褶皱石墨带的电子输运性质

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摘要: 利用递推格林函数方法, 我们研究了褶皱石墨带的电子输运性质. 当石墨带具有褶皱时, 对于锯齿型石墨带, 在第一个范霍夫奇点内, 发现了电导隙和伴随着电导振荡的微带. 然而, 对于金属性扶手型石墨带, 在费米能附近仅发现了电导隙, 说明扶手型石墨带发生了金属-半导体转变. 随着石墨带的褶皱加强, 无论是锯齿型还是扶手型石墨带, 平均电导都逐渐减小, 并趋于0. 结果有利于我们理解真实构型石墨带的电子输运性质, 并且有助于设计基于石墨带的纳米器件.

关键词: 紧束缚模型; 格林函数; 石墨带; 电导

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Transport Properties of Corrugated Graphene Nanoribbons

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Abstract: We studied the transport properties of corrugated graphene nanoribbons by the recursive Green function method. We show that in the presence of ripples the minigaps with zero conductance and minibands with conductance fluctuations form in the zigzag ribbons among the first Van Hove singularity. For the metal armchair ribbons a conductance gap is present in the vicinity of the Fermi energy, which corresponds to a metal-semiconductor transition. With the fluctuation of ripples intensifying the overall averaged conductance decreases for both the zigzag and armchair ribbons and it tends to be zero. These results are useful for a better understanding of the electronic transport properties of realistic graphene nanoribbons and will be helpful for the design of nanodevices based on graphene.

Key Words: Tight-binding model; Green function; Graphene-nanoribbon; Conductance

1 Introduction

Since the graphene sheets have been successfully isolated by Novoselov, Geim, and co-workers,^{1,2} this new material has attracted a great deal of attention. The electrons in graphene obey the relativistic Dirac equation instead of the Schrödinger equation.²⁻⁸ At the room temperature, quantum Hall effect was observed together with large coherence length and high electronic mobility.^{9,10} Therefore, in addition to being a tool for

studying fundamental physics, graphene is also of interest for device applications.

Peierls^{11,12} and Landau *et al.*^{13,14} predicted theoretically that two dimensional (2D) lattice can not exist at any finite temperature. The numerous followed experiments on thin films have been in accord with the theory.¹⁵⁻¹⁷ However, although the theory does not allow perfect 2D crystals existing in three dimensional (3D) space, it does not forbid nearly perfect 2D crystals in 3D space.

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In experiment, a single-atom-thick graphene sheet is usually studied by suspending it on a micron-sized metal grid or by supporting it on a substrate such as SiO₂.^{18–20} The sheet is not perfectly flat but contoured with intrinsic ripples. The ripple has been reproduced theoretically by Monte Carlo simulations method.²¹ It is argued that the anharmonic coupling between bending and stretching modes in graphene causes the rippling and is responsible for the stability of the 2D crystal. Theoretical calculations show that the existence of ripples in graphene will give rise to charge inhomogeneities.^{22,23} Charge anisotropies in monolayer graphene have also been recently observed in experiments.²³ Therefore, one can expect that the ripples in graphene have pronounced effects on electronic structure and thus the transport properties.

In this work, we carry out a numerical study of transport properties of the corrugated graphene nanoribbons (GNRs) with varying widths, which can be realized either by cutting mechanically exfoliated graphenes,^{24,25} or by patterning epitaxially grown graphenes.^{26,27} For simplicity, we focus here mainly on periodical sine/cosine structure corrugated GNRs, as shown in Fig.1, and many intrinsic physical properties are observed.

2 Model and method

To explore the electronic properties of the corrugated graphene ribbon, we divide the graphene ribbon into three regions (as shown in Fig.1): the left lead, the central sample, and the right lead. The width of corrugated GNRs in the central sample is labeled by N ,²⁸ which is consistent with the width of the two leads. The corrugated GNRs are made of P unit cells, and the number of atoms in a unit cell is $2N$.²⁸ The fluctuations of GNRs satisfy the sinusoidal function. The position of random carbon atoms in corrugated GNRs fits well to $A_z = A \sin(mA_x)$. A represents the amplitude of the corrugated GNRs. A_x and A_z are coordinates of carbon atoms along the x and z axes, respectively.

