Solid State Communications 233 (2016) 18–23

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Line defect induced conductance suppression in graphene nanojunction

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ARTICLE INFO

Article history:
Received 18 November 2015
Received in revised form
11 January 2016
Accepted 11 February 2016
by P. Hawrylak
Available online 17 February 2016

Keywords:
A. Graphene
C. Line defect
C. Staggered potential
D. Conductance suppression

ABSTRACT

Line defect induced conductance suppression in graphene nanojunction is investigated by means of Landauer–Bütikker formula and the nonequilibrium Green's function technique. With the increase of the longitudinal size of the device region, the conductance value decreases and tends to form two conductance valleys. Then we prove that the line defect can lead to localize states in the device region, which contributes to conductance valley at the point far away from Dirac point. And the zero conductance at the Dirac point is associated with the edge state localized at the zigzag-edged shoulder of the nanojunctions. The staggered potential can change energy spectrum structure of the device region, and produce strong conductance suppression. The line defect can efficiently enhance the conductance suppression, which can be utilized to realize the electron transport manipulation.

1. Introduction

Graphene is the first realization of truly two-dimensional crystal, which has became a subject of intense interest in the past ten years [1–6]. Previous studies showed that pristine graphene is a zero-gap semiconductor and has a linear dispersion relationship nearby the Dirac points [5,7], which makes electrons behave as relativistic Dirac particles. Such a carbon material presents many unusual physical properties in comparison with conventional materials, such as the quantum Hall effect and the nonzero conductivity [1,8,9]. Graphene also has been an important two-dimensional material for exploring condensed matter physical phenomena and is expected to be very useful in the next generation of electronic devices [3,5,10].

Recently, the experiment reported a peculiar topological line defect in graphene [11], which can be created by alternating the Stone–Thrower–Wales defect and divacancies, leading to a pattern of repeating paired pentagons and octagons [12]. In addition, first-principles calculation and experimental observations show that this defect acts as a one dimensional metallic wire [11], which motivates researchers to further discuss the electron properties or designs the schemes of valley polarization [13–15]. Moreover, the study also found that the metallic characteristics and Fabry–Perot oscillation phenomena can be observed due to the line defect [16]. Considering that the line defect has a simple geometry makes them suitable to observe the electron properties in graphene nanojunctions (GNJs). Thus receiving extensive attention, some interesting line defect based transport phenomena have been observed [12,17–20]. For example, Rodrigues et al. studied the low-energy electronic transport across periodic extended defects in graphene by a continuum approach. They found that the defect acts as infinitesimally thin stripes separating two regions where Dirac Hamiltonian governs the low-energy phenomena in the continuum low-energy limit [21,22]. Gargiulo and collaborator found the structural topological invariant of dislocations, and revealed a strong suppression of transmission at low energies upon decreasing the density of dislocations with the smallest Burger's vector [23]. Inspired by these fascinating physical phenomena and possible potential device applications, in this work, we theoretically investigate the impact of a line defect on the transport properties of GNJs. We found that such a system can be considered as a promising candidate for manipulating the electron transport.

In addition, the staggered potential has had extensive theoretical investigations in many systems. The study found that the staggered potential is very helpful in finding fascinating quantum phenomena and quantum phase transitions [24–26]. For example, it found that a staggered potential can help observe quantum spin Hall effect in graphene. Changes of the quantum phase shift can be induced by a quantum phase transition. It should be noted that in the experiment one can realize the potential staggered on graphene by an asymmetric interaction with a substrate [27–29]. Therefore, we also consider a general situation that the graphene bulk lattice can be subject to a staggered potential in this work.

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http://dx.doi.org/10.1016/j.ssc.2016.02.009
0038-1098/

Whereby we observe the staggered potential impact on the transport properties of GNJs containing the line defect.

2. Model and theory

The lattice structure that we consider is depicted in Fig. 1, two semi-infinite graphene nanoribbons (GNRs) at the left and the right sides serve as two leads for electronic transmission. Here, we define the parameters N_L and N_R as the width of the two semi-infinite GNRs, which are needed to characterize a clear junction. The armchair-edged GNRs are metallic when the width satisfy $N_{L(R)}=3p+2$ where p is an integer, otherwise, it is semiconducting [24]. The central region with one line defect constitutes the device region (shaded), where the electron tunneling is scattered. We use the parameters $N_{DL(R)}$ and $L_{DL(R)}$ as the latitudinal and longitudinal size, respectively.

The low-energy properties in graphene are mainly determined by the p_z orbital. The total Hamiltonian H can be divided into four terms, $H=H_C+H_L+H_R+H_T$, where H_C is the central region, H_L and H_R describe the left and the right leads, respectively, and H_T is the coupling of central region to the left and the right leads. Thus, we use a single-orbital nearest-neighbor tight-binding model to describe the electronic properties of the GNRs. They may take the following forms:

$$H_C=\sum_{i\in C}\varepsilon_i d_i^{\dagger}d_i+\sum_{\langle i,j\rangle}(td_i^{\dagger}d_j+\text{H.c.}), \tag{1}$$

$$H_{\alpha=L(R)}=\sum_{i\in\alpha}\varepsilon_\alpha d_i^{\dagger}d_i+\sum_{\langle i,j\rangle}(td_i^{\dagger}d_j\text{H.c.}), \tag{2}$$

$$H_T=\sum_{\langle i,j\rangle(i\in C,j\in\alpha)}(td_i^{\dagger}d_j+\text{H.c.}). \tag{3}$$

where we use $d_i^{\dagger}(d_i)$ as the electron creation(annihilation) operator, which is associated with the local atomic orbits i in graphene. $\langle i,j\rangle$ denote the summation that is restricted between the pairs of the nearest neighbor sites. ε_C, ε_L and ε_R are the on-site energies in the center region, the left and the right leads, respectively. In addition, we consider a general situation where the bulk lattice can be subject to a staggered sublattice potential: $\varepsilon_A=\Delta$ for lattice sites $A(\bullet)$, $\varepsilon_B=-\Delta$ for lattice sites $B(\circ)$, and ε_d is the on-site energies of the line defect. It should be noted that the rearranging of carbon atoms near the line defect induced bond distances changes very little, so in what follows we will select the hopping energy t as the units of the energy, the lattice constant a as the units of the length, and the zero point of the energies as the Fermi energy level. The on-site energy ε of all lattice points in GNJs are zero.

