Rev. Adv. Mater. Sci. 33 (2013) 38-41

ELECTRICAL CONTACTS COUPLING EFFECT ON SINGLE-WALLED CARBON NANOTUBE ELECTRON RESONATOR

Linfeng Yang,Tintai Wang, Haizhen Ren and Jingchang Zhang

Zhongyuan University of Technology, 450007, Zhengzhou, China

Received: October 17, 2011

Abstract. We have studied the electrical contacts coupling effect on a left lead/central single-walled carbon nanotubes(SWNTs)/right lead system by using the tight binding Green function approach. It is showed that at strong coupling strength between electrical contact and central SWNT, the system behaves as Fabry-Perot electron resonator, which can show distinct quantum conductance oscillations and complicate background as the Fermi energy is driven far from the charge neutrality energy point by the applied gate-voltage V_g, the shape of conductance background is dependent on the contacts coupling strength and the chirality of SWNT. For very weak contacts coupling strength, the system presents well defined resonant peaks, which is the limit of the quantum conductance oscillations.

1. INTRODUCTION

The behavior of traditional electronic devices can be usually understood in terms of the classical diffusive electron motion. However, as the size of a device continuously decreases and becomes comparable to the electron coherence length, the quantum interference between electronic waves becomes increasingly important, leading to dramatic changes in the device properties. This classical-to-quantum transition in the device behavior suggests the possibility of using quantum coherence in the nanometer-sized electronic elements [1-3]. Molecular electronic devices are promising candidates of realizing such devices because the electronic motion in them is inherently quantum mechanical and can be modified by well defined chemistry. One coherent electronic device is the Fabry-Perot electron resonator based on individual SWNT with near-perfect Ohmic contacts to electrodes [4-6], in which the nanotube acts as a coherent electron wave guide with a resonant cavity formed between the two nanotube-electrode interfaces.

2. RESULTS AND DISCUSSION

The geometrical structure under consideration is composed of two leads (left and right) plus SWNT, with all three parts being metallic SWNTs of the same chirality, which can be described by a tight-binding model with one ð electron per atom. The tight-binding Hamiltonian of the system is written as $H = -V_{pp\pi} \cdot \sum_{<i,j>} a_i^{\dagger} a_j + c.c$, where the sum over i,j is restricted to the nearest-neighbor site, and $V_{pp\pi}$ = 2.75 eV [7,8], Within this theory, the defect-free nanotubes have complete electron-hole symmetry with their Fermi levels at zero. The layers of carbon atoms between left and right leads are chosen to be 405 for armchair tubes and 470 for zigzag tubes (the length of nanotube L = 100 nm). For simplicity, On-site energies are set to zero, all

Corresponding author: Tintai Wang, e-mail: laodizhi@yahoo.com.cn

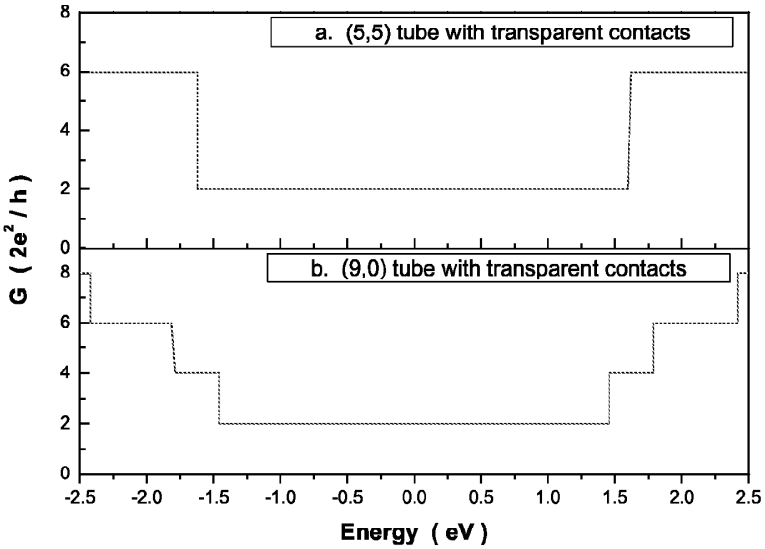

Fig. 1. Conductance *G* vs Fermi energy with ideal contacts α =1.0.

nearest-neighbor hopping parameters are assumed to be $V_{pp\pi}$ except those at contacts, which are taken to be $\alpha V_{pp\pi}$ with $0<\alpha<1$ is the coupling coefficient. Consequently, electrons will be scattered at the contact and central SWNT interfaces. The scattering will mix the π-binding channel and the π*-binding channel, and quantum interference between two channels will then take place.

