Electron transport of folded graphene nanoribbons

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Recently, the AA-stack bilayer graphene nanoribbon (BGN) with a closed edge is observed in experiment. This new type of GN, we called folded GN (FGN), can be formed by folding a monolayer GN (MGN). Electron transport of the folded structures with different edges is studied. The FGNs show unique transport properties different from those of MGNs and BGNs. A metallic MGN with armchair edge (MAGN) is still metallic after folding. However, a semiconducting MAGN can be either semiconducting or metallic after folding, which depends on the width of MAGN and strength of interlayer coupling in the folded structure. The energy gap decreases with the increase of the coupling strength or width. As to the MGNs with zigzag edge (MZGNs), after folding they exhibit interesting conductance characteristics. The conductance steps around the Dirac point are even multiple of $G_D=2e^2/h$, while other conductance steps are odd multiple of $G_D$. It indicates that the electron transport around the Dirac point in zigzag-edged FGNs is similar to that in zigzag-edged BGNs (BZGNs), while electron transport far from the Dirac point is similar to that in zigzag-edged MGNs (MZGNs). © 2009 American Institute of Physics. [doi:10.1063/1.3261757]

I. INTRODUCTION

Graphene, a monolayer sheet of graphite, has become of great interest to the scientific community due to experimental breakthroughs. By cutting mechanically exfoliated graphenes or patterning epitaxially grown graphenes, quasione-dimensional graphene nanoribbons (GNs) are obtained. The properties of monolayer GNs (MGNs) can range from metallic to semiconducting according to the widths and edges. MGNs with zigzag edge (MZGNs) are metallic with peculiar edge states on both sides of the ribbon regardless of its widths, while the MGNs with armchair edge (MAGNs) can be either metallic or semiconducting. A MAGN with width $N_A=3k+2$ ($k$ is an integer) is metallic; otherwise it is a semiconductor. By stacking a MGN on the other, one can obtain a bilayer GN (BGN) which shows quite different properties with monolayer structure in many respects such as the edge states, energy gap etc. There are two typical stacking forms for the BGNs, i.e., AA and AB stackings. Because AB-stacked graphene is stable while AA-stacked graphene has never been found experimentally, most recent studies are concentrated on the AB-stacked structures. Both MGNs and BGNs have attracted much attention due to their interesting transport properties and great potential technological applications. The GN-based nanoelectronics have been regarded as the alternative to silicon-based devices in the future.

Recently, a kind of AA-stack BGNs with closed edges are observed experimentally by means of a high-resolution transmission electron microscope. These new carbon nanostructures we called folded GNs (FGNs) can be obtained by folding MGNs. According to the edge form, the GNs after folding have two typical structures, i.e., FGN with armchair edge (FAGN) and FGN with zigzag edge (FZGN) as shown in Figs. 1(a) and 1(b), respectively. Due to existence of interlayer coupling the FGNs are obviously different from the MGNs in Figs. 1(c) and 1(d). They are also different from the AA-stacked BGNs in Figs. 1(e) and 1(f) due to the closed edges. Thus one can expect that FGNs should have unique electronic characteristics. However, to the best of our knowledge, transport properties of the FGNs have not been studied.

![Diagram](Image)

FIG. 1. (Color online) Schematic view of (a) a FAGN, i.e., an AA-stacked BAGN with a closed edge; (b) a FZGN, i.e., an AA-stacked BZGN with a closed edge; (c) a MAGN; (d) a MZGN; (e) an AA-stacked BAGN; (f) an AA-stacked BZGN. The FAGN (FZGN) can be formed by folding the MAGN (MZGN). $N_l$ represents the widths of both the MAGN (MZGN) and the FAGN (FZGN), and $W_Z=5$ ($W_Z=4$) describes the width of closed edge of the FAGN (FZGN). $N_l$ represents the width of the MAGN (MZGN). The bidirectional arrows display the direction of electron transmission. Inset between (c) and (f): Two hexagons in the AA-stacked BAGN or BZGN with hopping energies. $t$ and $V$ are the hopping energies between nearest-neighboring sites in the same and different layer(s), respectively.

