Physics Letters A 377 (2013) 2687–2691

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Transport properties in a line defect superlattice of graphene

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ARTICLE INFO

Article history:
Received 1 June 2013
Received in revised form 5 August 2013
Accepted 7 August 2013
Available online 14 August 2013
Communicated by R. Wu

Keywords:
Electronic transport
Line defect
Graphene

ABSTRACT

It was recently reported that a kind of graphene line defect can be fabricated in a controllable experimental way. In the present work we theoretically investigate the band structure and the electronic transport properties of a graphene superlattice formed by embedding periodically line defects in the graphene lattice. Based on the calculated results, we suggest that such a superlattice can be used as a quantum wire array which can carry much larger current than a single graphene nanoribbon. A remarkable advantage of this superlattice over other quantum wires is that the electronic transport in it is insensitive to scattering effects except that the scattering potential range is smaller than the graphene lattice constant. Moreover, we find that the anisotropy of the Dirac cone presented in this superlattice has a nontrivial influence on the universal minimal conductivity and the sub-Poissonian shot noise of graphene.

1. Introduction

Graphene possesses Dirac-cone-like band structure around two inequivalent touching points between the conduction and valence bands [1]. Thus the low-energy electron or hole excitation in the atomically thin two-dimensional carbon material behaves as a massless Dirac Fermion [2,3]. As a result, graphene presents some unique electronic and transport properties [4–6], in contrast with conventional semiconductor materials, for example, the nonzero conductivity at the vanishing carrier concentration, the sub-Poissonian shot noise [6,7], the reflectionless Klein tunneling [8] and the half-integer quantum Hall effect [9,10].

Just after the first experimental acquirement of the bulk graphene sample [11], various experimental means have been applied to modulate the electronic structure of graphene to meet the requirement of the device application and/or to further uncover interesting physical properties of graphene. For instance, in order to open a bandgap, a necessary step to realize the field effect transistor function, graphene nanoribbons are lithographically produced with well-ordered lattice edges [12]. When an electric and a magnetic field are applied simultaneously, a one-dimensional channel (quantum wire) can be created in graphene sheet. Such a quantum wire offers a unidirectional conductivity, robust to disorders. If the applied field is a spatially periodic one, a graphene superlattice (GSL) is formed which perhaps exhibits unusual electronic characteristics, unlike both the pristine graphene and the ordinary semiconductor material. Experimentally, many types of GSL have been fabricated and investigated. For example, electron-beam induced deposition of adsorbates on graphene creates a dot array with a period of 5 nm [13]; epitaxially growth of graphene on some metallic substrates can form periodic pattern of supercell [14–17]. These experimental progresses certainly make both the physical investigation and device applications of GSLs realistic. Accompanying the relevant experimental work, theoretical studies have predicted many interesting electronic properties of GSLs. For example, some recent theoretical works [18–21] focused on a simple GSL which is constructed by exerting a one-dimensional striplike or cosinusoidal periodic potential on a graphene sheet. It was found that such a one-dimensional GSL presents multiple Dirac points even in one valley of the pristine graphene. Then the conductivity and shot noise spectra of the GSL were theoretically studied to clarify the role of these new Dirac cones on the electronic transport properties [5], in contrast with the case of the pristine graphene.

Recently, the roles of various defects in graphene have drawn much attraction. So far an extended line defect of millimeter scale in an epitaxial layer of graphene has been successfully fabricated [22,23]. Subsequently, it was demonstrated that during the growth of graphene by chemical vapor deposition [24], the line defect can be patterned in a controllable way. These experimental results indicate that graphene in the presence of line defects is currently a practical structure, which certainly merits further investigations, both experimentally and theoretically. Some recent theoretical investigations [25,26] indicated that the line defect can be utilized as a valley filter because the transmission probability of a low-energy electron incident upon it shows notable valley polarization.

