Chin. Phys. B Vol. 19, No. 5 (2010) 057206

Size effect of quantum conductance in carbon nanotube Y-Junctions*

Liu Hong(刘 红)

Physics Department, Nanjing Normal University, Nanjing 210046, *China*

(Received 16 July 2009; revised manuscript received 10 October 2009)

This paper studies the quantum conductance properties of three-terminated carbon nanotube Y-junctions, which are built by connecting three (5,5) single-walled carbon nanotubes. The results show that the quantum conductance at the Fermi energy oscillates periodically with the junction's size, and the number of oscillating periodic layers is 3 which is the same as that in the two terminated $(10,0)/m(5,5)/(10,0)$ junctions. Moreover, this Y-junction with different size exhibits an obviously different distribution of electron current in the two drain branches, called shunt valve effect of electronic current. Thus the degree of this effect can be controlled and modulated directly by constructing the three branches' sizes or the distribution of defect. The results show in detail that the difference between the two drain currents can be up to two times for some constructions with special sizes. In addition, the uniform distribution of defects in the Y-junction leads to lower quantum conductance than that of other defect configurations.

Keywords: single-walled carbon nanotube, Y-junction, quantum conductance, local density of state
PACC: 7280R, 7360T

1. Introduction

Molecularly perfect materials such as single-wall carbon nanotubes (SWCNs) can provide new opportunities for designing nanometer-sized electronic devices. Carbon nanotube not only has the magnitude order of micrometer of length compared with the diameter of several nanometers, but also metallic nanotube is one good quantum conductor wire because the localization length of he telectron can be up to μm magnitude.[1] Based on the ballistic and phase-coherent natures of the electron transport, various interesting nanoelectronic devices, such as the directional coupler,[2] the quantum stub transistor,[3] and the three-terminal ballistic junction[4,5] have been proposed. As is well known, two nanotubes can be connected through the defects of pentagon and heptagon first postulated by Chico *et al.*[6] There are many works studying the electronic properties of two-terminal junction.[6−13] In particular, the Y-shaped three-terminal ballistic junction, also known as the Y-branch switch, was proposed as a promising alternative for future low-power, high-speed switching devices.[4] Recently, CNT Y-junctions were produced by Li *et al.*,[14] and theoretically studied by Refs. [15] and [16]. These tubular heterostructures called intramolecular heterojunctions offer new perspectives for nanoelectronic technology. So it could be envisioned to integrate an electronic circuit of nanotube based architecture. However, it is ambiguous of the growth mechanism and stability of defect distribution in multi-terminated junctions. Andriotis *et al.*[15] reported that the possible role of topological defects at the junction in insulating the current flow in primary channel is not entirely clear. The positions of the defects relative to the junction can be expected to be a factor in rectification. Valle *et al.*[16] investigated that the interference between the defective states and the extended continuum background leads to Fano resonances. In their work, the junctions based on CNT consist of the different chiral tubes, interface states between the two different chiral tubes. In recent years, super CNTs have been proposed by linking CNT Y-junctions into a tube structure.[17,18] They presented that for perfect Y-branched CNTs the angle between two neighbouring branches should be 120°, and the radii of the three branches should be equal. According to our knowledge, the interface states between two different chiral tubes generally lead to strong resonances.[17] Therefore these problems are still required to investigate in detail.

Physically, as we know, the band structure of armchair nanotubes consists of two non-degenerate bands which cross the Fermi level at $k = 2\pi/3a_0$, with lattice constant a_0. In our previous work, only when layer number is $m = 3 \times n + 2$ with n being integer, can one probe the Fermi level exactly where the

*Project supported by the Natural Science Foundation of Jiangsu Education Department (Grant No. 04KJB140065) in China.
© 2010 Chinese Physical Society and IOP Publishing Ltd

two bands overlap. This characteristic is obviously shown in those two terminated (10,0)/m(5,5)/(10,0) junctions.[7] In our previous work,[12] we connected the three limited-length (5,5) tubes with each other, called as Y-junction (5,5) nanotube. Through the three branches there is not oscillation in the conductance with the junction size since there is not the interface states. And the conductances through three branches are the same as each other because of the symmetry among three semi-infinite (5,5) tubes and are independent of the sizes of three tubes. The differences in conductance among the four kinds of Y-junction are mainly from their defect of geometric structures. However, when the electrodes connected with these junctions are taken place by three metal electrodes, we think that the periodic oscillation characteristic in electronic properties with the junction size still exists in these three-terminated (5,5) Y-junctions, due to the quantum confinement and the band mismatch at interface between the junctions and the metal electrodes. In this paper, we investigate the size effect in this Y-junction devices in detail. Furthermore, we find that it exhibits some interesting effects in their quantum conductance. Specially, these properties could be influenced and modulated by the junctions' size and the distribution of defect. Therefore, we believe that these properties are desirable for the design of nanoscale size molecular devices based on CNT.