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In this paper, we study electron transport of the FGNs as shown in Figs. 1(a) and 1(b). We first discuss the folding effect on the MAGN by comparing folded and unfolded structures. It is found that the folding effect destroys the symmetry of conductance and thus changes the energy gaps. Though a metallic MAGN is still a metal after folding, a semiconducting MAGN will become metallic after folding as the strength of interlayer coupling exceeds critical value. The dependence of energy gap on width of the FAGN is also discussed. We then study transport properties of FZGNs by comparing with MZGNs and zigzag-edged BGNs (BZGNs). Splitting edge states similar to those in the bilayer structure are found in the FZGN, which results in interesting conductance steps. The conductance steps around the Dirac point are even multiple of $G_0 = 2e^2/h$, because transport of these electrons is dominated by edge states. While the electrons far from the Dirac point will transport across the bulk of the FZGN and thus their corresponding conductance steps are odd multiple of $G_0$.

II. MODEL AND METHOD

Let us consider two type of FGNs: the FAGN in Fig. 1(a) and FZGN in Fig. 1(b). Obviously, the FAGN can be formed by folding the MAGN in Fig. 1(c). $N_A$ represents the width of both MAGN and FAGN. While the FZGN can be formed by folding the MZGN in Fig. 1(d), and their widths are represented by $N_Z$. The region between the two dashed lines in Fig. 1(c) or Fig. 1(d) corresponds to the closed edge of the FGN, while the regions out of the two dashed lines correspond to the two layers of the folded structure. It is noted that, to keep AA stacking, the width of FAGN $N_A$ should be odd number while the width of FZGN $N_Z$ should be even number. The AA-stacked armchair-edged BGN (BAGN) and BZGN are shown in Figs. 1(e) and 1(f) for comparison. Because each FGN consists of two sections, i.e., an AA-stacked BGN and a closed edge, the Hamiltonian $H_{\text{FGN}}$ of folded structure can be expressed as:

$$H_{\text{FGN}} = H_{\text{BGN}} + H_{\text{CE}} + H' ,$$

where $H_{\text{BGN}}$ is the Hamiltonian of BGN, $H_{\text{CE}}$ is the Hamiltonian of closed edge, and $H'$ is the interaction of the two sections. The nearest-neighbor tight-binding model is used to describe the electronic structure of the BGN

$$H_{\text{BGN}} = \varepsilon \sum_i (a_i^\dagger a_i + b_i^\dagger b_i) + \tau \sum_{\langle i,j \rangle} (a_i^\dagger a_j + b_i^\dagger b_j + \text{H.c.})$$

$$+ V \sum_{\langle i,j \rangle} (a_i b_j + \text{H.c.}),$$

where $a_i^\dagger$ and $b_i^\dagger$ are creation operators in top and bottom layers of BGN, respectively, $\varepsilon(=0)$ is the site energy, $\tau$ and $V$ represent intralayer and interlayer hopping energies in the BGN, respectively. As the curvature effect of the closed edge is omitted, the Hamiltonian $H_{\text{CE}}$ and $H'$ can be written as

$$H_{\text{CE}} = \varepsilon \sum_i c_i^\dagger c_i + \tau \sum_{\langle i,j \rangle} (c_i^\dagger c_j + \text{H.c.}),$$

$$H' = \tau \sum_{\langle i,j \rangle} (a_i^\dagger c_j + b_i^\dagger c_j + \text{H.c.}),$$

where $c_i^\dagger$ is creation operator in the closed edge.

