Electronic delocalization and resonant transmission in symmetric metallic nanowires

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We report here the theoretical studies on electronic delocalization and resonant transmission in symmetric metallic nanowires (SMNs). Resonant transmissions, which are characterized by multiple perfect transmission peaks, have been found in the electronic band gap. The resonant energy and the number of modes of resonant transmission therein can be manipulated, and the quality factor of the perfect transmission peak can be exponentially increased. We suggest that the resonant transmission originates from the electronic delocalization in SMNs, which is characterized by the extended wave function of electrons around the resonant energy. These features open a unique way to control quantum transport in nanodevices. © *2006 American Institute of Physics*.
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With the development of microfabrication technology, much progress has been achieved in the miniaturization of electronic devices.[1–4] Nowadays, the feature size of microelectronics devices may reach several tens of nanometers. It becomes very important to manipulate the electron transport on the nanometer scale, where semiclassical transport theory is invalid and the effect of quantum interference has to be taken into account. The electronic behavior in nanostructures can be described by the Landauer-Büttiker theory.[5–7] On the other hand, the localization-delocalization transition of electrons was first predicted by Dunlap *et al.* in one-dimensional (1D) random-dimer (RD) model in 1990.[8] It was shown that extended states may exist in a system with correlated disorder. Recently electronic delocalization has been experimentally demonstrated in RD GaAs–AlGaAs supperlattice.[9] Up to now, RD model has been generalized to twined disordered system, random trimer, random dimer-trimer, and even random n-mer models.[10,11] Physically, electronic delocalization in RD-like systems originates from the internal structural symmetry (or inverse symmetry) of the impurity cluster. Very recently, the electronic delocalization has also been found in a set of metallic clusters randomly attached to an adsorbed nanowire.[12] These investigations may explain the high conductivity in the system. In this letter we focus on the electronic delocalization and resonant transmission in a symmetric metallic nanowire (SMN) constructed as $S(m,n)=(BA)^m C^n (AB)^m$, where A, B, and C are three types of atoms, and m and n are the repeating numbers of the units.

Now we consider the electron behavior in a host monatomic chain, where a cluster of SMN is inserted. Assuming the host chain is composed of atom A only, in the on-site model, atoms A, B, and C have the energies of ε_a, ε_b, and ε_c, respectively. The nearest-hopping integral is taken as the same constant V. With tight-binding approximation, the Schrödinger equation for a spinless electron in 1D chain can be written in the matrix form of

$$\begin{pmatrix} \psi_{j+1} \\ \psi_j \end{pmatrix} = p_j \begin{pmatrix} \psi_j \\ \psi_{j-1} \end{pmatrix}, \tag{1}$$

with

$$p_j = \begin{pmatrix} (E-\varepsilon_j)/V & -1 \\ 1 & 0 \end{pmatrix}, \tag{2}$$

where ε_j depends on the atom which occupies the jth site, p_j is the transfer matrix that correlates the adjacent site amplitudes ψ_j and $\psi_{j\pm1}$. The whole chain contains three parts: the SMN cluster, its left part, and its right part. The amplitudes of wave functions can be described as $\psi_j = e^{ikj} + re^{-ikj}$ for the left part of the SMN cluster and $\psi_j = te^{ikj}$ for the right part of the SMN cluster. Here r and t are the reflection and the transmission amplitudes of the SMN cluster, respectively.

If the cluster of SMN occupies the sites from $h+1$ to $h+l$, the total transfer matrix across the SMN cluster can be expressed as $\bar{P} = p_{h+l-1} \cdot p_{h+l-2} \cdots p_h$. The correlation between the wave amplitudes at both ends of the SMN cluster can be described as

$$\begin{pmatrix} \psi_{h+l} \\ \psi_{h+l-1} \end{pmatrix} = \bar{P} \begin{pmatrix} \psi_h \\ \psi_{h-1} \end{pmatrix}. \tag{3}$$

