, ” Appl. Phys. Lett., **22**-11, 562/564 (1973); H. Mizuta and T. Tanoue, “ The Physics and Applications of Resonant Tunneling Diodes, " Cambridge University Press (1995).
[3] T. Umegaki, M. Ogawa, Y. Makino, and T. Miyoshi, “ Quantum Transport in Carbon Nanotubes with Arbitrary Chirality,” Memoirs Graduate School Science & Technology, Kobe University, 22-A, 103/114 (2004).

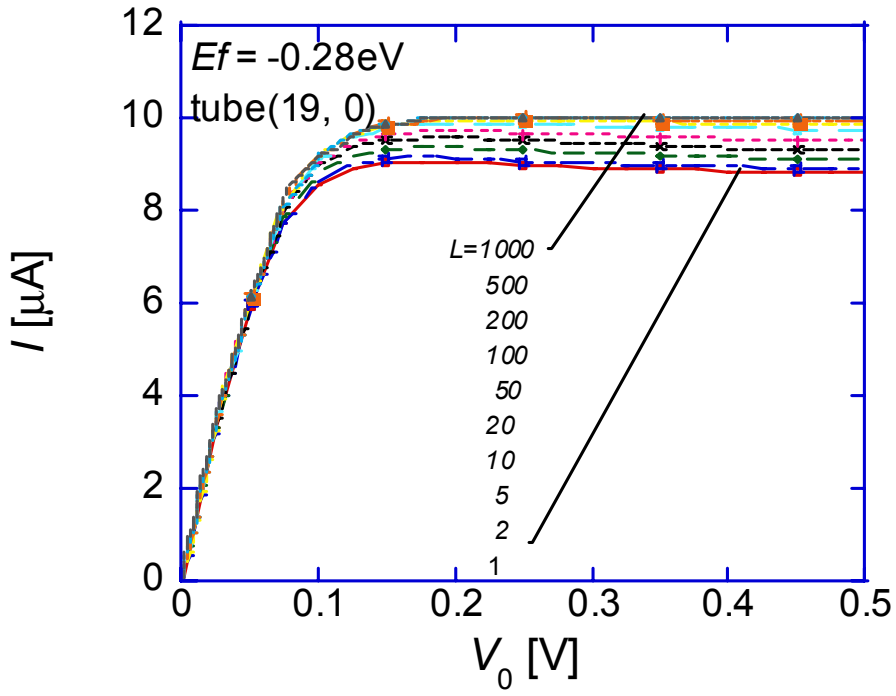

Figure 3. *I-V* characteristics without evanescent modes of the CNT. The chirality is (19, 0) and Fermi energy is assumed to be -0.28eV. Each characteristics are shown for the length *L* of 1, 2, …, 1000, respectively.

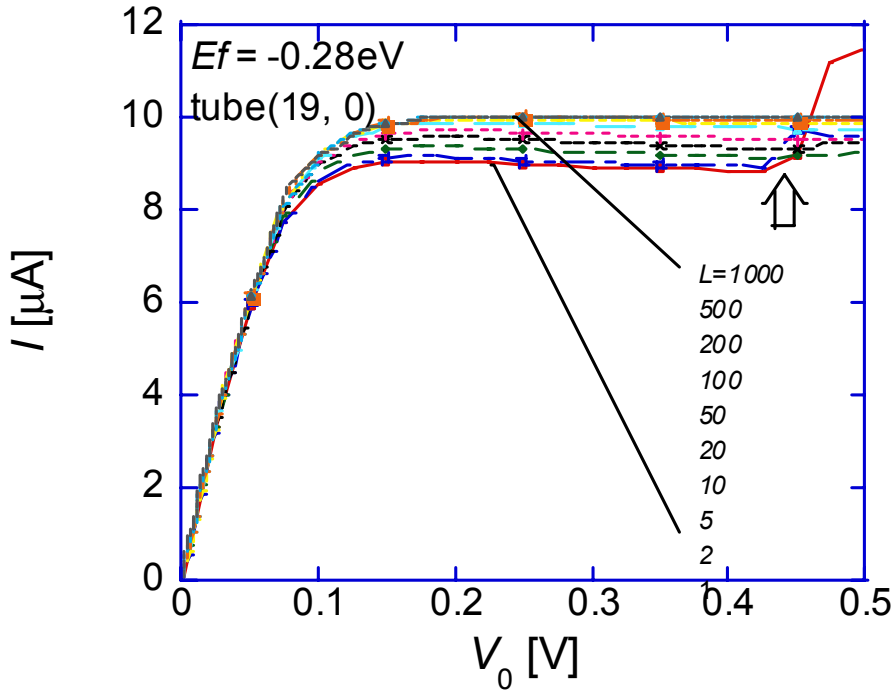

Figure 4. *I-V* characteristics when the evanescent modes of the CNT are taken into account. An abrupt increase in the current is observed around 0.43V as indicated by the arrow.