The lattice Green’s function method is used to calculate the transport properties of the FGN. Along the direction of electron transmission (as shown the bidirectional arrows in Fig. 1), one can divide the periodic FGN into three parts: a central region consisting of one or several unit cells of FGN, and two half infinite (left and right) leads at the two sides of the central region. According to the Green’s function scheme, the total Green’s function of a FGN can be expressed as

$$G_S = \left( E - H_c - \Sigma_L - \Sigma_R \right)^{-1},$$

where $H_c$ is the Hamiltonian of the central region, $\Sigma_L$ and $\Sigma_R$ are self-energy of the left or right lead, and $\Sigma_{L,R}$ is the Green’s function of the left or right lead, while $H_c$ is the interaction matrix between lead and central region. The Green’s function of lead can be calculated by the recursive Green’s function method. Once the total Green’s function is obtained, one can calculate the conductance $G$ and density of state (DOS)

$$G = \frac{2e^2}{h} \text{tr}[\Gamma_S G_S^2 \Gamma_A G_S],$$

$$\text{DOS} = -\text{Im} \text{tr}[G_S]/\pi,$$

where $\Gamma_{L,R} = i[\Sigma_L - \Sigma_L - \Sigma_R]$ is coupling function of the left (right) lead. The Green’s function method can be also used to calculate conductance and DOS of MGNs and BGNs. In the calculated results, all energies including electron energy and hopping energy will be measured in units of $t$.

III. RESULTS AND DISCUSSION

In Figs. 2(a) and 2(b), we show the conductance as a function of electron energy for the FAGNs with width $N_A = 17$ and 21, respectively. As a comparison, the conductance for the MAGNs are also shown (see the dashed lines). One can find that the conductance steps of MAGNs distribute symmetrically at the two sides of the Dirac point. After fold-
The folding effect of GNs is originated from the interlayer coupling existing in the folded structure. To clearly show the folding effect on energy gap of the semiconducting MAGN in Fig. 2(b), before folding a wide gap is exhibited in the conductance. The energy gap decreases after folding and the conductance step crosses the Dirac point, i.e., midgap is formed. If the midgap band is partially filled, the FAGN will behave like a metal. Thus, the folding effect results in the transition from semiconducting to metallic.

The folding effect of GNs is originated from the interlayer coupling existing in the folded structure. To clearly show the folding effect on energy gap of the semiconducting GN, in Fig. 3, we depict the DOS for FAGNs with different coupling strength \( V \). As \( V=0 \) (no folding), there is a wide gap in the DOS profile, and symmetric DOS peaks distribute at the two sides of the Dirac point (see the solid line). This coincides with the conductance of MAGN in Fig. 2(b). A weak interlayer coupling (\( V=0.05 \)) destroys the symmetry of DOS profile, as shown the dashed line, but the wide gap still exists. As \( V=0.1 \), the energy gap decreases and one DOS peak crosses the Dirac point (see the dotted line). In this case, so-called midgap states are formed in the FAGN, which coincides with the conductance of FAGN in Fig. 2(b). As the coupling strength is increased to \( V=0.16 \), the energy gap disappears, i.e., the FAGN exactly becomes metallic. This indicates that a semiconducting MAGN with certain width can be either semiconducting or metallic after folding dependent on the coupling strength. The enhanced interlayer coupling will lead to the FAGN transiting from semiconducting to metallic. In the inset of Fig. 3, the dependence of energy gap on the width of FAGN is shown. One can clearly find that the gap decreases with the increase of width. As the width is great than the critical width \( N_A = 31 \), the FAGN becomes metallic. The critical width is correlated with the coupling strength according to the former discussion.