For a given $\bar{P}$, the reflection amplitude r and transmission amplitude t can be written as

$$r = -\xi^{2h} \frac{\alpha^T \Gamma \bar{P} \alpha}{\alpha^T \Gamma \bar{P} \alpha^*}, \quad t = \frac{\xi^{-l} 2i \sin k}{\alpha^T \Gamma \bar{P} \alpha^*}, \tag{4}$$

where

$$\xi = e^{ik}, \quad \Gamma = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \alpha = \begin{pmatrix} \xi \\ 1 \end{pmatrix},$$

and α^T is the transpose of α. According to Eq. (4), it is obvious that the reflection and transmission coefficients are determined by the total transfer matrix $\bar{P}$. Moreover, the reflection coefficient will be zero in the following scenarios: (i) $\bar{P}$ is proportional to the unit matrix, (ii) $\bar{P}$ is proportional to

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the promotion matrix for the periodic system, and (iii) $\bar{P}$ is the linear combination of unit matrix and promotion matrix for the periodic system.[13]

It is necessary to pay attention to the total transfer matrix through the SMN cluster, i.e., $\bar{P}$. In the SMN cluster, the atoms are arranged as $(BA)^m C^n (AB)^m$. Define P_L, P_N, and P_R as the transfer matrices across the sites AB, the central atoms C^n, and the sites BA, respectively. It follows that

$$P_L P_N P_R = \begin{pmatrix} u & v \\ w & x \end{pmatrix} \begin{pmatrix} a_{n+1} & -a_n \\ a_n & -a_{n-1} \end{pmatrix} \begin{pmatrix} u & -w \\ -v & x \end{pmatrix} = \begin{pmatrix} G_1 & -H_1 \\ H_1 & -F_1 \end{pmatrix}, \tag{5}$$

where $v=-(E-\varepsilon_b)/V$, $w=(E-\varepsilon_a)/V$, $u=-vw-1$, $x=-1$, and $a_n=[(E-\varepsilon_c)/V]a_{n-1}-a_{n-2}$ with $a_0=0$ and $a_1=1$. The total transfer matrix of the SMN with the structure of $S(m,n)$ can be obtained as follows:

$$\bar{P} = \begin{pmatrix} G_m & -H_m \\ H_m & -F_m \end{pmatrix}. \tag{6}$$

Here, $G_m=u^2G_{m-1}+2uvH_{m-1}+v^2F_{m-1}$, $H_m=uwG_{m-1}+(ux+vw)H_{m-1}+vxF_{m-1}$, and $F_m=w^2G_{m-1}+2wxH_{m-1}+x^2F_{m-1}$. The matrix $\bar{P}$ in Eq. (6) can be further simplified in the following cases: (i) In the case of

$$H_m = 0 \text{ and } G_m = -F_m, \tag{7}$$

the matrix $\bar{P}$ of the SMN cluster will be a unit matrix. (ii) In the case of $H_m \neq 0$, the total transfer matrix $\bar{P}$ has the form

$$\bar{P} = H_m \begin{pmatrix} (G_m+F_m)/H_m & -1 \\ 1 & 0 \end{pmatrix} - F_m \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{8}$$

It is obvious that if

$$(G_m+F_m)/H_m = (E-\varepsilon_a)/V, \tag{9}$$

the total matrix $\bar{P}$ of the SMN will be a linear combination of both a unit matrix and a promotion matrix for the periodic system. Thereafter, if an electron possesses the energy satisfying Eq. (7) or (9), its reflection coefficient will be zero and electrons will transmit perfectly through the SMN cluster. We can conclude that the resonant transmission can happen in the SMN at the energies satisfying Eq. (7) or (9).

Based on the above analysis, we can carry out numerical calculation of electron transport. Figure 1 shows the transmission coefficient T as a function of electron energy in the SMN of $S(5,n)$. There are several interesting features. First, due to the substructures of $(BA)^m$ and $(AB)^m$ in SMN, there is an electronic band gap. Second, there indeed exist perfect transmission peaks in the band gap. Third, the central part C^n determines the peak number and the energy of perfect transmission peaks in the band gap. We find that in the case of even n, there are odd peaks of perfect transmission in the band gap. Whereas in the case of odd n, an even number of perfect transmission peaks appear in the band gap. For example, when we select $n=2,12,22,32$, there exist $2i+1(i=0,1,2,3)$ peaks within the electronic band gap [as shown in Figs. 1(a)–1(d)]. And when the SMN has $n=5,15,25,35$, correspondingly $2i(i=1,2,3,4)$ peaks occur in the band gap in Figs. 1(e)–1(h). Therefore, by increasing n, more and more perfect transmission peaks appear in the band gap of the SMN. This feature originates from the fact that the reflected wave at each interface has changed its phase when n increases. Once the phase difference of the reflected waves becomes an integer multiple of π, the total reflected wave at the interface reaches zero due to interference. As a result, more transmission peaks lie in the band gap by increasing the central part C^n in the SMN.