In this work, we adopt a tight-binding Hamiltonian and follow the single-particle Green's function formalism to obtain local density of states(LDOS) within real-space renormalization techiques.[13,19] Taking into account that electron transport on the molecular scale became a topic of intense and relevant applications, we also calculated the quantum conductance and the I–V characteristics of the four Y-junctions, adopting the Landauer–Kubo formalism.[20] This work is organized as follows: in Section 2, we present the theoretical method and the four symmetric geometrical configurations of (5,5) Y-junction. In Section 3, we proceed with the numerical calculations, and give discussions. Finally, the summary is given in Section 4.

2. Theoretical method

We performed the LDOS and quantum conductance to characterize the electronic properties within a tight binding description of the carbon bonds. Our tight-binding Hamiltonian is of the form:[7]

$$H = \sum_{<i,j>,s} V_{\mathrm{pp}\pi}(C^{+}_{i,s}C_{j,s} + C_{i,s}C^{+}_{j,s}), \qquad (1)$$

where the $\sum_{<i,j>}$ is restricted to nearest-neighbouring atoms, the two-centre hopping integral $V_{\mathrm{pp}\pi} = -2.75$ eV[7] for centre apart from Y-junction. On-site energy is set to zero, so $E = 0$ eV is the Fermi energy. The three electrodes are assumed to be one dimensional lead with a single channel. Among the nearest sites in the electrodes, the hopping integral is also set to be $V_{\mathrm{pp}\pi}$. We consider that the electrode is one-dimensional metallic chain. In this case, because we consider ballistic transmission, the bottleneck of the molecule–electrode contact should not be smaller than the order of the hopping integral $V_{\mathrm{pp}\pi}$. Thus the hopping integral $V'_{\mathrm{pp}\pi}$ between the atom at the edges of junction (shown in Fig.1) and the atom of the electrodes is taken as the half of the value $V_{\mathrm{pp}\pi}$. All the hopping parameters are independent of the bond length, curvature, or any rearrangement due to the presence of defects. Therefore, these results show the changes induced solely by the alterations in the topology of these Y-junctions.

Surface Green's functions for the metallic chains are calculated through the solution of matrix like Dyson equations obtained by successive decimation of unit cells. Let us consider a system composed of a heterojunction C connected to three semi-infinite one dimensional chains, i (i=1, 2, 3). A fundamental result in the theory of electronic transport is that the conductance through a region of interacting electrons is related to the scattering properties of the region itself via the Landauer formula: $\mathcal{T} = (2e^2/h)T_{ij}$, where $\mathcal{T}$ is the conductance, and the transmission function T_{ij} is expressed as

$$T_{ij} = \mathrm{Tr}(\Gamma_i G^{\mathrm{r}}_{\mathrm{C}} \Gamma_j G^{\mathrm{a}}_{\mathrm{C}}) \quad (i,j = 1,2,3), \qquad (2)$$

where $G^{\mathrm{r}}_{\mathrm{C}}$ and $G^{\mathrm{a}}_{\mathrm{C}}$ represent the retarded and advanced Green's function of the heterojunction, respectively, Γ_i and Γ_j represents the couplings of the heterojunction to the ith and jth branches, respectively. The Green's functions (G_{C}) as a function of energy E are calculated with a previously published surface Green's function matching technique.[13]

Subsequently, by introducing the pentagon and heptagon defects into the contacting region, we constructed four Y-junctions[12] with symmetric geometrical structure, which are shown in Fig. 1. The (Y-a), (Y-b) and (Y-c) all have six heptagon defects,

which are symmetrically distributed with respect to the cross-centre. But the distance between defect and the cross-centre is different for these three models, respectively. Among these three configurations, the distribution of six heptagon defects in (Y-a) is the most uniform one in the region of junction. For (Y-c) the six heptagons centrally localize near the cross-centre. Another (Y-d) model has three octagons, which are symmetrically distributed at the out-side of the connections, away from the cross-centre. According to the results of optimization of geometrical structure by using the universal force field,[21] and analysing both total energy and bond strength, we believe that the junction (Y-a) is the most stable one among these Y-junctions.