The conductance *G* of the SWNT system can be calculated by using the Landauer formula $G = (2e^2/h)T$, with T the transmission coefficient, expressed as follows [7,8]: $T = Tr(\Gamma_L G_C^r \Gamma_R G_C^a)$ where G_C^r, G_C^a are the retarded and advanced Green's functions of the SWNT, respectively, and Γ_L, Γ_R are the coupling of the SWNT to the left(right)lead. The Green's function of the SWNT can be explicitly written as $G_C(\varepsilon) = (\varepsilon - H_c - \Sigma_L - \Sigma_R)^{-1}$, where $\Sigma_L = h_{LC}^{\dagger} g_L h_{LC}$, $\Sigma_L = h_{LC} g_R h_{LR}^{\dagger}$ are the self-energy terms due to the semi-infinite leads [7,9].

We have calculated the conductance of metallic SWNT electron resonators with Landauer formalism of different coupling strength at zero temperature and zero bias. Since the transport property of armchair SWNT system and zigzag SWNT system are different, so we choose the armchair SWNT (5,5)tube and the zigzag SWNT as representatives of our calculation. First we calculated the conductance of (5,5) and (9,0) tubes with ideal electrical contacts(the coupling coefficient α = 1.0), the obtained results are plotted in Fig. 1, since there are two channels (π-binding and π*-binding channel) around the charge neutrality point, so the quantum conductance is $2G_0$. As the energy is driven far away from the charge neutrality point, new energy band will enter the observation window and the quantum conductance steps appear.

However, the actual electrical contacts are not exact transparent, then the coupling coefficient α<1.0, electron will be scattered at the interface and thereby reduces the conductance, the system behaves as fabry-Perot electron resonator. At stronger coupling strength (we choose α = 0.80 for representative), the calculated results can be seen in Fig. 2a for the armchair type (5,5) SWNT resonator and Fig. 2b for the zigzag type (9,0) SWNT resonator, which illustrate several characteristics shared by all metallic SWNTs resonators: all metallic SWNT electron resonators can show the slow oscillations except the zigzag ones and the slow oscillation period is inversely proportional to Fermi energy *E*, which is driven by the gate-voltage V_g. Also all the metallic SWNT electron resonators exhibit pronounced fast oscillations with the maximum conductance approaching $2G_0$. The fast conductance oscillations period $\Delta E \approx 0.018$ eV for the length *L* = 100 nm have been obtained, coinciding very well to the experimental data and the previous theoretical prediction $\Delta E = (hV_F)/(2L) \approx (1.68\text{eV.nm})/\text{L}$ [1,2]. It is the manifestation of electron scattering only at the SWNT-electric contact interface and passing through SWNT ballistically. The ratio of the slow oscillation period to the fast one is independent of the coupling strength between the SWNT and electric contacts, but is relevant to the SWNT length *L*. Since now neither disorder nor defect exist in the central SWNT, the slow and fast conductance oscillations can only be manifestations of the

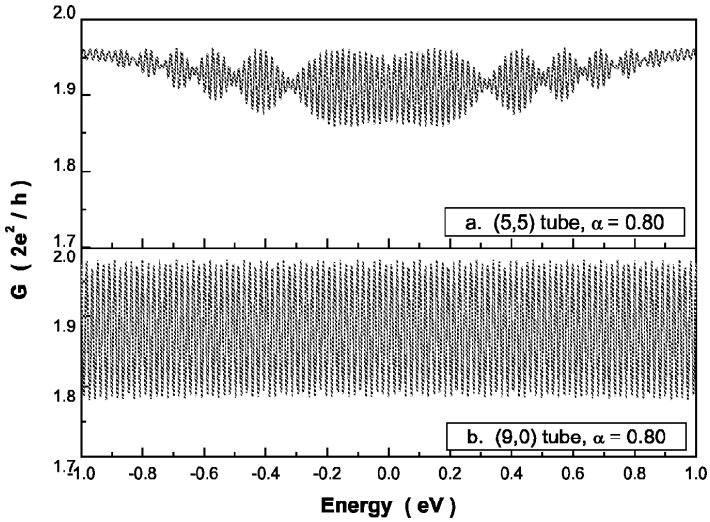

Fig. 2. Conductance *G* vs Fermi energy with coupling coefficient $\alpha = 0.80$.

intrinsic quantum interference in the conducting SWNTs.

The weaker the contacts coupling strength, the stronger the electron interfacial scattering, the quantum conductance will decrease as the coupling strength decreases. As the Fermi energy is driven far away from the charge neutrality point, the strong contacts interfacial scattering will make the electron have the probability hop to the higher energy subband and result in the conductance decrease [1,2,6] as the energy being far away from charge neutrality point and show complicated background for armchair system (as seen in Fig. 3a for $\alpha = 0.40$). And the zigzag system has relative simple result (see Fig. 3b with $\alpha = 0.40$).

We also studied SWNT system with very weak contacts coupling ($\alpha = 0.01$ for representative), the results can be seen in Fig. 4, it is found that the SWNT system demonstrates well defined resonant peaks, showing resonant transmission and it behaves like a quantum dot which is the limit of conductance oscillations.

