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ELECTRICAL CONDUCTANCE OF ZIGZAG NANOGRAPHITE RIBBONS WITH LOCALLY APPLIED GATE VOLTAGE

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The electric conductance of the graphite ribbon with locally applied gate voltage has been studied in terms of the Landauer approach. In the low-energy region, nano-graphite ribbon with zigzag boundaries exhibits the single electronic transport channel due to the edge states. The chemical potential dependence of the electric conductance shows qualitatively different behavior, depending on whether the magnitude of the potential barrier (gate voltage bias) V_g is larger than the energy gap Δ of the single channel region of the zigzag ribbon. For positive V_g with $V_g < \Delta$, the zero-conductance resonances appear for $0 \leq E \leq V_g$, and average transmission probability is quite small in this region. However the transmission probability is almost one, i.e. perfect transmission, for $E > V_g$. This step-function-like behavior of the conductance shows that it is possible to fabricate a nano-graphite-based switching device by the application of weak gate voltage bias.

1. Introduction

Nanometer-sized carbon systems such as carbon nanotubes[1,2] and nano-graphites[3–7,9,10] have attracted much attention due to their possibilities as carbon-based molecular-electronic devices. In these systems, the topology of sp^2 carbon networks has much influence on the electronic states near the Fermi level. Recent theoretical studies indicate that in nano-size carbon systems with open boundaries, the size of the system and shapes of graphite edges strongly affect their π-electronic states.[3] For the model of graphite ribbons, it has been shown that ribbons with zigzag edges (zigzag ribbon) possess localized edge states with energies close to the Fermi level.[3,9,10] These edge states correspond to the non-bonding molecular orbitals, where the electrons are strongly localized near the zigzag edge. Although the non-bonding state cannot carry the electric currents, the overlap of two edge

states from the two edges of a ribbon yields bonding and anti-bonding states and gives the single channel for electron transport.[11,13]

Recently there are some experimental attempts to control and fabricate the nano-size carbon systems.[6–8] One is the preparation of a single nano-graphene derived from heat-treated nano-diamond particles on a highly oriented pyrolytic graphite (HOPG),[6] another is the fabrication of the nano-graphite ribbon on the metallic substrate using the epitaxial growth techniques.[7] The progress of experimental research becomes the basis of the fundamental technology toward the nanographite-based electronic devices. Therefore, from theoretical and experimental point of view, it is interesting to study the electronic transport properties of nanographite ribbons.[11,13] In this paper, we study the electrical conductance of the zigzag nanographite ribbons with local application of gate voltage, which suggest the possibility of nanographtie-based switching electronic devices.

2. Electronic States of Zigzag Ribbons

We use tight-binding Hamiltonian defined by

$$H = \sum_{i,j} t_{i,j} |i\rangle\langle j| + \sum_{g} V_g |g\rangle\langle g| \tag{1}$$

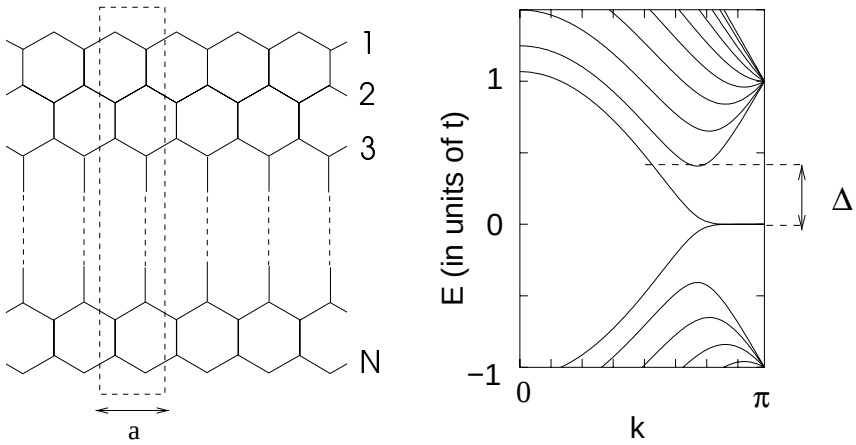
where $t_{i,j} = -t$ if i and j are nearest neighbors, otherwise 0, and $|i\rangle$ is a localized orbital on site i. The summation $\sum_g$ is taken for all sites applied gate voltage. We incorporate the effect of the application of local gate voltage via the variation of the onsite potential in this tight binding model. The nearest-neighbor hopping integral t is used as the unit of energy throughout this paper. Electrical conductance is evaluated using the Landauer formula,[12]

$$G(E) = \frac{e^2}{\pi\hbar} T(E) = \frac{e^2}{\pi\hbar} |t(E)|^2 \,, \tag{2}$$

where T and t are the transmission probability and transmission coefficient. We use the recursive Green function techniques for the calculation of transmission coefficients.[14] Here, E is the chemical potential of the lead lines. We take $e^2/\pi\hbar$ as the unit of conductance throughout this work.

