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Conductance growth in metallic bilayer graphene nanoribbons with disorder and contact scattering

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Abstract

By using a decomposition elimination method for Green's function matrix, we explore the effects of both disorder and contact scattering on electronic transport in metallic bilayer graphene nanoribbons (BGNRs) and related structures, in the limit of phase-coherent transport. Due to the inter-layer interaction, a conductance gap is observed at Fermi energy in primary metallic zigzag BGNRs. It is found that the fashion of the conductance variations with disorder depends strongly on the type of disorder and contact scattering. In the edge disordered BGNR, the conductance decreases monotonically with the disorder increasing and finally tends to disappear, while a nonmonotonic behavior is obtained in the single-layer disordered BGNR, first decreasing then increasing. In the presence of contact scattering, especially, an abnormal growth of the conductance appears at much lower disorder in both edge and single-layer disordered BGNRs, which may be due to the destruction of coherence by the introduction of disorder.

1. Introduction

Recently, there have been many experimental reports on the production of few-layer graphene (monolayer, bilayer), that enables us to access its exotic electronic properties [1, 2]. Monolayer graphene, owing to the unique honeycomb structures, exhibits an unconventional quantum Hall effect. Some new phenomena had been predicted, such as the Josephson effect [3], the photon-assisted electron transport [4], composite Dirac fermions [5], the n–p junction [6], the fractional quantum Hall effect [7], and the spin–orbit gap [8]. For bilayer graphene, some unexpected properties were found to be essentially different from those of a monolayer [9, 10]. For example, there exist anomalies in its integer quantum Hall effect and minimal conductivity on the order of e^2/h.

More recently attention has turned to graphene nanoribbons (GNRs), which can be realized either by cutting [11] mechanically exfoliated graphenes [12], or by patterning epitaxially grown graphenes [13, 14]. Based on the simple tight-binding model or Dirac's equation, the electronic structure [15, 16] and transport properties [17, 18] of single-layer GNRs (SGNRs) were explored. It was shown that SGNRs with zigzag shaped edge are metallic, and that SGNRs with armchair shaped edge can be either metallic or semiconducting depending on their widths. Due to recent progress in preparing few-layer graphene on conventional device setups, multilayer GNRs (MGNRs) of various widths can be realized in the same ways. In a bilayer GNR (BGNR), there exists a relatively weak inter-layer interaction, similar to that in multi-walled or in bundled nanotubes [19–21]. Electronic conduction through a BGNR is complicated by inter-layer interactions and possible wavefunction interference between electronic states on the different layers. Some new characteristics may be expected on the electronic structure and transport in such BGNRs.

For a BGNR, there may exist various types of disorder. One type of disorder is edge disorder. Due to two open edges on one side, a BGNR can be usually passivated by hydrogen and/or other atoms at its open edges. As a result, the σ bonds between hydrogen and carbon, and the on-site energies at the edge carbons would be different from those in the middle of the BGNRs. The bonding distances between carbon atoms at the edges change accordingly. Another type of disorder is single-layer disorder. In this case, dopant atoms are distributed uniformly for the disordered layer and the other

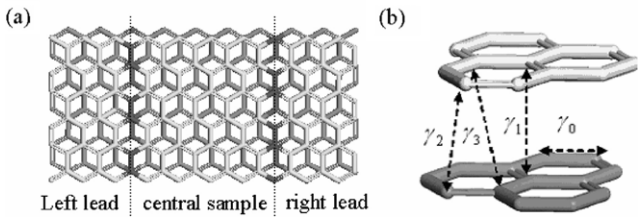

Figure 1. (a) Geometry of a zigzag BGNR device ($N = 4$). (b) The interaction integrals between atoms, indicated by γ_0, γ_1, γ_2 and γ_3.

layer is thought to be perfect. How about the influence of both the edge and single-layer disorder upon the conductance? This is an interesting problem in the applications of GNR devices. For the conductance measurement and device applications, in addition, the studied system must be connected to two electronic reservoirs. When electrons transmit through the central sample, each interface between a lead and the central sample may be regard as contact barrier existing there [22]. Therefore, the influence of both the disorder and the contact scattering on conductance should be considered.

By using a decomposition elimination method for Green's function, in this paper we have performed simulations to assess the effects of both the disorder and the contact scattering on the conductance of BGNRs. Our calculations show that the inter-layer interaction plays an important role in determining the transport properties of BGNRs. Importantly, it is found that the fashion of the conductance variations with disorder depends strongly on the type of disorder and contact scattering.