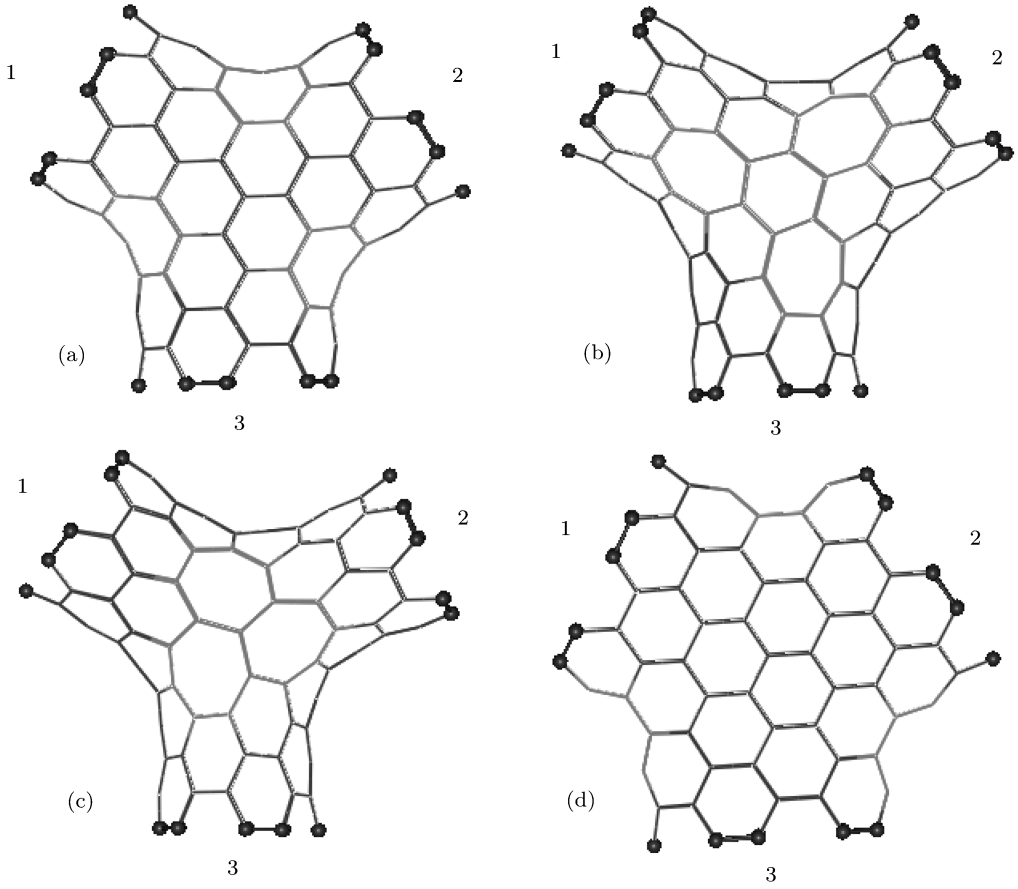


Fig. 1. Four models of three-terminated symmetric Y-junction CNT, in which the solid spheres at three ends will be connected with three semi infinite metal chains, respectively. The sizes of these models shown here are noted by 0/0/0, which is the smallest size for each model in this present work.

Then we use three integers $l/m/n$ to note the Y-junction size. The three integers l, m and n represent the layer numbers of the three branches, respectively. In our present work, each layer includes 10 atoms in (5,5) tube.

3. Results and discussion

Only when layer number $m = 3 \times n + 2$ with n being integer, can one probe the two bands crossed at the Fermi level exactly in armchair tube. In Y-junction (5,5) nanotube, we think there still exists the size effect in its conductance because of the existence of quantum confinement and the interface states. Firstly, we take the first branch as the source one and the two others as two drains. For metal chains its band structure is

$E = -2V'_{pp\pi}\cos(ka)$ with $a = 1$. Due to the flat band structure of chain, there is no any sharp peaks near the Fermi energy in the quantum conductance in Y-junctions. So the quantum conductance is mainly infected by the mismatch between two kinds of states of chain and junction.

3.1. The four situations of three branch sizes

Now we investigate the electronic properties and the quantum conductance of these three-terminal Y-junctions (shown in Fig. 1). At different energies the quantum conductance is very complicated for different size $l/m/n$.

Since the size of Y-junction is controlled by the lengths of three branches, respectively, we increase the junction size according to the following four situations: (i) $m/m/m$ with the same layers in the three branches; (ii) $m/m/n$ with the same layers in the source branch and one of two drain branches. (iii) $l/m/m$ with the same layers in the two drain branches; (iv) $l/m/n$ with the three integers different from each other.