3. CONCLUSION

In conclusion, our numerical calculations demonstrate the quantum conductance of the SWNTs system with different coupling strength between electrical contacts. Our numerical calculations demonstrate that at strong coupling

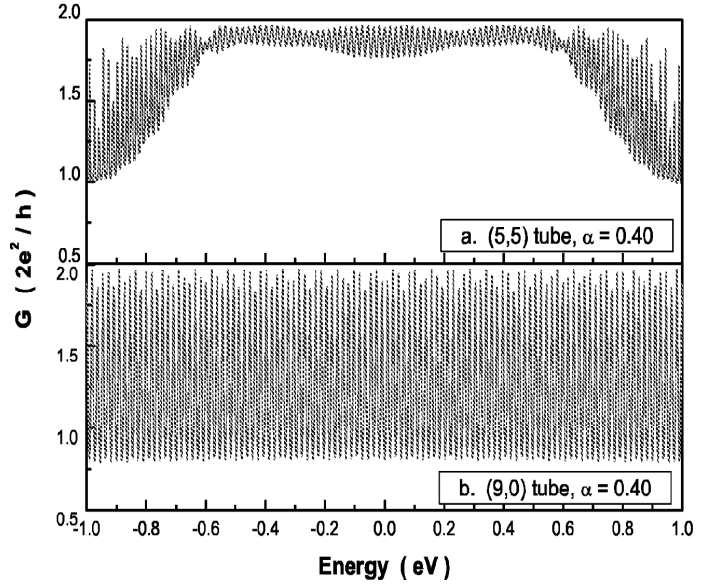

Fig. 3. Conductance *G* vs Fermi energy with coupling coefficient $\alpha = 0.40$.

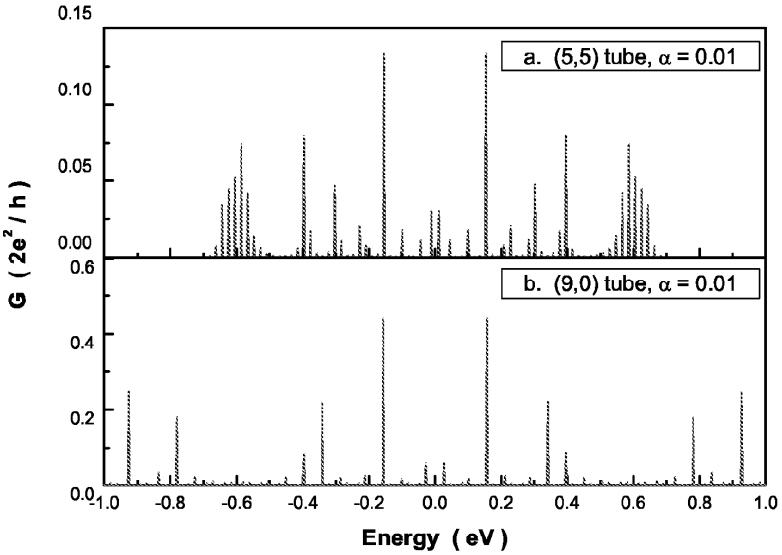

Fig. 4. Conductance *G* vs Fermi energy with coupling coefficient $\alpha = 0.01$.

strength between electrical contact and central SWNT, the system behaves as Fabry-Perot electron resonator, which can show distinct quantum conductance oscillations. For very weak contacts coupling strength, the system presents well defined resonant peaks, which is the limit of the quantum conductance oscillations.

ACKNOWLEDGEMENT

This work was supported by the Natural Science Foundation of China under Grant No. 51077134 and No. 50977093.

REFERENCES

[1] Jie Jiang, Linfeng Yang, Jinming Dong and Dingyu Xing // *Phys. Rev.* **B68** (2003) 054519.
[2] Linfeng Yang, Jiangwei Chen, Huatong Yang and Jinming Dong // *Eur. Phys. J.* **B43** (2005) 399.
[3] Linfeng Yang, Jiangwei Chen, Huatong Yang and Jinming Dong // *Phys. Stat. Sol.* **B242** (2005) 1476.
[4] Linfeng Yang, Jiangwei Chen, Jizhou Zhang and Jingchang Zhang // *Phys. Stat. Sol.* **B243** (2006) 1306.
[5] W. Liang, M. Bockrath, D. Bozovic, J.H. Hafner, M. Tinkham and H. Park // *Nature(London)* **411** (2001) 665.
[6] J. Kong, E. Yenilmez, T.W. Tombler, W. Kim, H. Dai,. R.B. Laughlin, L. Liu, C.S. Jayanthi and S. Y. Wu // *Phys. Rev. Lett.* **87** (2001) 106801.
[7] M.B. Nardelli // *Phys. Rev.* **B60** (1999) 7828.
[8] L. Chico, V.H. Crespi, L.X. Benedict, S.G. Louie and M.L. Cohen // *Phys. Rev. Lett.* **76** (1996) 971.
[9] Y. Meir and N.S. Wingreen // *Phys. Rev. Lett.* **68** (1992) 2512.