2. Model and method

The AB-stacked BGNR is shown in figure 1, which is held by the van der Waals forces in the AB sequence along the z axis. The distance between the two layers is 3.35 Å. The BGNR device system is composed of a central sample with P unit cells, connected to two semi-infinite leads, as shown in figure 1(a). If the BGNRs are commensurate, the translational symmetry can be still remained. Here we focus on the primary metallic BGNRs. For simplicity, the central sample is taken to be a commensurate zigzag edge BGNR, and the two leads are assumed to be made of the same kind of BGNR. The sample length L is then given by $L = P \times L_0$ with L_0 the unit cell length.

The BGNR is described by a tight-binding model with one π electron per atom. In the absence of edge disorder, the on-site energy ε_i is set to be the Fermi energy E_{F}. The values of hopping integrals are taken from those of the graphene bilayer [23], i.e. $\gamma_0 = 2.9$ eV, $\gamma_1 = 0.3$ eV, and $\gamma_2 = 0.12$ eV, $\gamma_3 = 0.1$ eV, as indicated in figure 1(b). In the presence of edge disorder, the on-site energies ε_i are randomly distributed within the interval $[-\xi, \xi]$ only for the edge atoms of the BGNR. In the single-layer disordered BGNR, the random values are distributed within the interval $[-\xi, \xi]$ for the disordered layer and the on-site energies are taken to be E_{F} for the ordered layer. To model the barrier potential at the lead contact, the nonzero site energies u_1 and u_2 are assumed for the interface atoms, as in [22]. For simplicity, we put the same values of u_1 and u_2 for the upper and lower layers of graphene.

The transmission coefficient between the left and right leads can be calculated by [24–28]

$$T = \mathrm{Tr}(\Gamma_{\mathrm{L}} G^{\mathrm{r}} \Gamma_{\mathrm{R}} G^{\mathrm{a}}), \tag{1}$$

where $\Gamma_{\mathrm{L,R}}$ are the coupling of the device to the left and right leads. $G^{\mathrm{r,a}}$ are the retarded and advanced Green's function matrices of the device. Based on Landauer theory, the conductance G through the central sample is given by $G = (2e^2/h)T$ at zero temperature.

Based on the generalized Landauer approach, the tunneling current at a finite temperature is given by

$$I = \frac{2e}{\hbar} \int \mathrm{d}E T(E) \left[f_1(E - u_{\mathrm{L}}) - f_2(E - u_{\mathrm{R}}) \right], \tag{2}$$

where the factor of 2 accounts for degeneracy; $f_1(E - u_L)$ and $f_2(E - u_R)$ are the Fermi energy functions of the waves incident from the two contacts to the device. Note that in the present work we calculate only the phase-coherent transmission coefficient. The effect of electron–phonon interaction is neglected and the temperature dependence is only via the Fermi factors of electrons.

Close to equilibrium ($u_L \approx u_R \approx E_{\mathrm{F}}$), the conductance can be obtained from equation (2) by

$$G(V \approx 0, T) = \frac{2e^2}{h} \int T(E) \left(-\frac{\partial f(E - E_{\mathrm{F}})}{\partial E} \right) \mathrm{d}E, \tag{3}$$

with a zero bias voltage ($V \approx 0$).

The key of the problem is to evaluate the transmission coefficients of interest. To calculate effectively the conductance of a much larger sample, a decomposition elimination method for Green's function matrix is newly developed by Xu *et al* [28]. By using the method, we can calculate effectively the conductance of a much longer disordered BGNR system.

3. Results and discussion

As a typical example, we consider only the commensurate zigzag BGNR molecular device. The central sample contains P primitive unit cells ($P = 203$–1626), of which $L \approx 50$–400 nm is comparable to the length of a real system measured experimentally.

To explore the effects of both edge disorder and contact scattering, in figure 2 we show the conductance of the edge disordered zigzag BGNR ($N = 14$) in (a) the absence and (b) the presence of the contact scattering. In the absence of contact scattering ($u_1 = u_2 = 0$), it is seen from figure 2(a) that the conductance of the perfect BGNR ($\xi = 0$) exhibits a perfect step-like feature with two units of quantum conductance, due to two open channels. Also, a small conductance gap is observed, a metal–semiconductor transition existing there. It is the inter-layer interaction that induces an energy gap, leading to a conductance gap [29]. Therefore, the inter-layer interaction plays an important role in determining the electronic structure