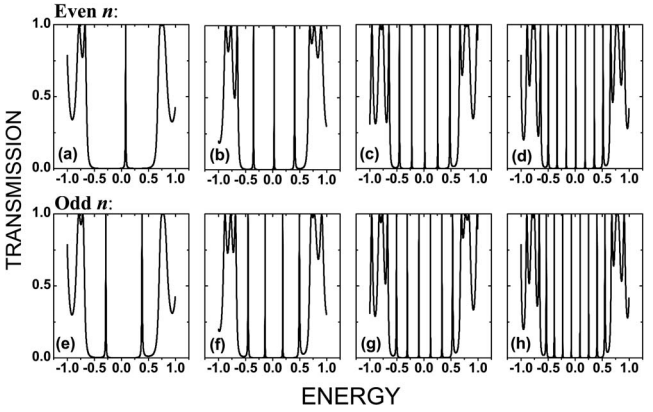

FIG. 1. Transmission coefficient T as a function of the electron energy for the SMN of $S(5,n)$, where $\varepsilon_a=-\varepsilon_b=0.5$, $\varepsilon_c=0$, and $V=1.0$. For even n, (a) $n=2$, (b) $n=12$, (c) $n=22$, and (d) $n=32$, respectively. For odd n, (e) $n=5$, (f) $n=15$, (g) $n=25$, and (h) $n=35$, respectively.

If we define the energy deviation of the nearest peak from the on-site energy of C site as δE, δE will depend on the structural parameter of the SMN. Figure 2(a) shows the relation between δE and n in the SMN with $m=4$, 5, and 8, respectively. Obviously, the nearest peak to $\varepsilon_C=0$ gradually approaches the center of the band gap as n increases. It is interesting to note that δE shows a significant difference for odd n and even n in Fig. 2(a). The main reason is that there is a transmission peak around $E=\varepsilon_C$ in the SMN with even n, but no such peak in the SMN for odd n (as shown in Fig. 1). In order to explain this feature, we consider a case that an electron with energy of $E=\varepsilon_C$ transports through the SMN, where m is supposed to be infinite. Obviously, the central part C^n acts as a well of potential energy, where the width is related to n. At the boundary of the well, there are multiple

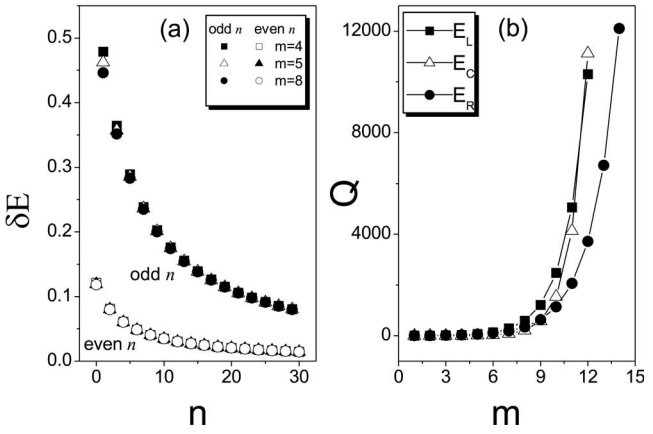

FIG. 2. (a) Relation between δE and n in the SMN $(BA)^m C^n (AB)^m$ with $m=4$, 5, and 8, respectively. δE is the energy deviation of the nearest peak from $\varepsilon_C=0$. (b) The relation between the quality factor Q of the perfect transmission peaks in the band gap and m in the SMN with $S(m,12)$. There are three perfect transmission peaks in the band gap of $S(m,12)$ as shown in Fig. 1(b). These three peaks are located at the electron energies $E_L \cong -0.3520$, $E_C \cong 0.030\,40$, and $E_R \cong 0.4082$, respectively.