In Fig. 1(a), the graphite ribbon with zigzag edges (zigzag ribbons) is shown. The ribbon width N is defined by the number of zigzag lines. We define the length of the unit cell as a, which is set as unity. We show the energy band structure of the zigzag ribbon for $N = 10$ in Fig. 1(b). The zigzag ribbons is metallic for all N. One of the remarkable features is the appearance of partly flat bands at the Fermi level ($E = 0$), where the electrons are strongly localized near zigzag edges.[3] Although the edge state has non-bonding character, the overlap from the two sides of the ribbon yields bonding and anti-bonding configurations. As a result a weak dispersion of these states along the ribbon is realized, which leads to one channel for electron transport. We define the magnitude of the single-channel energy region as Δ. This Δ decreases with increasing ribbon width, i.e. $\Delta \propto 1/N$.[15]

The effect of the gate voltage is represented by rectangle potential with length L and height V_g, as shown in Fig. 2. The length L of the potential barrier is defined by the number of slices of applied gate voltage.



(a) (b)

Fig. 1. (a) Graphite ribbon with zigzag edges, the rectagle with dashed line is the unit cell. (b) The energy band structure of zigzag ribbon for $N = 10$.

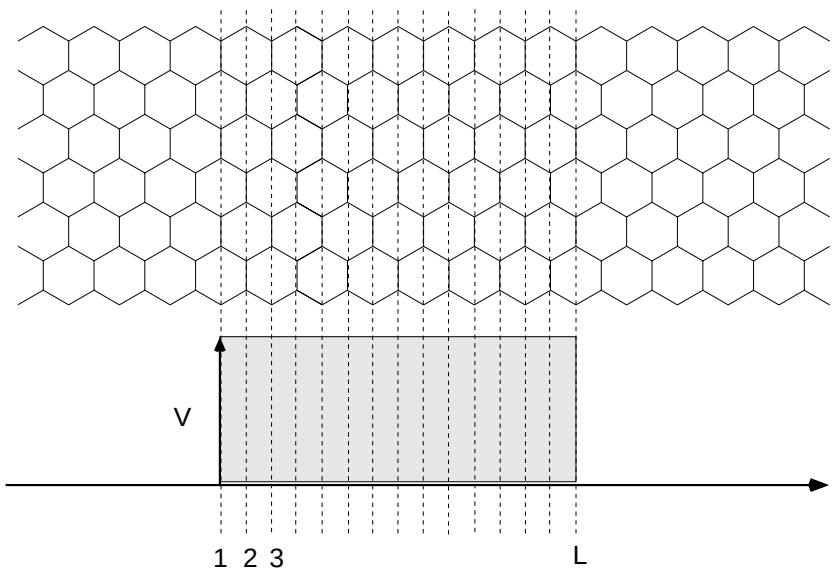


Fig. 2. The rectangle potential with the magnitude V_g is applied from 1st slice to Lth slice.

3. Numerical Calculation

In this section, we demonstrate the result of numerical calculation on the electrical conductance through the zigzag nanographite ribbon with locally applied gate voltage. The application of the local gate voltage can make the single or double potential barrier in the graphite ribbon. The chemical potential dependence of the electric conductance shows qualitatively different behavior, depending on whether the magnitude of the potential barrier (gate voltage bias) V_g is larger than the energy gap of the single channel region of the zigzag ribbon Δ. In the case of the single-barrier potential with positive V_g of $V_g < \Delta$, the zero-conductance resonances appears in the $0 \leq E \leq V_g$, and average transmission probability is quite small in this region, but the transmission probability becomes almost one for $E > V_g$. This result supports that it is possible to make a switching device by the application of weak gate voltage bias. In the case of the double-barrier potential, we found the clear resonant tunneling behavior of the conductance. This result supports that we can fabricate a quantum dot system on the nanographite zigzag ribbon by using the two seperate gate.