The common characteristics in these four cases are that the space between conductance peaks reduces and the number of peaks increases around the Fermi energy level with the increase of size, as shown in the Fig. 2. Another interesting feature is that the quantum conductance at the Fermi energy periodically oscillates with the size of the junction. Comparing 3/3/3 with 0/0/0, they have the similar behaviour of quantum conductance at the Fermi energy. Similar characteristic also exists in 0/1/1 and 0/4/4 in Fig. 2. Moreover, we also calculate the quantum conductance of the Y-junction with larger size in order to obviously observe this oscillation. Figure 2 shows that this periodic oscillation with increasing size exists along the three directions of three branches in (Y-a) junction, respectively. And the oscillating periodic length along three branches all is 0.369 nm about the distance between 3 layers.

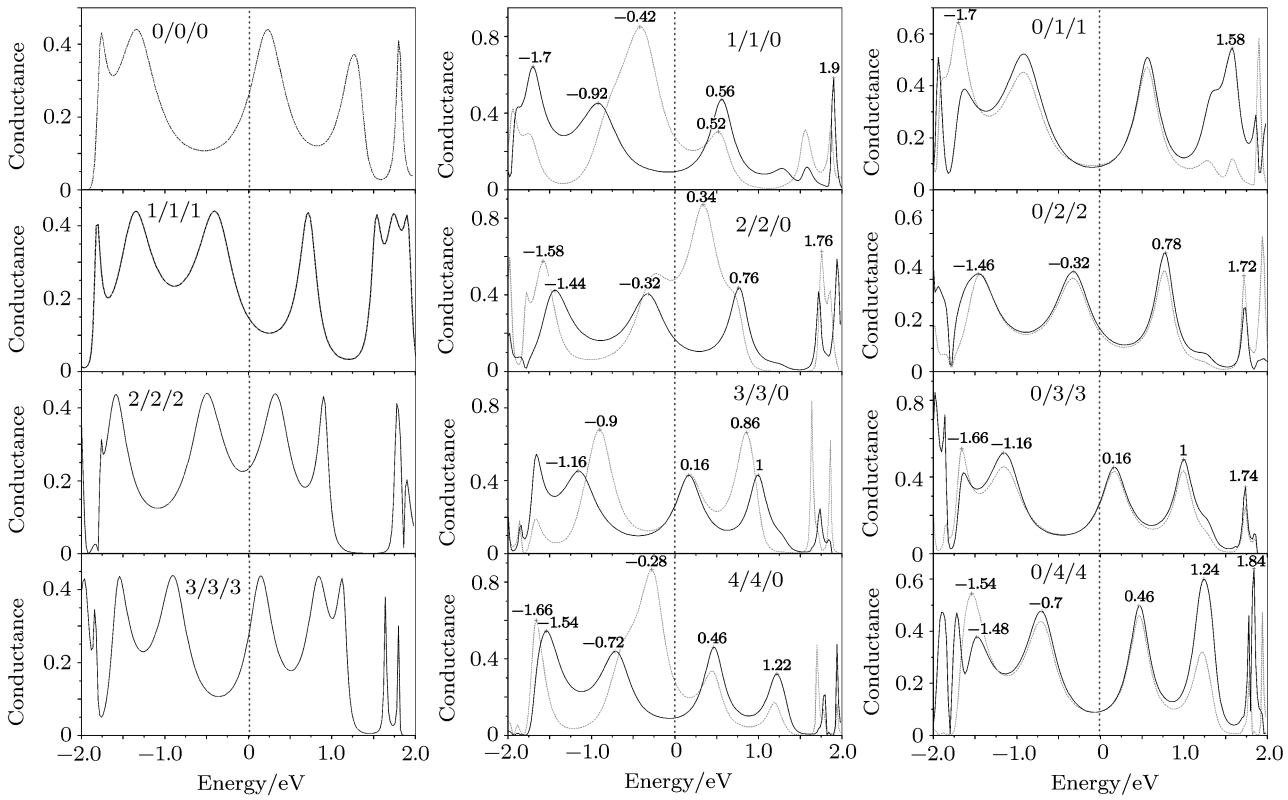


Fig. 2. The quantum conductance of (Y-a) junctions for (i), (ii) and (iii) situations, respectively. The grey dotted line corresponding to T_{12} and the black solid line corresponding to T_{13}.

