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Manipulation of resonant tunneling by substrate-induced inhomogeneous energy band gaps in graphene with square superlattice potentials

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ABSTRACT

We investigate the resonant transmission of Dirac electrons through inhomogeneous band gap graphene with square superlattice potentials by transfer matrix method. The effects of the incident angle of the electrons, Fermi energy and substrate-induced Dirac gaps on the transmission are considered. It is found that the Dirac gap of graphene adds another degree of freedom with respect to the incident angle, the Fermi energy and the parameters of periodic superlattice potentials (i.e., the number, width and height of the barriers) for the transmission. In particular, the inhomogeneous Dirac gap induced by staggered substrates can be used to manipulate the transmission. The properties of the conductance and Fano factor at the resonant peaks are found to be affected by the gaps significantly. The results may be helpful for the practical application of graphene-based electronic devices.

1. Introduction

In recent years, there has been a great deal of interest in studying graphene due to its remarkable properties and potential applications. Graphene is a single two-dimensional layer of carbon atoms arranged in a hexagonal lattice structure [1–3]. At low energy, the electron in graphene can be described by an effective massless Dirac equation, having a linear energy dispersion. Electrons behave like relativistic and chiral particles, and make graphene quite different from conventional materials. A novel electronic transport property in graphene is the perfect transmission in tunneling through an arbitrarily high and wide graphene barrier at normal incidence [4]. However, the transmission probability as a function of incidence energy has a gap when Dirac electrons transport through an electrostatic potential barrier in monolayer graphene at nonzero angle. This transmission gap can be controlled by the incidence angle, the height and width of the potential barrier. Meanwhile, graphene exhibits other unusual electronic properties, such as anomalous quantum Hall effect [5,6], minimum conductivity [7,8], and trembling motion (or Zitterbewegung) [9,10], etc. These are expected to play an important role in the future fabrications of graphene-based nanoelectronic devices.

However, some other properties of graphene are detrimental for its nanoelectronic applications, such as the zero-gap semiconductor nature, which prevents the pinch off of charge current as requested in conventional electronic devices. Different attempts have been therefore tried in order to induce a energy band gap at Dirac point (Dirac gap), for instance by quantum confinement of electrons and holes in graphene nanoribbons [11–13] or quantum dots [14,15]. These patterning techniques are unfortunately affected by the edge roughness problem, namely, the edges are extensively damaged and the resulting lattice disorder can even suppress the efficient charge transport. Another approach is substrate-induced band gap for graphene supported on hexagonal boron nitride (h-BN) [16] or silicon carbide (SiC) [17,18] by making two carbon sublattices (A and B sublattices) unequivalent. With this approach, a band gap of 260 meV has been experimentally demonstrated. There are also theoretical works to engineer the tunable band gap by strain [19,20]. In addition, a recent experiment demonstrates that patterned hydrogen adsorption on graphene induces a band gap of at least 450 meV around the Fermi energy [21].

Beside tackling the zero-gap problem in graphene, how to control the electronic behaviors is another critical issue needs to be solved in its nanoelectronic applications. Since superlattices are very successful in controlling the electronic structures of many conventional semiconducting materials, we may expect that using

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superlattice would be a good way to manipulate the electrons in graphene. Therefore, the transport characteristics of Dirac fermions in graphene superlattices with electrostatic potential [22–24] and magnetic barriers [25,26] have been widely studied theoretically. In gapless graphene-based superlattices, researchers have found that a one-dimensional periodic-potential superlattice possesses some distinct electronic properties, such as the strong anisotropy for the low-energy charge carrier's group velocities [27], the formation of the extra Dirac points and new zero energy states [28,29], and the unusual properties of Landau levels and the quantum Hall effect for these extra Dirac fermions [30]. The transmission gap also exists in graphene electric superlattices which can be modulated by the incidence angle, the number, width and hight of the barriers [31–34]. Moreover, graphene superlattices have been realized experimentally, e.g., graphene grown epitaxially on metal surfaces demonstrate superlattice patterns with about a several nanometer period [35,36]. Recent scanning tunneling microscopy studies of a corrugated graphene monolayer on Rh foil show that the quasiperiodic ripples generate a weak one-dimensional electronic potential in graphene leading to the emergence of the superlattice Dirac points [37].

From previous studies, one has known that for gapless graphene superlattices there is no transmission gap at the normal incidence due to the Klein tunneling. New electronic properties in gapped graphene-based devices have been discovered since Klein tunneling is suppressed due to the presence of a Dirac gap [32]. However, most of the studies about graphene with superlattice potentials still mainly focus on the homogenous Dirac gaps at present, i.e., the gaps don't rely on the positions of the potential barriers. Recently, a graphene-based superlattice formed by a periodic gap modulation is studied theoretically by using a Dirac-type Hamiltonian in Ref. [38]. The forbidden minibands and extra Dirac points arise in the electronic spectrum of the superlattice with equal widths of the gapless and gapped graphene fractions under certain conditions. This interesting new result raises a question: what role the inhomogeneous Dirac gap plays in the resonant tunneling of the Dirac electrons through graphene with superlattice potentials. With this question in mind, in this Letter, we investigate the resonant transmission inside graphene superlattices with inhomogeneous Dirac gaps induced by staggered substrates. We design two new open-gap schemes to construct inhomogeneous band gap at Dirac point. One is realized on the base of graphene deposited on a strip substrate combined from two different materials, while the other is by varying the distance between the graphene and the substrate at different position. It is shown that the adjustability of the Dirac gaps provides us a new degree of freedom for modulating the transmission of the Dirac electrons in graphene. The impact of the number of potentials, incident angle, Fermi energy, and the height and width of the potential on the transmission properties of Dirac electrons in these inhomogeneous band gap graphene superlattices is also discussed in detail.