3.1. *Single potential barrier*

It is instructive to study the electron tunneling through the potential barrier with $L = 1$. There are two types of carbon slices in the zigzag ribbons, which called α and β slice as shown in Fig. 3. For even N, the α and β-slice are not equivalent. However, for odd N, the α and β-slice are equivalent, because of the mirror symmetry with respect to the translational axis of the zigzag ribbon. Figure 4 shows the chemical potential dependence of the conductance through the $L = 1$ potential barrier, for (a) $N = 10$ and (b) $N = 11$. For even N, there are differences in the behavior of the

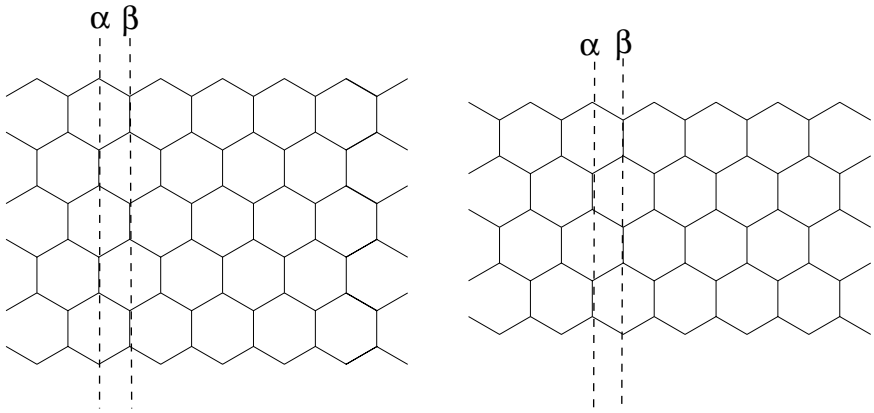
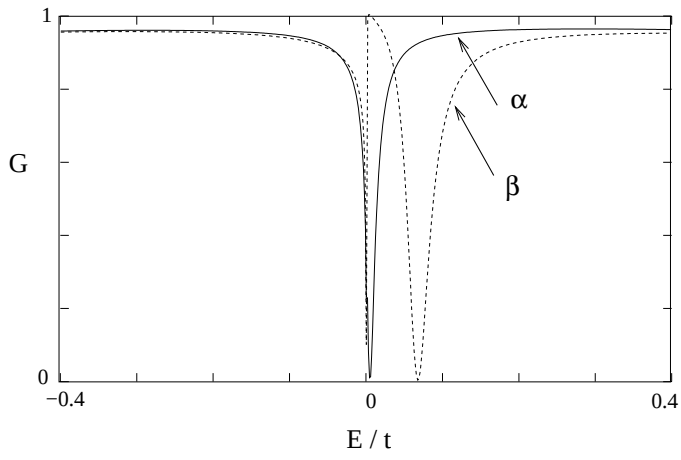
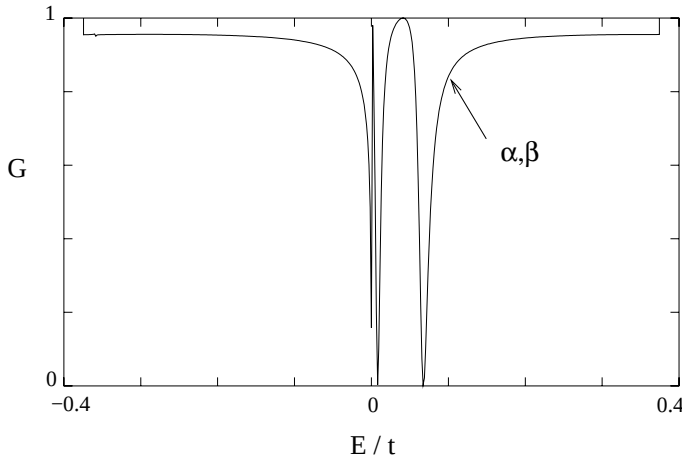


Fig. 3. Two kinds of slices in a zigzag ribbon for N is (a) even and (b) odd.



(a)



(b)

Fig. 4. The chemical potential dependence of the conductance of zigzag ribbon with the potental barrier of $L = 1$ and $V = 0.3$, for (a) $N = 10$ and (b) $N = 11$.

conductance between α and β-slice. But, for the odd N, both α and β-slice work equivalently as expected. This even-odd effects rapidly disappear with the increase in the length of the potential barrier. It should be noted that these dip structures are perfect reflection, i.e. zero-conductance resonance.[11,13] We have also checked that the phase of the transmission coefficient has the clear π-phase jump at each zero-conductance energy point. The π-phase jump guarantees perfect reflection.[11] Since the simple 1D free electron systems with single electron channel do not show such dip structures, these dip structures are originated from the topological nature of the hexagonal lattice.[13] It is also mentioned that the results for negative V_g can be obtained by reversing the sign of the chemical potential, i.e. $E \to -E$.

Figure 5 shows chemical potential dependence of the conductance for the potential barrier with $L = 10$. We change the height of the potential in the range $0.1 \leq V_g \leq 1.0$. Here we restrict the chemical potential in the single-channel energy region of the left lead line, i.e. $|E| < \Delta$, where $\Delta \sim 0.4$ in this case.