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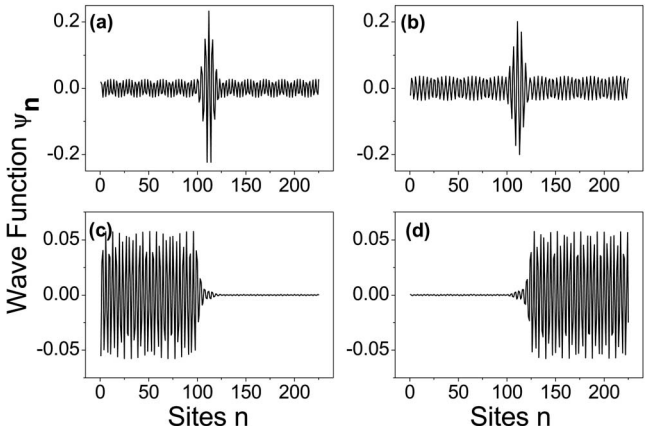

FIG. 3. Wave functions of the electron in the nanowire $S(5,5)$. The electronic states are almost extended when (a) $E_1 \cong -0.285\,371\,35$ and (b) $E_2 \cong 0.383\,400\,33$, respectively. The electronic states are localized when (c) $E_3 \cong 0.014\,571\,411$ and (d) $E_4 \cong -0.019\,991\,903$, respectively.

transmissions and reflections. For transmission waves, the phase difference is $n\pi$ at the boundary of the well. Thereafter, if n is odd, the total transmission wave reaches zero due to the interference and there is no transmission peak at $E=\varepsilon_C$. But if n is even, the total transmission wave is enhanced due to the interference, which is also in agreement with the result based on the transfer-matrix method. The transfer matrix across the central part is $P_N=(-1)^{n/2}I$ in the case of $E=\varepsilon_C$ (here I is a unit matrix). The electron will transmit perfectly through the central part C^n. Moreover, this wave has a resonant tunneling through the left and right substructures of $(BA)^m$ and $(AB)^m$. Therefore, there is indeed a transmission peak at $E=\varepsilon_C$ in the case of even n.

On the other hand, the quality factor Q of perfect transmission peak is determined by parameter m in the SMN. By increasing m, the number of peaks in the band gap does not change and the peak position only shifts slightly [as shown in Fig. 2(a)]. However, increasing m may lead to a significant change of the quality factor Q of the peak, which is defined as $Q=E/\Delta E$, and E is the energy of the peak and ΔE is the half-width of the peak, respectively. Figure 2(b) illustrates the relation between the quality factor Q of the peak in the electronic band gap and the number of m in the SMN for $S(m,12)$. Obviously, the quality factor of the peak increases exponentially by increasing m in the SMN. In some sense, the mode number, the mode energy, and the quality factor Q of the resonant transmissions are related to the structure of the system, which can be described with a "phase diagram."

In order to understand the behavior of electrons in the SMN clearly, the electronic wave function has been studied. The wave function of electrons can be obtained by using the triangular matrix.[14] Figure 3 presents the wave functions in the SMN with $S(5,5)$ when the electron is close to or far away from the resonant energies. As shown in Fig. 1(e), there are two resonant transmission peaks in the electronic band gap of $S(5,5)$, and the resonant modes in the band gap are at the energies with E_1 and E_2, respectively. It is shown that the electronic wave function is almost extended when its energy is close to the resonant energy E_1 [as shown in Fig. 3(a)] or E_2 [as shown in Fig. 3(b)]. In other words, electron with the energy of E_1 or E_2 can propagate through the whole nanowire $S(5,5)$. Meanwhile, a localized wave function can be observed when the electronic energy is far away from the resonant energy E_1 or E_2, as shown in Figs. 3(c) and 3(d), respectively. It is known that electrons with the energy of E_1 or E_2 cannot propagate in the periodic nanowires $(AB)^m$ or $(BA)^m$. Therefore, the electronic localization-delocalization transition has indeed happened at the resonant energies E_1 and E_2 in the SMN of $S(5,5)$. It is the internal symmetry in the SMN that leads to the electronic delocalization, and eventually to the perfect transmission at the resonant energy. We can control the resonant mode, the number of the mode, and the quality factor of the mode in the nanowire by tuning the structural parameter of the SMN. The perfect transmissions with tunable mode and high Q can be obtained by designing a suitable SMN in the system. One may build the high-quality metallic nanowire experimentally by using probes of scanning tunneling microscope[3,15] or by the step decoration on vicinal surfaces.[16] Our investigation opens a unique way to control electronic propagation in nanodevices.

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