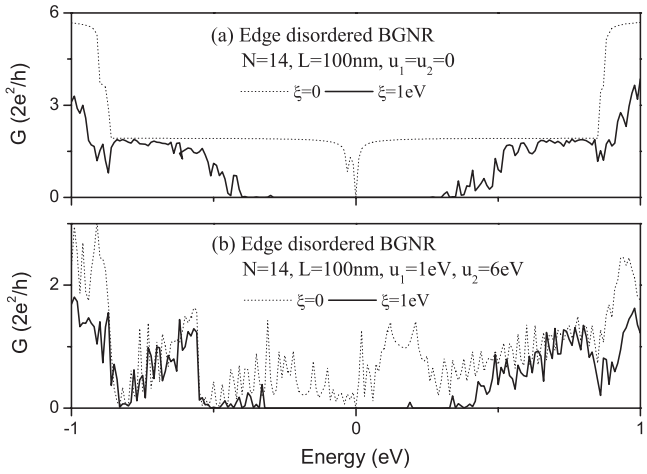

Figure 2. Conductance versus energy in (a) the absence and (b) the presence of a contact barrier.

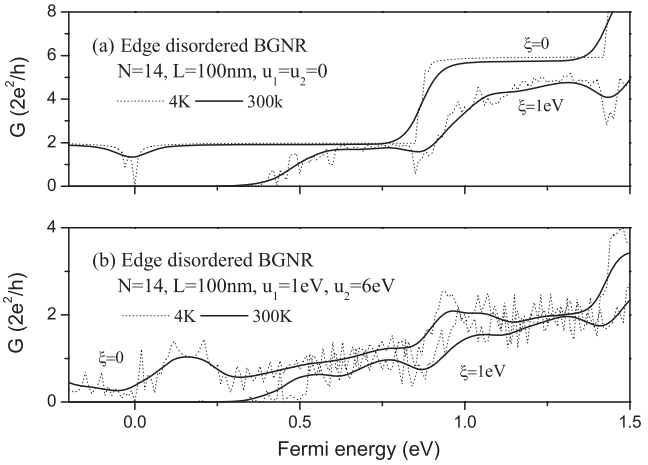

Figure 3. Conductance versus Fermi energy in (a) the absence and (b) the presence of a contact barrier.

and thus the transport properties of BGNRs, which should be considered to explore the performance of GNR devices. For the edge disordered BGNR, the conductance is averagely decreased, which is attributed to the mismatch in the energies of the resonances by the disorder. Some resonance peaks are created by the disorder. From figure 2(a), importantly, it is found that the conductance gap is broadened to be about 0.69 eV at $\xi = 1$ eV, much larger than that at $\xi = 0$. This may be due to the fact that the electrons at about E_F are localized at the ribbon edges with almost zero group velocity, just as in a zigzag SGNR [10, 17]. The edge disorder induces the localization of the electrons at the ribbon edges, leading to a large conductance gap at about E_F. This means that some new characteristic of the conductance can be expected, especially at low energy and low temperature.

In the presence of contact scattering ($u_1 = 1.0$ eV, $u_2 = 6.0$ eV), as expected, an overall decrease of conductance is observed from figure 2(b) even at $\xi = 0$, due to the contact reflection. Also, it is found that the conductance oscillates between 0 and $4e^2/h$ for -0.88 eV $\leqslant E \leqslant$ 0.88 eV. The rapid conductance fluctuations are superimposed on a slow fluctuation background, similar to that in a single wall nanotube [30]. Both the rapid and slow conductance fluctuations may be attributed to antiresonance of an incoming channel with beating standing waves in the central sample region. Therefore, it is shown that the contact scattering cannot be neglected to explore the performance of the GNR devices.

At high temperature, phonon scattering plays an important role in determining electronic transport, while it is not significant at low temperature. In a conductance experiment, the effect of the temperature should be considered. In the present work, we calculate only the phase-coherent transport (the effect of electron–phonon interaction is neglected). In figure 3, we show the conductance versus the Fermi energy at various temperatures. In equilibrium, the ability to vary the Fermi energy had been demonstrated experimentally by changing the gate voltage [31]. In the absence of contact scattering, one can clearly see from figure 3(a) that the conductance of the perfect BGNR is quantized at both low and high temperatures, while the conductance step is smoothed at high temperature. Also due to the inter-layer interaction, a small conductance gap is observed at low temperature, a metal–semiconductor transition existing at about $E_F = 0$. Interestingly, the small gap disappears at high temperature, no transition existing there. This is because the electronic transport occurs over a few k_BT around E_F. In the presence of edge disorder ($\xi = 1$ eV), the whole conductance is decreased, and a large conductance gap appears there, due to the Anderson localization induced by the disorder. At low temperature, the conductance fluctuations are observed, due to the quasibound resonances in the disordered region, while such conductance fluctuations are averaged out at high temperature. For an almost zero group velocity, a series of conductance dips exists at the beginning of the next subband [27]. As a result, the conductance steps are evolved into some plano-convex peaks.