In Fig. 5, it is found that the behavior of the conductance is quite different irrespective of the height of potential V_g as compared to the energy width of a single-channel region Δ. When the potential V_g is smaller than Δ, we can find the clear dip structures in the region of $0 \leq E \leq V_g$. Interestingly, the conductance has the almost perfect transmission except for the region $0 \leq E \leq V_g$. These results remind us that the application of gate voltage can be a good switching method in zigzag nano-graphite ribbons. On the other hand, when the height of the potential V_g is larger than Δ, quite irregular dependence of the conductance appears.

Here we explain the reason behind the qualitative change of the conductance behavior based on the energy band structures of zigzag ribbon. Figure 6 shows

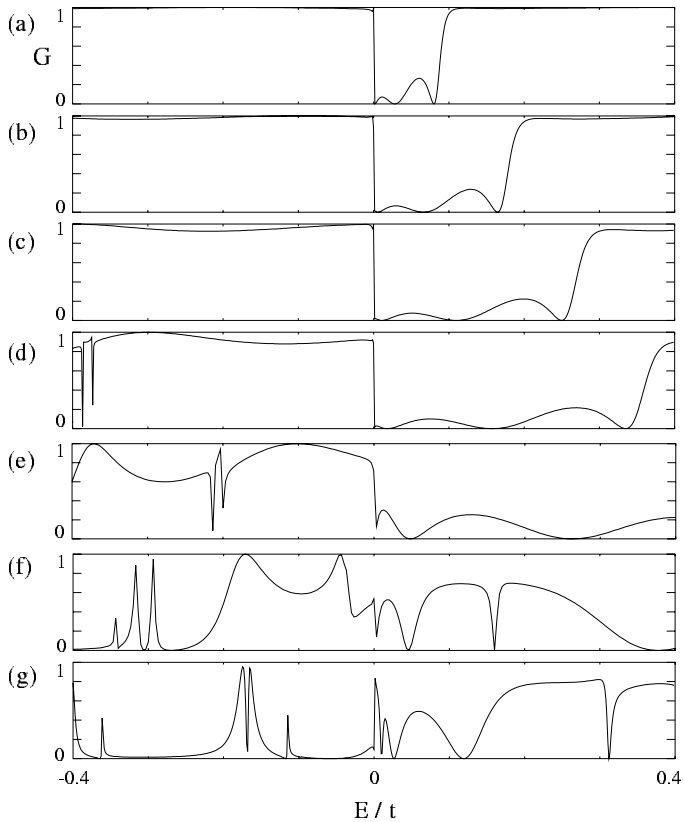


Fig. 5. The chemical potential dependence of the conductance of zigzag ribbon ($N = 10$ and $\Delta \sim 0.4$), where the potential barrier is $L = 10$, (a) $V_g = 0.1$, (b) $V_g = 0.2$, (c) $V_g = 0.3$, (d) $V_g = 0.4$, (e) $V_g = 0.6$, (f) $V_g = 0.8$ and (g) $V_g = 1.0$.

energy band in (a) the lead line and (b) the region applied where the gate voltage $V_g \leq \Delta$. The energy band in the potential barrier shifts with the magnitude V_g, in accordance to the magnitude of the gate voltage. It should be noted that an electron with energy $E \in (0, \Delta)$ passes through the single channel in the whole sample. However, when $V_g > \Delta$ (Fig. 7), an electron with energy of $E \in (0, \Delta)$ in the lead comes to multi-channel in the potential. Therefore the multiple scattering of the electrons with inter-band transition occurs in the potential barrier region, resulting in the complicated behavior of conductance for $V_g \geq \Delta$. In addition, if the potential V_g is larger than the half of the bandwidth ($\sim 3t$), there is no conducting channel in the potential barrier region. As a result, no electron transmission occurs.

Figure 8 shows the chemical potential dependence of the conductance for $N = 10$, $V_g = 0.3$ and $\Delta \sim 0.4$. Here we change the length L of the potential barrier in the range of $1 \leq L \leq 50$. The perfect reflection appears in the range where the width of the potential L is almost equal to the width of the ribbon N. Furthermore,