The electronic properties of GNRs have been explored in the context of various methods.^{28,29} We adopt the simplest tight binding model in this paper, which assume the graphene ribbon to be sp^2 bonded network. The corresponding single particle Hamiltonian is

$$\mathbf{H} = \sum_i \varepsilon_i c_i^\dagger c_i + \sum_{i,j} \gamma_0 f(r_{ij}) c_i^\dagger c_j \quad (1)$$

where ε_i is the on-site potential. To consider the variations of bond length, the constant hopping parameter γ_0 between the first neighbor sites is multiplied by a modified factor $f(r_{ij}) = e^{-3.37(r_{ij}/r_0 - 1)}$.³⁰ The value of r_{ij} is the bond-length between

Fig.1 Schematic of an armchair corrugated GNR connecting to semi-infinite leads

the sites i and j . $\{c_i^\dagger, c_j\}$ are the creation and annihilation operators at site i and j . In our model, ε_i is set to be zero and hopping parameter $\gamma_0 = -2.7$ eV.

The transmission coefficient between the left and right leads can be calculated by³¹

$$T = \text{Tr}(\Gamma_L G^r \Gamma_R G^a) \quad (2)$$

where $\Gamma_{L(R)} = i[\Sigma_{L(R)}^\dagger - \Sigma_{L(R)}]$ are the coupling of the corrugated GNRs to the left and right leads. $G^{r,a}$ is the retarded and advanced Green function matrices of the device. Based on Landauer-Büttiker theory, the conductance G through the corrugated GNRs is given by $G = (2e^2/h)T$.

The density of states (DOSs), of the corrugated GNRs is calculated by

$$\text{DOS} = -\frac{1}{\pi} \text{Im}[\text{Tr}G^r(E)] \quad (3)$$

Eq.(1) can be written as a block tridiagonal matrix, which follows that $(\varepsilon I - H_{II} - \sum_L \delta_{L,1} - \sum_R \delta_{P,P})G_{IP}^r - \sum_J H_{IJ}G_{JP}^r = I\delta_{IP}$, with $I=1, 2, \dots, P$. P is the number of unit cell and I is the random unit cell. To calculate the transmission coefficients of interest, the key of the problem lies in the calculations of submatrix $G_{1,P}$ in the Green function for a much larger sample. In the present paper, we employed a recursive Green function method to decimate all the intermediate parameters of a much large system. According to the Dyson equation $G = G^0 + G^0 \hat{V} G$, a set of recursive formula can be obtained:

$$\begin{aligned} \langle i+1 | G^{i+1} | i+1 \rangle^{-1} &= E - H_{i+1,i+1} - \langle i | G^i | i \rangle H_{i,i+1} \\ \langle 1 | G^{i+1} | i \rangle^{-1} &= \langle 1 | G^i | i \rangle H_{i,i+1} \langle i+1 | G^{i+1} | i+1 \rangle \end{aligned} \quad (4)$$

($i=1, 2, \dots, P-1$). In actual calculations, the unit cell can be enlarged in two-, three- and even many-fold size. By using the method, we can calculate effectively the conductance and DOS of a much long disordered irregular system.

3 Results and discussion

There are two basic shapes for graphite edges, namely, zigzag and armchair edges. Theoretical calculation and the first-principles self-consistent pseudopotential simulation show that the electronic properties of GNRs depend strongly on the shape of edges.²⁹ The GNRs with zigzag shaped edges are metallic with peculiar edge states on both sides of the ribbons regardless of its width. The group velocity of electrons is close to zero in the vicinity of Fermi energy. However, the GNRs with armchair shaped edges can be either metallic or semiconducting depending on their width. The group velocity of electrons is up to $10^6 \text{ m} \cdot \text{s}^{-1}$ around Fermi energy, which has been confirmed in experiment.^{29,32} Since the ripples in GNRs give rise to redistribution of electrons,^{22,23} one can expect that the ripples in GNRs have pronounced effects on its transport properties.