In the presence of contact scattering ($u_1 = 1$ eV and $u_2 = 6$ eV), it can be seen from figure 3(b) that at low temperature the whole conductance decreases even at $\xi = 0$, due to the contact reflection. Also, it is observed that the slow conductance fluctuations are superimposed on the rapid ones. Such fluctuations had been observed in a single wall carbon nanotube [30], which arise from the quantum interference by the contact reflection [22]. At higher temperature ($T = 300$ K), interestingly, there appear some conductance peaks even for perfect BGNRs ($\xi = 0$) due to the quantum interference, while the rapid conductance fluctuations are smoothed by the temperature. The results show the importance of the contact scattering, leading to the quantum interference and thus the conductance fluctuations.

In the presence of both edge disorder ($\xi = 1$ eV) and contact scattering ($u_1 = 1$ eV and $u_2 = 6$ eV), in addition, the results are present in figure 3(b), which are very similar to those in the absence of contact scattering. Importantly, new conductance peaks are observed on a conductance plateau, induced mainly by the disorder. This further shows that both the edge disorder and contact scattering play an important role in determining the transport properties of BGNRs, which should be taken into account in the application of BGNR devices.

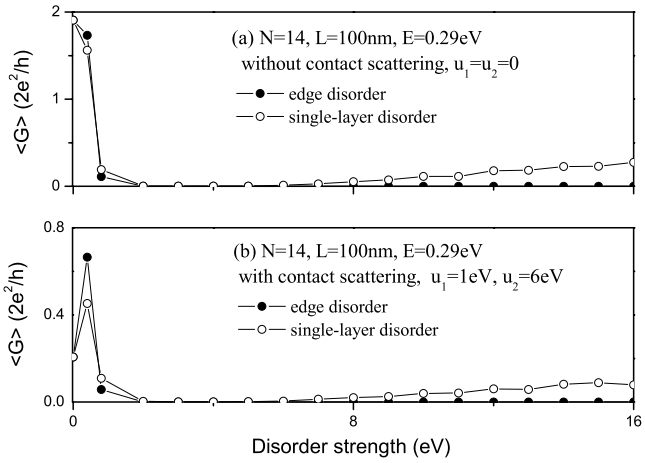

Figure 4. Average conductance $\langle G\rangle$ of a zigzag BGNR ($N = 14$) as a function of disorder strength in (a) the absence and (b) the presence of a contact barrier.

For the control of carrier mobility in BGNRs, we further calculate in figure 4 the average conductance $\langle G\rangle$ versus edge disorder strength in (a) the absence and (b) presence of the contact scattering. The conductance is averaged over more than 200 disorder configurations. To explore the influence of various disorder, the result of single-layer disordered BGNR is also presented. At the energy $E = 0.29$ eV, it is found from figure 4(a) that in the absence of contact scattering the average conductance of the edge disordered BGNR drastically decreases with disorder at $\xi < \xi_C \approx 1$ eV and finally tends to disappear at $\xi > \xi_C$. The disappearance of conductance may contribute to the disorder induced energy gap and thus a zero conductance in the gap. In the case of single-layer disordered BGNR, the system behaves remarkably differently from edge disordered BGNR. A localization/quasi-delocalization transition is observed at critical disorder ($\xi_C = 4$ eV). In the regime of stronger disorder ($\xi > \xi_C$), the average conductance increases with disorder, while it decreases in the regime of weaker disorder ($\xi < \xi_C$). Even in the presence of the contact scattering, a similar transition is also obtained, independent of the values of u_1 and u_2. Such transitions had been found in shell-doped nanowires and order–disorder separated quantum films [32, 33], which can be understood by the same consideration. Therefore, the conductance variations with disorder may indicate the types of disorder, and thus determine the presence of the edge disorder or the single-layer disorder in BGNR systems.

In the presence of contact scattering, especially, an abnormal growth of the conductance is obtained from figure 4(b) at much lower disorder strength. This behavior can be understood by the following consideration. In the absence of disorder, these energies correspond to the lower and even minimal conductance due to the quantum interference. For such energies, the introduction of disorder destroys the coherence, which leads spontaneously to a little increase of the lower and minimal conductance. Therefore, it is shown that the electron transport in GNR devices can be controlled through modulation of the disorder strength.