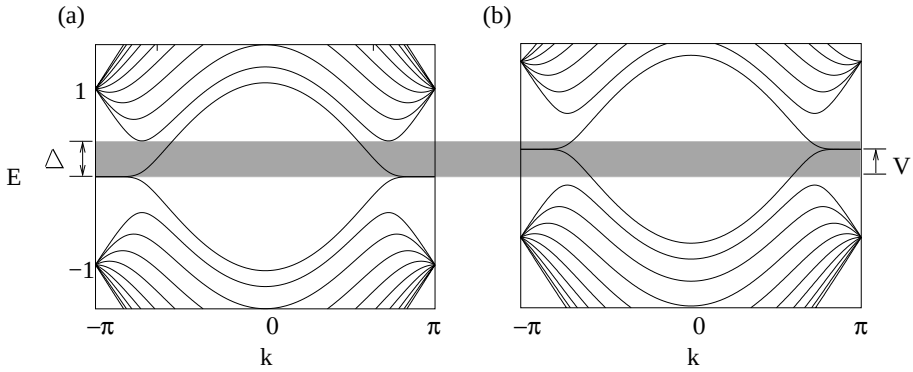


Fig. 6. The schematic energy band structure of zigzag ribbon with $N = 10$ in the (a) lead line and (b) potential barrier when $V_g \leq \Delta$.

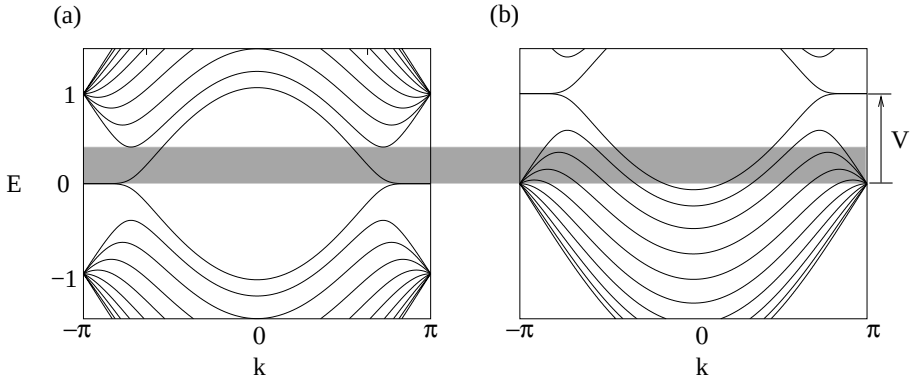


Fig. 7. The schematic energy band structure of zigzag ribbon with $N = 10$ in the (a) lead line and (b) potential barrier when $V_g > \Delta$.

for $L \gg N$, the transmission probability becomes close to zero with the energies lower than V_g.

Now let us consider rather a more realistic potential barrier than the simple rectangle potential barrier. In the realistic system, both ends of the potential might have a certain amount of inclination. Here we express both ends of the potential by the Gaussian function $V_g e^{-\alpha(x-x_0)^2}$ as shown in Fig. 9. Here, V_g is the maximum of potential energy, L is the length between centers of two gaussian functions, and α is the Gaussian parameter.

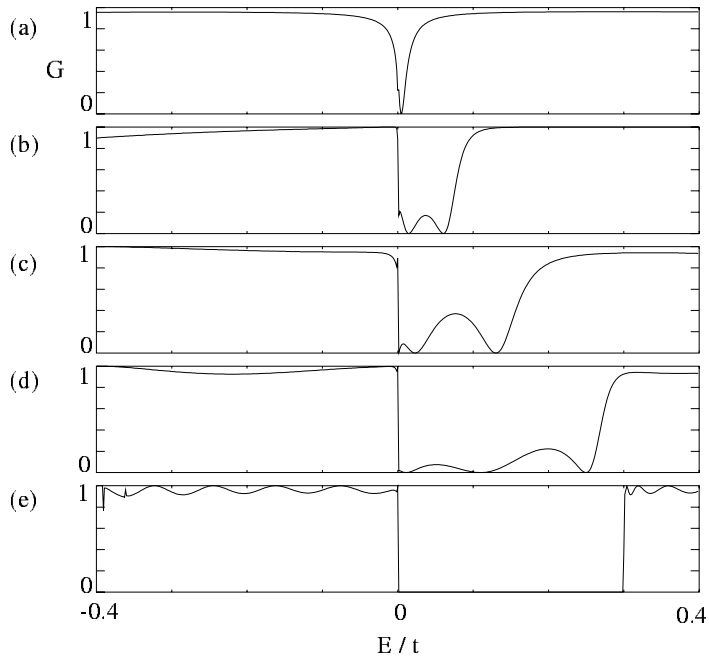


Fig. 8. The chemical potential dependence of conductance of zigzag ribbon with $N = 10$, $V_g = 0.3$ for (a) $L = 1$, (b) $L = 2$, (c) $L = 3$, (d) $L = 10$ and (e) $L = 50$.