For the former three situations, the two quantum conductances through two drain branches are shown in Fig. 2. In the first case $m/m/m$, T_{12} and T_{13} are always equal due to symmetric geometric structures. The

conductance at Fermi energy through each drain branch is about $0.26(2e^2/h)$ for 0/0/0, $0.14(2e^2/h)$ for 1/1/1, and $0.23(2e^2/h)$ for 2/2/2, respectively. The maximum of the total conductance at the Fermi energy through two drain branches is not high only about $0.50(2e^2/h)$. However, the electronic current through two drains has the same value at different voltages and increases smoothly with the increase of voltages, shown in the Fig. 3. Thus the (Y-a) junctions with the size of the first situation could be as one stable perfect like-metal junction under any voltage.

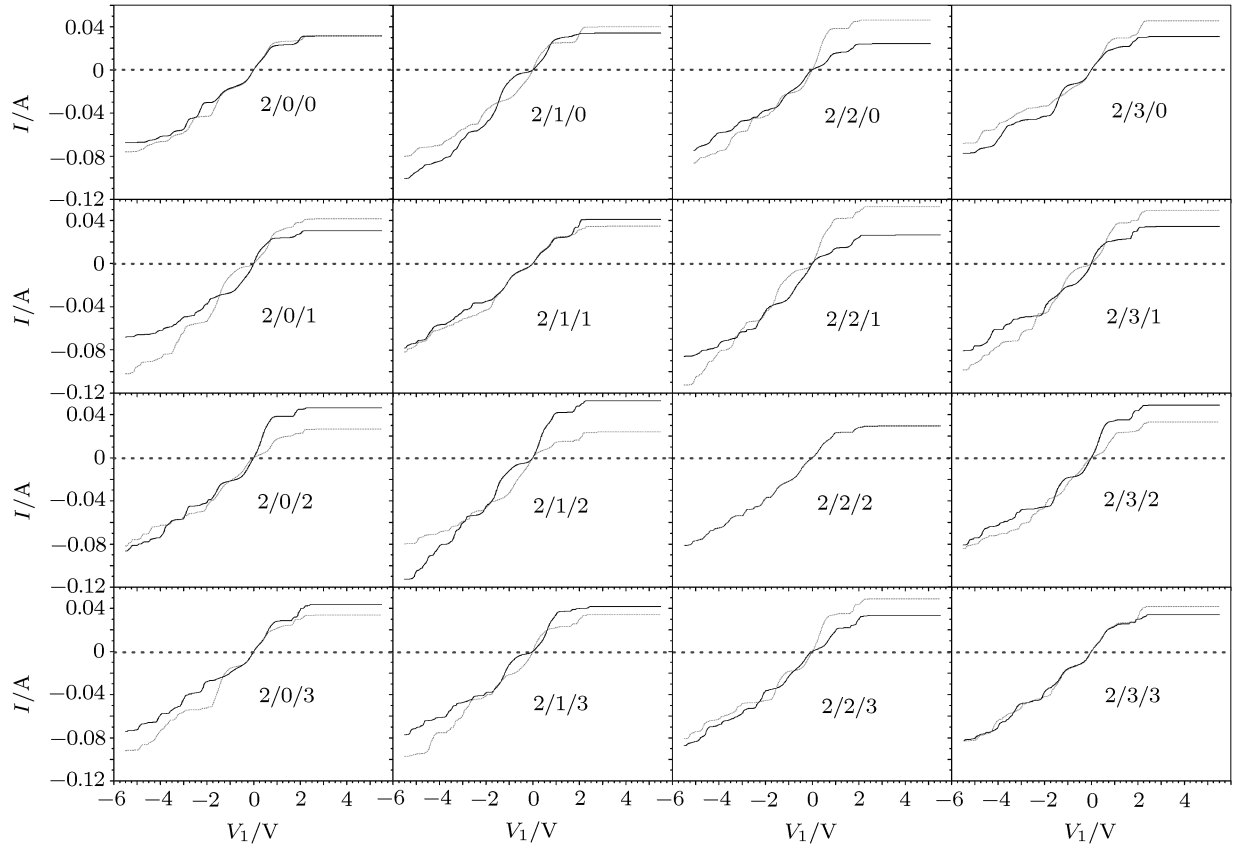


Fig. 3. At $V_2 = 0$ eV, $V_3 = 0$ eV the currents through two drain branches in (Y-a) junctions with $2/m/n$ $(m, n = 0, 1, 2, 3)$ sizes vary with the voltage V_1 on the source branch, respectively. The grey dotted line corresponds to I_{12} and the black solid line corresponds to I_{13}.