2. Theoretical model

Let us consider a one-dimensional graphene superlattice with period d_1+d_2 formed by position-dependent electrostatic potential and Dirac gap. For gapped graphene superlattices, we assume that the potential $V(x)$ is comprised of periodic potentials with square barriers as shown in Fig. 1. The potential $V(x)$ can be controlled by the electrostatic voltage imposed on the electrodes. In Refs. [32] and [38], they reported that the energy band gaps can be realized, e.g., on the base of graphene deposited on a strip substrate combined from SiC and h-BN (Fig. 1(a)). Another method for obtaining inhomogeneous band gap is using SiC or h-BN but either fraction of periodic unit of the potential is suspended. The separation distance h can be adjusted according to our needs for the size of the band gap (Fig. 1(b)). Decreasing this distance increases the Dirac gap, as expected for a physical picture based upon a symmetry-breaking substrate potential [16,18]. For the experimental data, we know that the maximum energy band gap could be ~ 260 meV due to the sublattice symmetry breaking for SiC substrate [17].

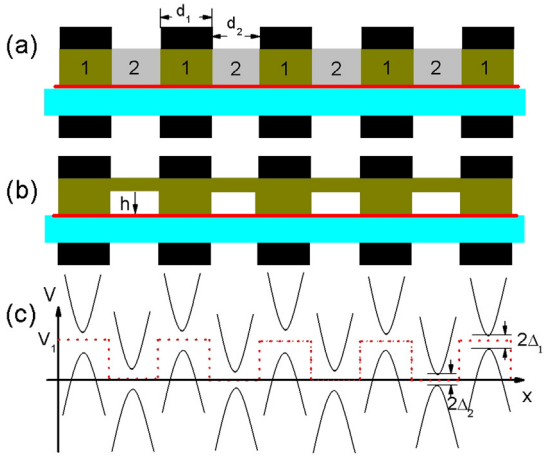

Fig. 1. (a) and (b) are schematic diagrams of unequally gapped graphene superlattice with black periodic electrodes. The thick red line denotes graphene, the gray and deep green rectangle denote SiC or h-BN, and the wathet blue rectangle denotes substrate SiO_2. (c) Schematic diagram of the electronic spectrum of the gapped graphene superlattice, and the pink dotted line denotes the periodic potentials of squared barriers. (For interpretation of the references to color in this figure, the reader is referred to the web version of this Letter.)

The superlattice electronic structure in the vicinity of the $\mathcal{K}$ point of the Brillouin zone is described by the Dirac-like Hamiltonian

$$\widehat{H} = v_f \hat{\sigma}\cdot\hat{p} + V(x)\hat{I} + \Delta(x)\sigma_z, \tag{1}$$

where $\hat{p} = (p_x, p_y) = (-i\hbar(\partial/\partial x), -i\hbar(\partial/\partial y))$ is a momentum operator with two components, $\hat{\sigma} = (\sigma_x, \sigma_y)$. Here, σ_x, σ_y and σ_z are Pauli matrices, $\hat{I}$ is a 2×2 unit matrix, and v_F is the Fermi velocity. $\Delta(x)$, $V(x)$ are periodic functions equal to Δ_1 and V_1, respectively, at $0 \leqslant x \leqslant d_1$, and Δ_2 and V_2 at $d_1 \leqslant x \leqslant d_1+d_2$. The potential V_j $(j=1,2)$ define the shifts of the forbidden band center in the gapped graphene with respect to the Dirac point in the gapless graphene. We set $V_2 = 0$ for convenience in the following context (see Fig. 1(c)). Generally speaking, the Fermi velocity can differ in graphene modifications placed on different substrates. In our model, however, we neglect the dependence v_F on x supposing $v_F \simeq 10^8$ cm/s in both graphene frictions [38].

The above Hamiltonian acts on the state of a two-component pseudo-spinor, $\Psi = (\tilde{\psi}_A, \tilde{\psi}_B)^{\mathcal{T}}$, where $\tilde{\psi}_A$ and $\tilde{\psi}_B$ are the smooth envelope functions for two triangular sublattices in monolayer graphene, and the symbol $\mathcal{T}$ denotes the transpose operator. In the y direction, because of the translation invariance, the wave functions $\tilde{\psi}_{A,B}$ can be factorized by $\tilde{\psi}_{A,B} = \psi_{A,B}(x)e^{ik_x y}$. Therefore, from Eq. (1), we obtain

$$\frac{d\psi_A}{dx} - k_y\psi_A = i\eta_+\psi_B, \tag{2}$$

$$\frac{d\psi_B}{dx} + k_y\psi_B = i\eta_-\psi_A, \tag{3}$$

where $\eta_\pm = [E - V(x) \pm \Delta]/(\hbar v_F)$ are the coupling parameters from ψ_B (ψ_A) to ψ_A (ψ_B), E is the incident electron energy, and $k_0 = E/\hbar v_F$ corresponds to the incident electronic wavenumber.

Insides the jth barrier, $V_j(x)$ and $\Delta_j(x)$ is a constant, therefore, from Eqs. (2) and (3), we have

$$\frac{d^2\psi_{A,B}}{dx^2} + \left(k_j^2 - k_y^2\right)\psi_{A,B} = 0, \tag{4}$$