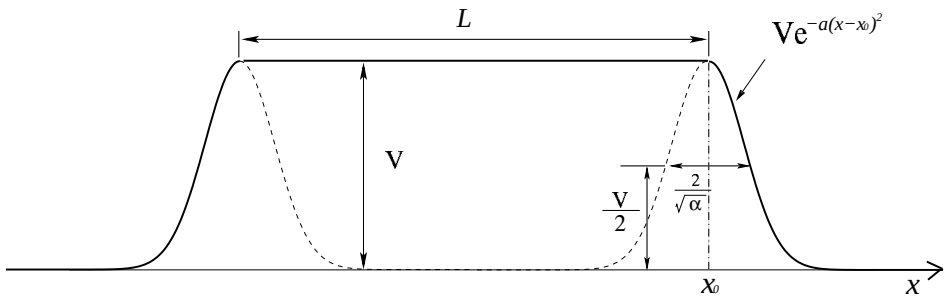


Fig. 9. The potential barrier both ended with Gauss function

Figure 10 shows chemical potential dependence of conductance for $N = 10$, $L = 10$ and $\alpha = 0.1$. Here we change the potential height V. Also in this case, an anti-resonance state appears in the domain of $V \leq \Delta$. For $V > \Delta$, the conductance irregularly depends on the chemical potential. Since similar behavior as the case of rectangle potential has been observed, the rectangle potential can well-reproduce the realistic cases in the low-energy electron transport of the nanographite ribbon systems.

Figure 11 shows the chemical potential dependence of conductance for $N = 10$, $L = 10$ and $V = 0.3$. Here we change the Gaussian parameter in the range of $0.01 \leq \alpha \leq 5.0$. For $0 < E < V$, the conductance becomes quite small, otherwise

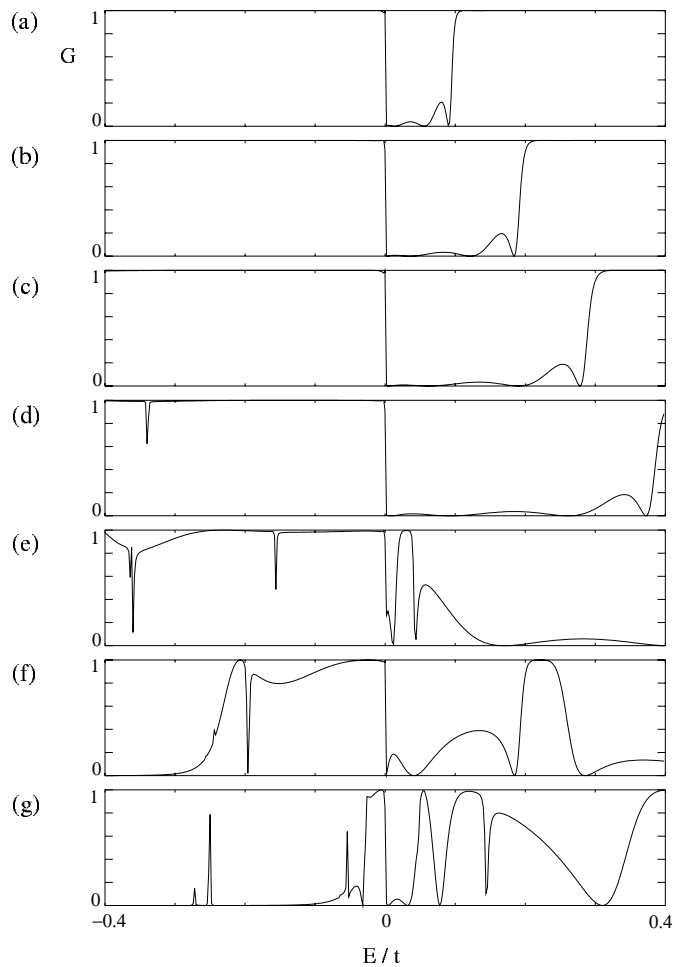


Fig. 10. The chemical potential dependence of the conductance of the zigzag ribbon ($N = 10$, $L = 10$) with Gaussian potential barrier of (a) $V_g = 0.1$, (b) $V_g = 0.2$, (c) $V_g = 0.3$, (d) $V_g = 0.4$, (e) $V_g = 0.6$, (f) $V_g = 0.8$, and (g) $V_g = 1.0$, where $\alpha = 0.1$.