In the second situation $m/m/n$, the source branch and one drain branch are symmetric with respect to another drain branch. Although the drain has the same size as the source, its quantum conductance is not always larger than that of another drain branch. From Figs. 2 and 4, we find that the T_{12} at Fermi energy in $2/2/3n$ and $1/1/3n$ are larger than T_{13}, even three times larger than T_{13} in $2/2/3n$. But in $0/0/3n+1$ (or 2) the T_{12} at Fermi energy is three times lower than T_{13}. Now comparing the total conductance values at Fermi energy, we find that it is about $0.55(2e^2/h)$ in 0/0/3, $0.34(2e^2/h)$ in 1/1/3, and $0.58(2e^2/h)$ in 2/2/3, respectively. But in $2/2/3m+1$, its total conductance is up to $0.90(2e^2/h)$, and its two conductance through two drain branches are about the same value. These features are also obviously shown in the current–voltage characteristic of two drain branches in Fig. 3. In 2/2/3 and 2/1/2 the I_{12} at large voltage is larger than I_{13}. Specially, in 2/2/1 the I_{12} is $0.53A$ even about two times of I_{13}. The results show that the junction with the size in this situation is not like metal junction. However, this difference between the electronic current of two drains is like the shunt valve of electronic current. Therefore, according to the results above obtained, we can propose one way to control the two different drain's current by designing the two drain branches with different sizes, such as 2/2/1.

In the third situation $l/m/m$, the two drain branches are symmetric with respect to the source branch. So the two quantum conductances have the similar behaviours near the Fermi energy. This mirror symmetry can

also be seen in the two junctions with sizes $2/k/i$ and $2/i/k$ in the fourth situation. The quantum conductances T_{12} and T_{13} in $2/i/k$ correspond to the T_{13} and T_{12} in $2/k/i$, respectively. From Fig.4, comparing the total conductance at Fermi energy for 0/3/3, 1/3/3 and 2/3/3, for the case $3l + 2/m/m$, we find that its total conductance is the highest among these three cases. So by designing the source branch size we can control the distributary properties of electronic current in this Y-junction. Furthermore, analysing the size types with the similar quantum conductance through two drains near the Fermi energy, such as $l/m/m$ in the third situation and the $m/m/m$ in the first situation, we find that the total conductance in $l/m/m$ is up to about $0.9(2e^2/h)$ higher than the value in the first situation $m/m/m$. And from Fig. 3, its electronic currents through two drains have not any difference near the zero voltage, but have more obvious step-like characteristic with voltage than that in $m/m/m$. Therefore, the (Y-a) junctions with these sizes $l/m/m$ also could be as one stationary perfect like-metal junction near zero voltage.