In the present work, we study the electronic and transport properties of a one-dimensional superlattice formed by patterning

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0375-9601/$ – see front matter
http://dx.doi.org/10.1016/j.physleta.2013.08.010

graphene lattice with a periodic line defect array (hereafter such a superlattice is abbreviated to LDGSL). From the calculated band structure we find that the lowest conduction subband of the superlattice has dispersionless part between two inequivalent Dirac points. This is reminiscent of the flat-bottomed subband of a zigzag-edged graphene nanoribbon (ZEGNR). Besides, in contrast with the case of the pristine graphene, the two Dirac cones in the LDGSL at K and K' points show more notable anisotropy. By calculating the transmission probabilities of the LDGSL we find that the electronic transport along the longitudinal direction (i.e. the direction parallel to the line defects) shows well-defined staircases as a function of the incident electronic energy. This means that the LDGSL can be viewed as an array of one-dimensional quantum wires which can carry larger current than an individual graphene nanoribbon. Moreover, the longitudinal electronic transport is insensitive to a long-range scattering potential, which is ascribable to the flat-bottomed band structure of the LDGSL. We also study the minimum conductivity and shot noise of the LDGSL at the Dirac point (the Fermi level in the case of charge neutrality). We find that the anisotropic Dirac cone of the LDGSL causes nontrivial difference of both the minimum conductivity and the Fano factor as a function of the sample size, in comparison with the case of the pristine graphene.

2. Model and theory

The lattice structure of the LDGSL is illustrated in Fig. 1(a). It is formed by periodically embedding extended line defects along y axial direction in the hexagonal lattice of the pristine graphene. Each extended line defect, consisting of the periodic repetition of a pair of pentagons plus an octagon, is infinitely long along x axial direction. The shadow region denotes the unit cell of LDGSL. The size of the unit cell in x axial direction is $2a$, with a being the graphene lattice constant; And in y axial direction the size of the unit cell is measured by an integer N, as explained in Fig. 1(a).

We employ the single π-orbital tight-binding model to describe the electronic properties around the Fermi level. Thus, the Hamiltonian in the nearest-neighbor approximation is given by

$$\mathcal{H} = \sum_{\mu} \varepsilon_{\mu} |\mu\rangle\langle\mu| + \sum_{\mu} U(r_{\mu}) |\mu\rangle\langle\mu| + \sum_{\langle\mu,\mu'\rangle} (-t) |\mu\rangle\langle\mu'| \qquad (1)$$

where ε_{μ} and r_{μ} denotes the on-site energy and coordinate of a carbon atom labeled by the index μ respectively, and $U(r_{\mu})$ accounts for the scattering potential which changes the onsite energies of the carbon atoms in the tight-binding model; $|\mu\rangle$ stands for the p_z atomic orbital localized at the μth carbon atom; The notation $\langle\mu,\mu'\rangle$ means the summation is restricted within the nearest-neighbor atomic pairs, and t (≈ 2.8 eV) denotes the corresponding hopping energy. By this simple model, the profiles of the valance and conduction subbands of the LDGSL can be readily calculated.

To study the electronic transport properties in the LDGSL along a specific direction, say x direction, we select a strip of size L in x direction in the LDGSL as the device region. And the other two parts of the LDGSL, on both sides of the device region, are regarded as the left and right leads. Due to the translational symmetry, the electronic wavevector component along y direction, i.e. k_y, is a conserved quantity. The TB Hamiltonian can be projected into a Hilbert subspace with a specific k_y. After such a treatment, we encounter an electronic transport structure with a finite transverse size which is just equal to the period of the LDGSL. Thus, the electronic transmission probability through the device region in a given k_y subspace can be evaluated by the Landauer–Büttiker formalism. It is given by

$$T(E,k_y) = \mathrm{Tr}\left[\Gamma^L(E,k_y) G^r(E,k_y) \Gamma^R(E,k_y) G^a(E,k_y)\right] \qquad (2)$$