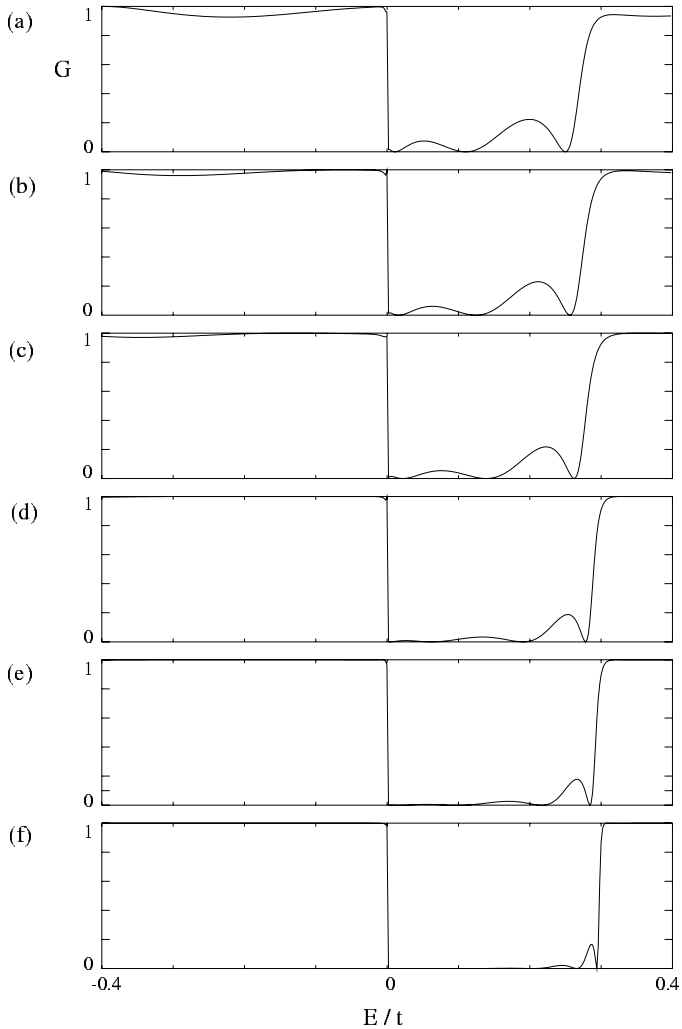


Fig. 11. The chemical potential dependence of the conductance of the zigzag ribbon ($N = 10, L = 10, V_g = 0.3$) for (a) $\alpha = 5.0$, (b) $\alpha = 1.0$, (c) $\alpha = 0.5$, (d) α=0.1, (e) $\alpha = 0.05$ and (f) $\alpha = 0.01$.

the conductance becomes almost one. Thus, we can recognize that the rectangular potential is simple, but can well-reproduce the results of more realistic potential cases.

3.2. *Double barrier system — quantum dot*

In this section, we briefly mention the electronic transport through the double potential barrier system as shown in Fig. 12. In this system, the region sandwiched by the barriers plays the role of a quantum dot. The electron can tunnel through the discrete energy levels, resulting in resonant tunneling. In Fig. 13, it is shown that

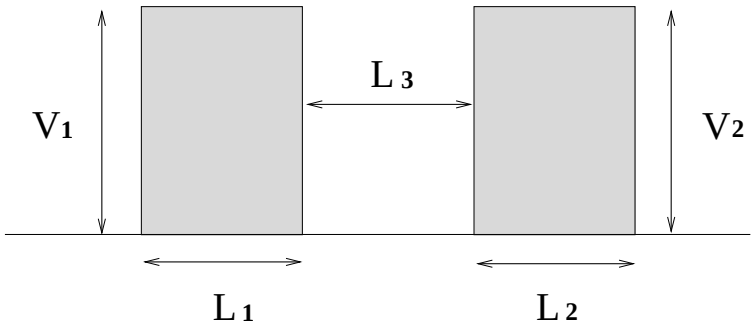


Fig. 12. The geometry of the double barrier potential system.