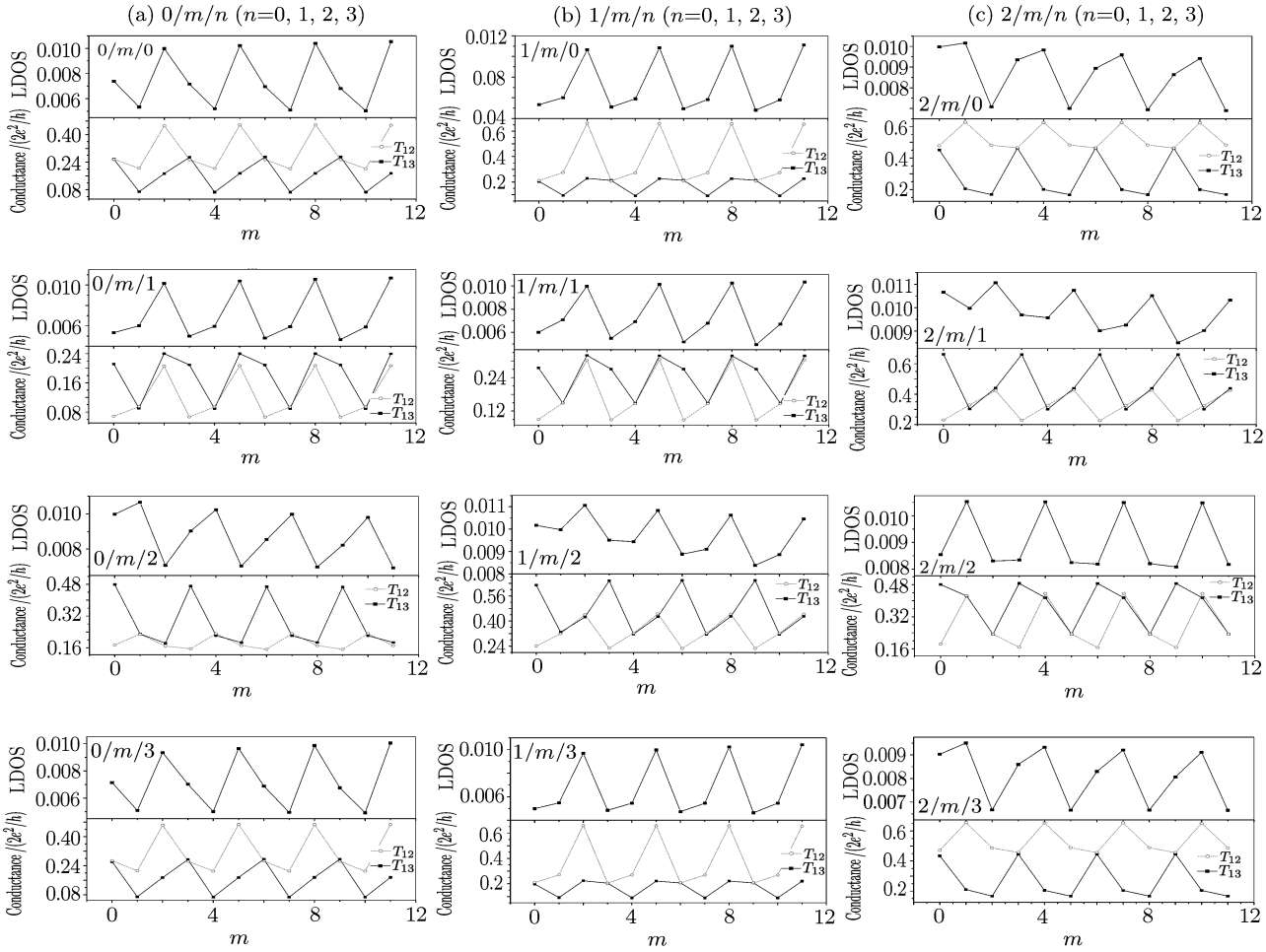


Fig. 4. The conductance and LDOS at the Fermi energy of (Y-a) junctions with different sizes noted by three integers $l/m/n$, taken as three layer numbers in three branches, respectively.

For the fourth situation, the sizes are $3l + 1/3m + 2/3n(l, m, n$ are three different integers), and three integers can exchange their positions under holding of one drain branch size being multiples of 3. Then from Fig. 3, we can find that the conductance T_{12} in 1/2/3 is $0.22(2e^2/h)$, about three times lower than $0.68(2e^2/h)$ of T_{13}. However, as shown in Fig. 3, we find that near zero voltage I_{12} is larger than I_{13}, but at larger positive voltage I_{13} is larger than I_{12}. So we can design the junction with this size as the one kind of device that can modulate the relative value of two drains' current like the shunt valve controlled by voltage.

3.2. The influence of defect distributions

Due to both the various types of size and the complex defect distribution, it is difficult to illustrate the influence in detail in one short paper. In this subsection, we only consider the four Y-junction models with the same size $0/i/0$ to investigate the influence of defect distribution on the quantum conductance.

In Fig. 5, it obviously shows the oscillation characteristic of quantum conductance at the Fermi energy with the size. From the distribution of the six heptagon defects in the three models shown in the Fig. 1, for the uniform spreading situation in the (Y-b) model, the conductance through two drains is two times lower than that of other models. Comparing the relative centralized distribution of the six heptagon defects in (Y-a) with the most centralized (Y-c) model, we find that their total quantum conductances are very similar, but the geometric structure of (Y-a) is more stable than the (Y-c) model.

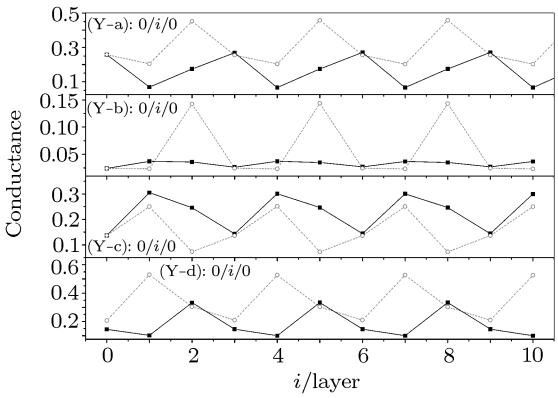


Fig. 5. The conductance at the Fermi energy of four Y-junctions with sizes $0/i/0$, i is the layer number in the second branch, respectively. The grey dotted line corresponds to T_{13} and the black solid line corresponds to T_{12}.