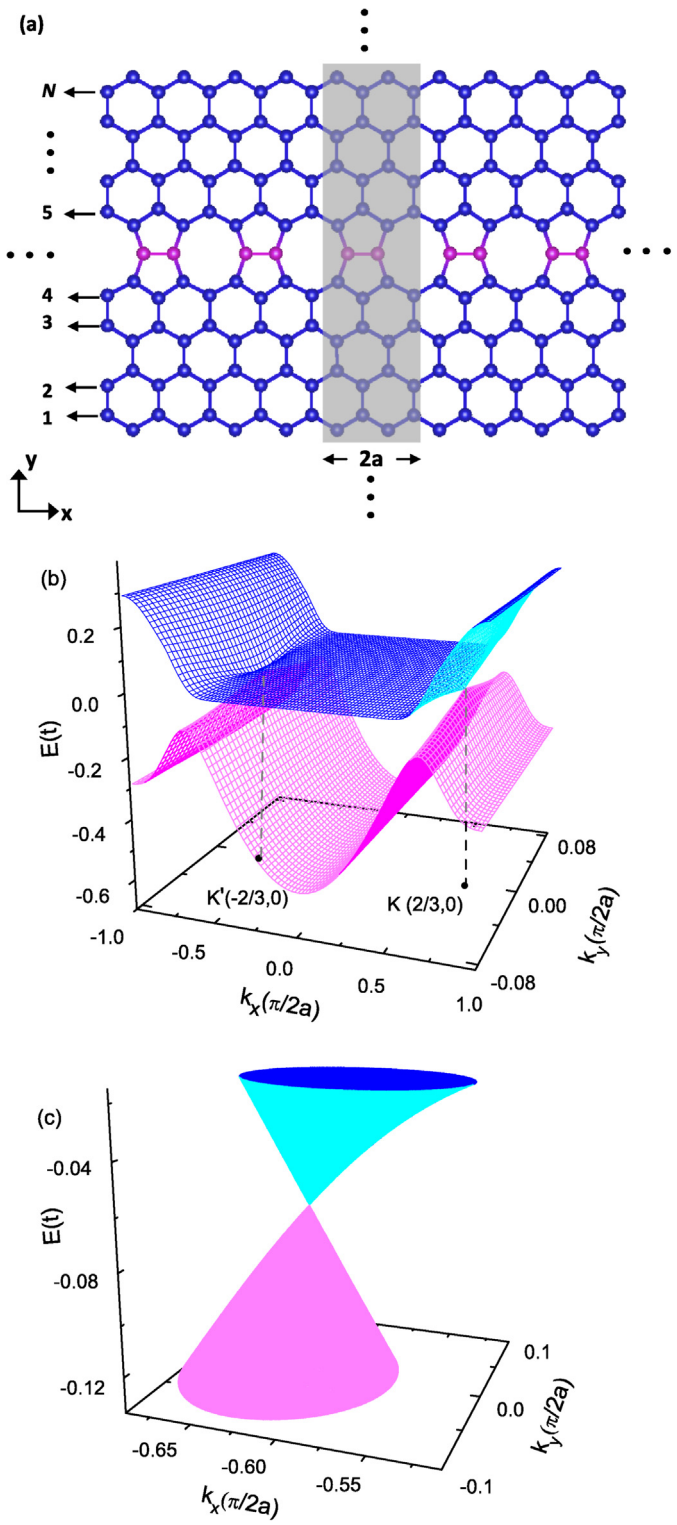

Fig. 1. (Color online.) (a) Schematic of the lattice structure of LDGSL. The shadow region denotes the unit cell of such a superlattice. The number N denotes the transverse size of the unit cell. And its longitudinal size is $2a$, with a being the graphene lattice constant. (b) Three-dimensional plot of the lowest conduction subband and the highest valence subband of the LDGSL ($N = 14$) in the Brillouin zone (BZ) of the superlattice. (c) Blowup of the Dirac-cone-like subband structure close to one of the Dirac point.

with the retarded Green function being defined as

$$G^r(E,k_y) = \left[E + i0^+ - \mathcal{H}(k_y) - \Sigma_L - \Sigma_R\right]^{-1} \qquad (3)$$