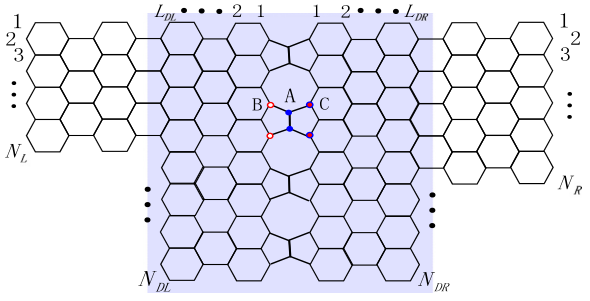

Fig. 1. (Color online) Schematic of the graphene nanojunctions, the parameters $N_{L(R)}$ and $N_{DL(R)}$ are the width of the two semi-infinite graphene nanoribbons and the central region (shaded), L_{DL} and L_{DR} are the longitudinal size of the intermediate segment. N_{DM} is the lattice points in the line defect. The carbon atoms belonging to the two distinct sublattices A and B are distinguishingly labeled as A: $\bullet$ and B: $\circ$, where C: $\circledcirc$ for labeling atom A or B, which can possess either positive or negative staggered potentials.

The conductance of the GNJs is calculated based on the Landauer–Bütikker formula in the discrete lattice representation [31,30]. It gives

$$\mathcal{G}(E)=\frac{2e^2}{h}T(E). \tag{4}$$

Here $T(E)=\text{Tr}(\Gamma_L G\Gamma_R G^{\dagger})$ is the transmission coefficient. $G=[E+i0^{+}-H_d-\Sigma_L-\Sigma_R]^{-1}$ is a retarded Green function, E is the incident electron energy, and H_d is the tight-binding Hamiltonian of the device region. $\Sigma_{L(R)}$ are the two self-energy terms which are associated with the coupling functions $\Gamma_{L(R)}$ by $\Gamma_{L(R)}=i[\Sigma_{L(R)}-\Sigma_{L(R)}^{\dagger}]$. The two self-energy terms can be evaluated by the recursive method [31]. The current through the junction is calculated as $I=\frac{2e}{h}\int[f(\mu_L)-f(\mu_R)]T(E)\,dE$ by Green's function, here f is the Fermi distribution functions, μ_L and μ_R are the chemical potential of the left and the right leads, respectively. The local density of states (LDOS) at site i can be found: $\rho_i=-\frac{1}{\pi}\text{Im}[G_{(i,i)}]$, where $G_{(i,i)}$ is the matrix element of Green's function at site i.

3. Results and discussion

According to these theories, first in Fig. 2 we plot a comparison of the conductance spectrum of the GNJs. From Fig. 2(a) we can see that the conductance spectra exhibit staircase-like structures in the absence of a line defect ($N_L=N_R=17, nc$), which can be readily explained by matching the subband structures of the two component ribbons. When the line defect appears in the device region

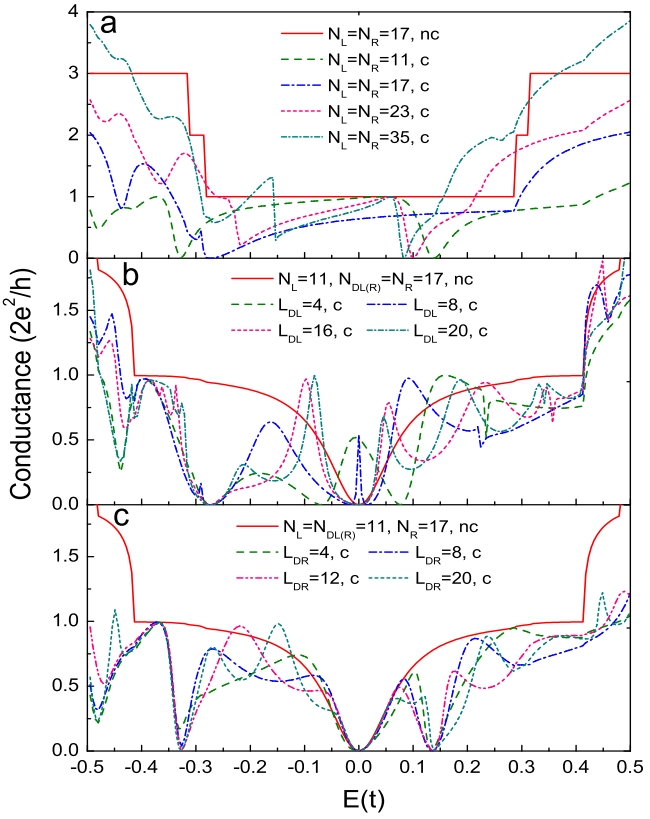

Fig. 2. (Color online) The comparison of the conductance spectra of the graphene nanojunctions, here we use *nc* to represent not contain line defects, and use the *c* to indicate containing line defect. (a) The conductance spectrum of equal width $N_L=N_R$. (b) and (c) The comparison of the conductance spectrum by changing the longitudinal size L and the width of the central region $N_{DL(R)}$. ($N_{DL(R)}=N_R=17$) indicates the line defect that exists in the wide side.