According to these results, the uniform distribution of defects is disadvantageous to the transport of carriers. It also shows that the defect distribution can change the scattering path of the carriers. In addition, in the (Y-c) model the conductance through the branch with the 0 size is lower than another drain branch, being contrary to other three models. When there are only three octagons at the out-side of the connections, the total conductance in (Y-d) model is about $0.68(2e^2/h)$ which is higher than that in the above three models. And the difference between two drains' quantum conductance can be up to five times in (Y-d) model with size $0/1/0$. It shows that the size effect in (Y-d) model is more remarkable.

Although there are different defect distributions in these four models and the behaviour of oscillation are different from each other, the oscillating periodic length is the same about 3 layers.

4. Summary

In our conclusion, for these (5,5) Y-junctions, the quantum conductance at Fermi energy periodically oscillates with the junction size. Furthermore, with different sizes Y-junction exhibits some interesting effects in their quantum conductance such as shunt effect. These properties could be influenced and modulated by three branch sizes and defect distribution. For some special sizes, the difference between two currents through two drain branches may be up to two times. So these special sizes could have an obvious electronic shunt effect in these nanoscale-size molecular devices, which is useful for the design of nano-scale size molecular devices connected with metal chain.

Acknowledgments

We thank Prof. Huang Wei-Cheng for his contributions to the discussion about this work.

References

[1] Tans S J, Devoret M H, Dai H, Thess A, Smalley R E, Geerligs L J and Dekker C 1997 *Nature* (London) **386** 474
Bockrath M, Cobden D H, McEuen P L, Chopra N G, Zettl A, Thess A and Smalley R E 1997 *Science* **275** 1922

[2] del Alamo J A and Eugster C C 1990 *Appl. Phys. Lett.* **56** 78.

[3] Sols F, Macucci M, Ravaioli U and Hess K 1989 *J. Appl. Phys.* **66** 3892

[4] Palm T and Thylen L 1992 *Appl. Phys. Lett.* **60** 237

[5] Worschech L, Weidner B, Reitzenstein S and Forchel A 2001 *Appl. Phys. Lett.* **78** 3325
Xu H Q 2001 *Appl. Phys. Lett.* **78** 2064
Hieke K and Ulfward M 2000 *Phys. Rev.* B **62** 16727

[6] Chico L, Crespi V H, Benedict L X, Louie S G and Cohen M L 1996 *Phys. Rev. Lett.* **76** 971

Chico L, Lopez Sancho M P and Munoz M C 1998 *Phys. Rev. Lett.* **81** 1278
[7] Liu H and Tao Y C 2003 *European Phys. J.* B **36** 411
[8] Liu H and Chen J W 2003 *Acta Phys. Sin.* **52** 664 (in Chinese)
[9] Liu H, Chen J W and Yang H T 2004 *Phys. Stat. Sol.* B **241** 127
[10] Fa W, Chen J W, Lin H and Dong J M 2004 *Phys. Rev.* B **69** 235413
[11] Liu H and Tao Y C 2005 *Nanotechnology* **16** 619
[12] Liu H 2005 *Phys. Lett.* A **339** 378
[13] Nardelli M B 1999 *Phys. Rev.* B **60** 7828
Nardelli M B and Bernholc J 1999 *Phys. Rev.* B **60** 16338
[14] Li J, Papadopoulos C, Rakitin A and Xu J 1999 *Nature*(London) **402** 253
[15] Andriotis A N, Menon M, Srivastava D and Chernozatonskii L 2001 *Phys. Rev. Lett.* **87** 066802
[16] del Valle M, Tejedor C and Cuniberti G 2005 *Phys. Rev.* B **71** 125306
[17] Yin Y J, Chen Y L, Yin J and Huang K Z 2006 *Nanotechnology* **17** 4941
[18] Zhao Q, Feng X Q, Zou J, Yin Y J and Yu S W 2007 *Appl. Phys. Lett.* **91** 043108
[19] Ferreira M S, Dargam T G, Muniz R B and Latge A 2000 *Phys. Rev.* B **62** 16040
Ferreira M S, Dargam T G, Muniz R B and Latge A 2001 *Phys. Rev.* B **63** 245111
[20] Kubo R 1957 *J. Phys. Soc. Jpn.* **12** 570
[21] Yao N and Lordi V 1998 *J. Appl. Phys.* **84** 1939