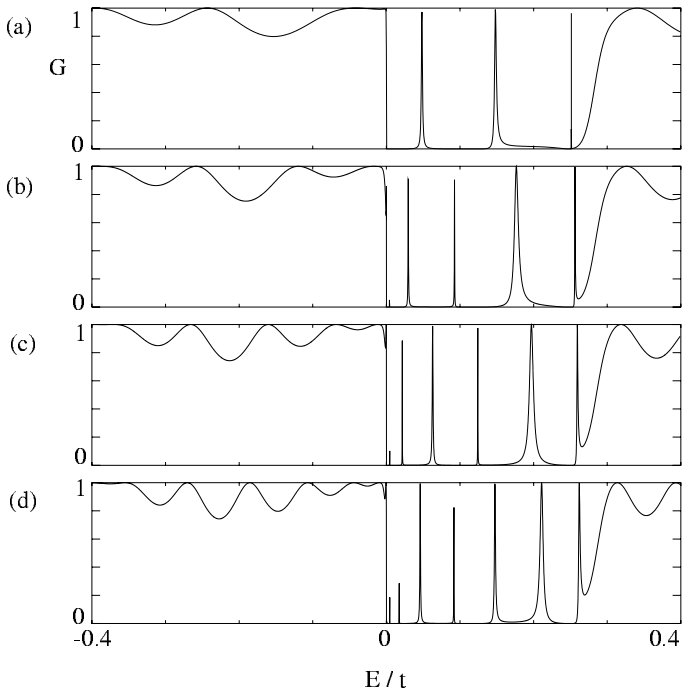


Fig. 13. The chemical potential dependence of the electrical conductance in the double barrier system, where V_3, $N = 10$, $V_1 = V_2 = 0.3$ and $L_1 = L_2 = 10$ for (a) $L_3 = 10$, (b) $L_3 = 20$, (c) $L_3 = 30$ and (d) $L_3 = 40$.

the chemical potential dependence of the double barrier system with $V_1 = V_2 = 0.3$ and $L_1 = L_2 = 10$ for various L_3. The clear resonant tunneling states are found in the energy region with $E \leq V_1$. This result demonstrates that it is possible to fabricate the quantum dots in the zigzag graphite ribbons by the application of two separate gate voltage.

4. Summary

In this work, we have studied the electrical conductance of zigzag graphite ribbons through locally applied gate voltage. The chemical potential dependence of the electrical conductance shows qualitatively different behavior, depending on whether the magnitude of the potential barrier V_g is larger than the energy gap of the single channel region of the zigzag ribbon Δ. For single potential barrier with positive V_g of $V_g < \Delta$, zero-conductance resonances appears in the $0 \leq E \leq V_g$ region, and average transmission probability is quite small in this region, otherwise the transmission probability is almost one. This result supports the fact that it is possible to make a switching device by applying a very weak gate voltage bias. For $V_g > \Delta$, the transmission probability shows quite irregular behavior, which is due to the multiple inter-subband electron scattering in the potential region. Futhermore, we have also also studied the double-barrier potential problem, we found the clear resonant tunneling behavior of the conductance. This result supports that we can fabricate a quantum dot system on the nanographite zigzag ribbon by using the two seperate gates.

Acknowledgments

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References

1. M. S. Dresselhaus, G. Dresselhaus and P. C. Eklund, *Science of Fullerenes and Carbon Nanotubes* (Academic Press, San Diego, 1996).
2. R. Saito, G. Dresselhaus and M. S. Dresselhaus, *Physical Properties of Carbon Nanotubes* (Imperial College Press, London, 1998).
3. M. Fujita, K. Wakabayashi, K. Nakada and K. Kusakabe, *J. Phys. Soc. Jpn.* **65**, 1920 (1996).
4. Y. Shibayama, H. Sato, T. Enoki and M. Endo, *Phys. Rev. Lett.* **84**, 1744 (2000).
5. O. E. Andersson, B. L. V. Prasad, H. Sato, T. Enoki, Y. Hishiyama, Y. Kaburagi, M. Yoshikawa and S. Bandow, *Phys. Rev.* **B58**, 16387 (1998).
6. A. M. Affoune, B. L. P. Prasad, H. Sato, T. Enoki, Y. Kaburagi and Y. Hishiyayma, *Chem. Phys. Lett.* **348**, 17 (2001).
7. M. Terai, N. Hasegawa, M. Okusawa, S. Otani and C. Oshima, *Appl. Sur. Sci.* **130–132**, 876 (1998); C. Oshima, private communication.
8. E. Dujardin, T. Thio, H. Lezec and T. W. Ebbesen, *Appl. Phys. Lett.* **79**, 2474 (2001).
9. K. Nakada, M. Fujita, G. Dresselhaus and M. S. Dresselhaus, *Phys. Rev.* **B54**, 17954 (1996).
10. K. Wakabayashi, M. Fujita, H. Ajiki and M. Sigrist, *Phys. Rev.* **B59**, 8271 (1999).
11. K. Wakabayashi and M. Sigrist, *Phys. Rev. Lett.* **84**, 3390 (2000).
12. M. Büttiker, Y. Imry, R. Landauer and S. Pinhas, *Phys. Rev.* **B31**, 6207 (1985).

13. K. Wakabayashi, *Phys. Rev.* **B64**, 125428 (2001), references all therein.
14. A. MacKinnon, *Z. Phys. B - Condensed Matter* **59**, 385 (1985); T. Ando, *Phys. Rev.* **B44**, 8017 (1991).
15. The zigzag (bearded) ribbons at $k = \frac{2\pi}{3a}$ can be mapped to a finite one-dimensional chain with $2N$ $(2N + 1)$ sites, which can be solved analytically (see the appendix of Ref. 10). From this analytic solution, the form of Δ_z (Δ_b) is easily derived.