To explore the effects of ripples on the electronic transport, in Fig.2, we first calculate the conductance spectra and DOS of zigzag corrugated GNRs with $N=8$, $P=100$, and $A=0.1$ nm. For comparison, the result of the flat zigzag GNRs is also shown. As expected, the flat zigzag GNRs exhibits the perfect step-like features

Fig.2 (a) Conductance of zigzag corrugated GNRs with $m=0, 0.8$ and 1.6 ; (b), (c) and (d) the corresponding DOS
zigzag ribbon $N=8, P=100, A=0.1$ nm

with one unit of quantum conductance at about E_F due to one open channel. In Fig.2(b), a sharp peak of DOS is observed at about E_F due to states localized at the ribbon edges, which is consistent with the previous results. In the presence of ripples in GNRs, the period $2\pi/m$ of ripples in GNRs decreases with m increasing. The charge redistributions induced by the effect of curvature change the conductance spectra dramatically. Two conductance gaps are observed between the first Van Hove singularities at $m=0.8$, which is close to the beginning of the second subbands. In the vicinity of E_F , the ripples almost have no effect on the conductance spectra and the corrugated GNRs remain the ballistic characteristic. With m increasing, the conductance gaps between the first Van Hove singularities, induced by minigaps, move closer to the Fermi energy. It is shown that at $m=1.6$, the conductance gap is observed at around E_F . The corresponding DOSs are shown in Fig.2(b–d). It can be seen that, corresponding to the minigaps, the DOS tends to

Fig.3 (a) Conductance of armchair corrugated GNRs with $m=0, 0.5$ and 1 ; (b), (c) and (d) the corresponding DOS
armchair ribbon $N=14, P=100, A=0.1$ nm

be zero. Much more resonant peaks are found in conductance spectra. Through comparative analyses of the conductance and the corresponding DOS, we find that the conductance fluctuations are attributed to local resonances created by quasi-bound states.

In Fig.3, we plot the conductance spectra and DOS of armchair corrugated GNRs with $m=0.5, 1$, respectively. For comparison, the result of the flat armchair GNRs is also shown. As expected, the flat armchair GNRs exhibit the perfect steplike features with one unit of quantum conductance at about E_F due to one open channel, which is consistent with the previous results. At the edge of very subbands, in Fig.3(b), the DOS peaks are observed due to degeneracy of energy level. In the presence of ripples in GNRs, a conductance dip is observed at around E_F for armchair GNRs with $m=0.5$. A corresponding DOS dip is observed at around E_F , as shown in Fig.3(c). With m increasing, the conductance dip turns into conductance gap

Fig.4 Conductance of corrugated GNRs with varying width and length in central sample
(a) and (c) are the zigzag corrugated GNRs; (b) and (d) are the armchair corrugated GNRs.

and the corresponding DOS is close to zero. This is because the energy bands in the vicinity of E_F separate gradually with m increasing. These results illustrate that armchair GNRs can change from metal to semiconductor by modulating the ripples.

To explore the quantum-size effect on transport properties, in Fig.4, we plot conductance as a function of energy in corrugated GNRs with varying width and length in central sample. In these samples, the amplitude and period of corrugated GNRs are 0.1 nm and $2\pi/m \approx 0.628$ nm, respectively. From Fig.4, it can be seen that the width N plays an important role in determining the conductance spectra. For corrugated zigzag GNRs, it changes from metal to semiconductor with the width N , while for armchair corrugated GNRs, it remains to be semi-conducting properties. A conductance gap is found in the vicinity of E_F . At the higher energy region, the conductance changes dramatically for both the zigzag and armchair ribbons. The overall averaged conductance increases with N , just as expected. This is because the number of paths by which electrons can travel across the central sample increases with width N . In addition, it is shown that the conductance spectra vary slightly with the number P of central sample. Much more resonant peaks are observed due to resonance of quasi-localized states.

4 Conclusions

In summary, we have studied the transport properties of corrugated graphene nanoribbons by using Landauer-Büttiker formula, based on tight binding model. Our results show that the ripples in graphenes have an important effect on conductance of corrugated graphene nanoribbons. It is shown that in the presence of ripples, the minigaps with zero conductance and minibands with conductance fluctuations are formed for zigzag ribbons among the first Van Hove singularity. The corresponding DOS is zero for minigaps due to energy bands separating. While for metal armchair ribbons, a conductance gap is observed in the vicinity of Fermi energy, which is corresponding to a metal-semiconductor transition. With the fluctuation of ripples intensifying, the overall averaged conductance tends to be zero for both the zigzag and armchair ribbons. These results are useful for better understanding the properties of realistic graphene nanoribbons, and will be helpful for designing nanodevices based on graphene.

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