In Fig. 4, we show the folding effect on the transport properties of MZGNs. The solid and dashed lines in Fig. 4(a) represent the conductance of FZGN and MZGN (\( N_Z = 22 \)), respectively, while the dotted line represents the conductance of AA-stacked BZGN (\( N_Z = 11 \)). It is found that the conductance steps of MZGN and BZGN are odd and even multiple of \( G_0 \), respectively. However, the conductance steps of the FZGN are dependent on the electron energy. In energy region \(-0.1 < E < 0.1 \) the conductance step is even multiple of \( G_0 \), while out of the region the conductance steps are odd multiple [see the solid line in Fig. 4(a)]. In other words, the electron transport around the Dirac point in the FZGN is similar to that in the BZGN, while the transport of other electrons is similar to that in the MZGN. To explain this interesting transport phenomenon, DOS profiles of the three type of GNs are depicted in Fig. 4(b). It is known that there exists edge state in the MZGN. So in the DOS profile of MZGN there is a sharp peak induced by the edge state at the Dirac point (see the dashed line). Except this peak, other peaks induced by the Van Hove singularities correspond to the conductance steps of MZGN. In the BZGN the edge state splits into two states due to the interlayer coupling. As a result at the two sides of the Dirac point two sharp splitting peaks appear in DOS profile of the BZGN, as shown the dotted line in Fig. 4(b). While other DOS peaks correspond to the conductance steps of bilayer structure. Seen from the DOS profile of FZGN [solid line], one can find that at the two sides of the Dirac point there also exist two sharp peaks which are superposed with the two splitting DOS peaks of BZGN. The calculations of local DOS indicate that the two peaks are induced by two splitting edge states in the FZGN (not shown here). As to the electrons in energy region between the two DOS peaks, their transport is dominated by edge states. This is similar to the case of electron transport in the BZGN. Therefore, the conductance step in the energy region is even multiple of \( G_0 \). However, the electrons out of the region will transmit across the bulk of FZGN including
the closed edge. Because the interlayer coupling is relatively weak, their transport will be similar to that in the MZGN.

In Fig. 5, the conductance and DOS as a function of electron energy for FZGNs with different interlayer coupling are shown. Similar to the case of FAGNs, the conductance steps and DOS peaks are tightly associated with the coupling strength. Here, we only discuss the conductance steps with even multiple of $G_0$ and corresponding DOS peaks. As the coupling is weak ($V=0.01$), the conductance step is narrow, and the two splitting DOS peaks are very near the Dirac point. With the increase of coupling strength, the energy difference of two edge states is enlarged. Thus, as $V=0.1$, the splitting DOS peaks induced by edge states are far from the Dirac point. Correspondingly, the conductance step becomes wide. As the coupling strength is increased to $V=0.2$, the two splitting DOS peaks are further away from the Dirac point, meanwhile other two DOS peaks induced by the Van Hove singularities appear between them. Due to existence of the Van Hove singularities, three conductance steps with even multiple of $G_0$ are exhibited in conductance profile [see dotted line in Fig. 5(a)]. From the results one can conclude that there are more steps of even multiple in conductance profile as the interlayer coupling is strong. In addition, the inset in Fig. 5(a) shows the dependence of the conductance step of even multiple on width of the FZGN. It is found that the conductance step does not change with the variation of width. It is result from the fact that the energies of splitting edge states are mainly determined by the interlayer coupling strength while unsensitive to the width of FZGN.

IV. CONCLUSIONS

In conclusion, the transport properties of the FGNs are studied by using the Green’s function method. Though the nearest-neighbor tight-binding model we used is simple, many unique electronic structures and interesting transport properties of folded structures are found. The folding effect has obvious influence on both MAGN and MZGN. The energy gaps of FAGNs vary with the interlayer coupling in

the structure. Although a metallic MAGN is still a metal after folding, a semiconducting MAGN can be either semiconducting or metallic after folding. The energy gaps of semi-conducting MAGNs decrease with the increase of the coupling strength and structural width. As the coupling strength or width exceeds critical value, the FAGN will become metallic. The FZGNs show interesting conductance steps which are different from those of both MZGNs and BZGNs. Around the Dirac point the conductance steps are even multiple of $G_0$, while other conductance steps are odd multiple. This is due to the fact that there exist splitting edge states in the folded structure. The energies of splitting states are dependent on the interlayer coupling while unsensitive to the structural width. So the even-multiple conductance steps change with the coupling strength but is independent of the width.

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