To clarify the conduction mechanism in the edge disordered BGNRs, we further study the localization length L_0 of the electrons. It is well known that in an infinite 1D system all states are localized even for weak disorder. The conductance is expected to decrease exponentially with length, $G = G_0 \exp(-|L|/L_0)$ [27, 34]. In figure 5, we present the average conductance $\langle G\rangle$ versus length L at lower energy ($E = 0.29$ eV) both in (a) the absence and (b) the presence of contact scattering. From figure 5(a), it is shown that in the absence of contact scattering the average conductance at various ξ depends strongly on the sample length, decreasing with L increasing. From a more careful analysis, it is found that the

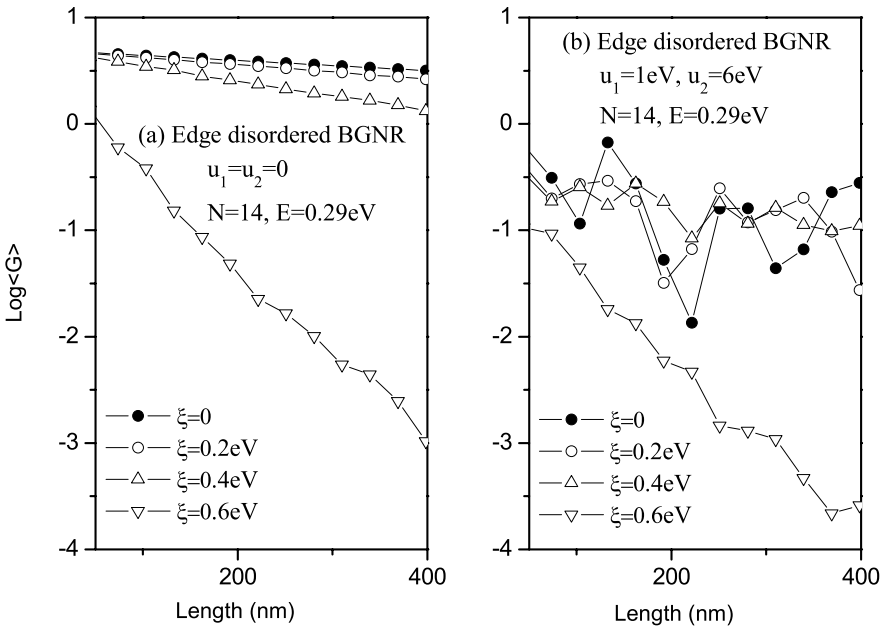

Figure 5. Average conductance $\langle G\rangle$ of the zigzag BGNR ($N = 14$) as a function of length L at $E = 0.29$ eV with various disorder strengths in (a) the absence and (b) the presence of a contact barrier.

data of $\langle G\rangle$ versus L are well fitted to $G = G_0 \exp(-L/L_0)$. The localization length L_0 is obtained to be 1476.25, 714.29 and 112.87 Å, respectively, corresponding to the disorder strength of 0.2, 0.4 and 0.6 eV. It is shown that L_0 is decreased with edge disorder strength, indicating a localization ($L_0 = 0$) at large enough ξ. In the presence of contact scattering, in figure 5(b), the average conductance $\langle G\rangle$ is decreased, lower than that in the absence of contact scattering, which is attributed to the contact reflection. Interestingly, it is found that the average conductance $\langle G\rangle$ periodically oscillates with L at small disorder strength. Even at $\xi = 0$ eV such an oscillatory behavior is obtained, due to the quantum interference by the contact reflection. Similar behavior has always been observed in carbon nanotube devices [22]. At larger disorder ($\xi = 0.6$ eV), however, the disorder scattering suppresses the effect of contact reflection, no oscillation appearing there. The average conductance $\langle G\rangle$ declines exponentially with L increasing, and L_0 is obtained to be 124.22 Å. Obviously, the contact reflection strengthens the interference, but the edge disorder scattering destroys the interference. Both of them together determine the appearance and/or disappearance of the oscillations, which may give an implication for the understanding of the experimental observation.

4. Conclusion

We calculate the phase-coherent transmission through zigzag BGNR that can include the effect of semi-infinite leads and can handle many defects and junctions with relative ease. It is shown that the conductance variation with disorder depends strongly on the type of disorder and contact scattering. In the edge disordered BGNR, the conductance decreases monotonically and tends to disappear, while a nonmonotonic behavior is observed in single-layer disordered BGNR, first decreasing then increasing. In the presence of contact scattering, an abnormal growth of the conductance is obtained at much lower disorder strength. These results are useful for better understanding the properties of BGNR, which could open up new possibilities for the design and application of the BGNR molecular devices and device wiring.

Acknowledgments

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