Enhanced Back Scattering due to Inter-Tube Interaction in Double-Wall Carbon Nanotubes

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Metallic single-wall carbon nanotubes (SWCN's) are considered to be good conductors because any weak long-rage potentials do not cause back scattering in carbon nanotubes (CN's) with large diameter [1,2]. Usually, the case of complex of CN's, for example, double-wall carbon nanotubes (DWCN's), multi-wall carbon nanotubes (MWCN's), CN bundles and so on, is considered to be similar to SWCN's due to the weak interaction and the quasi-periodicity though back scattering can arise from the off-diagonal elements in terms of the effective mass model [3]. The situation can be changed, however, in the case of CN systems with both of inter-tube interaction and impurities because the system is considered to become an ordinary one-dimensional system with disorder. In this paper, we present numerical demonstrations of conductance of DWCN's exhibiting that back scattering in DWCN's can be considerably enhanced comparering to SWCN's.

We perform calculations of conductance for DWCN's with long-range impurities with the use of recursive Green's function method and the Landauer-Büttiker formalism in the one-particle tight-binding model. An impurity with the center at the origin is modeled as a gaussian form:

$$V(\mathbf{R}_i) = \frac{vS'}{\pi d^2} \exp\Big(-\frac{R_i^2}{d^2}\Big),$$

where $\mathbf{R}_i$ is a position of site i, v a factor determining the amplitude, $S' = \sqrt{3}a^2/4$ the area of an atom with $a = 2.46\mathring{A}$ being the lattice constant, and d the width of the potential. Fixing v, repulsive and attractive impurity potentials with $\pm v$ are randomly distributed on lattice points with the probability p. We use long-range impurities $d/a = 1.7$ and $p = 0.01$ in the followings. Our system is a two-terminal system in which the inner tube is finite with the length A and the outer tube is infinitely long and plays a role of ideal leads. Figure 1 shows a schematic illustration of the system.

Calculated conductances for (10,0)-(4,16) DWCN near the Fermi energy as a function of the length A in units of circumference length of the outer tube L are shown in Fig. 2(a) and those for (4,16) SWCN same as the outer tube are also shown in Fig. 2(b) for reference. In the DWCN without impurities, the conductance is $G \approx 2e^2/\pi\hbar$ showing that the transmission is nearly perfect as plotted by a dotted line in Fig. 2(a). In the presence of impurities with $v/\gamma_0 = 3$ and 6 where $\gamma_0 \sim 3$eV, the conductance is considerably reduced. In the corresponding

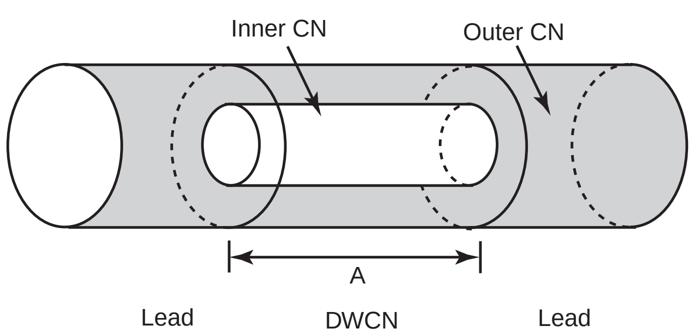

Figure 1: Schematic illustration of two-terminal DWCN. The inner tube is finite with the length A and the outer tube is infinitely long and connected to reservoirs. In the region without the inner tube, the outer tube plays a role of ideal leads.

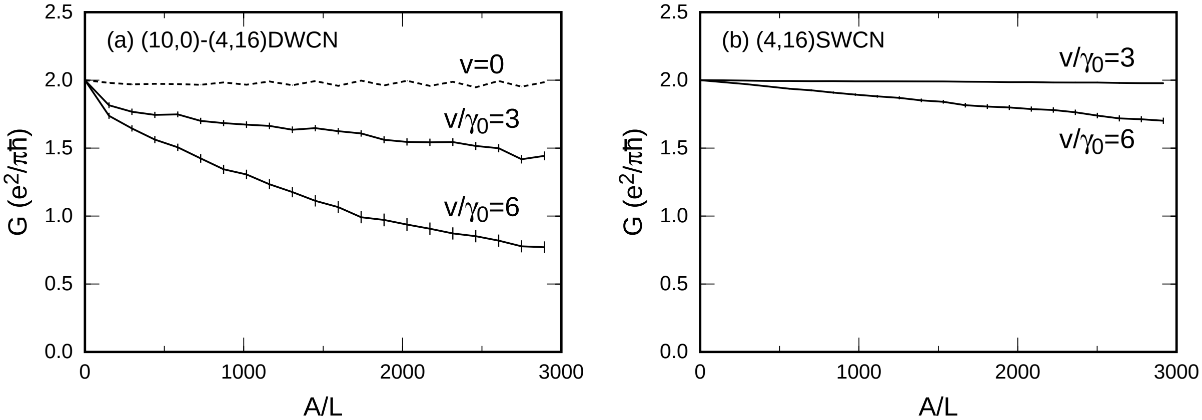

Figure 2: Conductace for (a)(0,10)-(4,16) DWCN and (b)(4,16) SWCN's as a function of the length A at the energy $EL/2\pi\gamma = 0.2$ where $2\pi\gamma/L$ is the bottom of the first excited subbands measured from the Fermi energy $E = 0$. In this case, $L = 4\sqrt{21}a = 45.1\mathring{A}$. A dotted line in (a) is the conductance in the absence of impurities.

case of SWCN in Fig. 2(b), on the ohter hand, the transmission is nearly perfect for $v/\gamma_0 = 3$ and decrease of the conductance is still small for $v/\gamma_0 = 6$.

The results reveal that in DWCN's the inter-tube interaction can lead to prominent enhancement of back scattering by the combination with impurities. The reduction of the conductance is attributed to the Anderson localization in quasi-one-dimensional systems. It should be noted that we can also see that either the inter-tube interaction or impurities cannot considerably contribute to the back scattering. This is because the strength of inter-tube interaction is weak and not random but quasi-periodic and there is no back scattering from long-range impurities in SWCN's.

It is considered that these results can be applied to multi-wall CN's and CN bundles. There are only a few reports that the quantization of conductance was clearly observed in spite of advances in technique to make contacts [3,4]. It is possible that the resistance in complex systems of CN's comes from coexistence of inter-tube interaction and impurities. However, our results are preliminary ones. Since the inter-tube interaction strongly depends on the structure, further systematic study of DWCN's is needed.

References

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