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Dc conductance of ordered and disordered silicene superlattices

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HIGHLIGHTS

- We drive analytically the transmission probability for SSL.
- There are resonance picks (RP) in transmission probability.
- The number of RP increases with increasing the number of SSL barriers.
- The oscillating conductance suppresses with imposing disorder in SSL.
- Dc conductance of the system depends on structural parameters.

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ABSTRACT

This paper studies the conductance of charge carriers through silicene-based superlattices consisting of monolayer silicene by means of transfer matrix method. At first, we consider the ordered superlattices and drive analytically the transmission probability of Dirac fermions. We show that the number of resonance picks increases with increasing the number of superlattice barriers. In order to the best understand of the appearance of the picks, we exactly studied transmission properties of the silicene superlattice. Also, the effect of disorder on the probability of transmission through the system of various sizes is studied. The short-range correlated disorder is applied on the thickness of electron doped silicene strips as quantum barriers which fluctuates around their mean values. We show that the oscillating conductance as a function of barriers hight suppresses with imposing the disorder in the silicene superlattice. Also, the effect of structural parameters on the conductance of the system is studied.

1. Introduction

Two-dimensional carbon crystals are hosts for Dirac type electrons, whose unusual properties have been studied extensively in graphene monolayers [1]. Recently, a close relative of graphene 2D honeycomb lattice of Si atoms called silicene has attracted a lot of research interest since the nanoribbons of silicene have been synthesized successfully [2–5].

Similar lattice structures between graphene and silicene bring up their similar band structures with Dirac cone type of dispersion near the Fermi surface, leading to similar physical properties between them. Theoretical calculations show that silicene has also graphene-like electronic band structure, supporting charge carriers behaving as massless Dirac fermions [6,7]. Due to the lattice structure, electrons in silicene obey the Dirac equation around the K and K' points at low energy [8].

However, it has two salient features absent in graphene. One is the relatively large spin–orbit interaction, which enables quantum spin-Hall effects to realize. Unfortunately, spin–orbit interaction of graphene is tiny so that the quantum spin Hall effect in a graphene has not been experimentally observed. In contrast, spin–orbit interaction of silicene is 1000 times larger than that of graphene [12,13]. So, the quantum spin Hall effect in silicene is experimentally accessible [6]. The other is its buckled structure, while the graphene layer forms a regular plane, the silicene layer instead takes the form of noncoplanar buckled structure, with the sublattices A and B forming two separate planes. This buckled structure enables us to control the mass of the Dirac electrons by applying an external electric field perpendicular to the silicene sheet [9]. As electric field increases, the Dirac mass decreases linearly, and vanishes to a critical value, and then increases linearly. These massive Dirac fermion systems lead to a quantum spin Hall insulator, which is originally proposed in a graphene [10,11]. These characteristics can be useful for device applications. The most fundamental electronic device is a field effect transistor. Field

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effect transistor made by silicene has an advantage that it has a large band gap due to spin–orbit interaction compared with graphene which is a zero gap semiconductor.

Charge [14] and spin [15] transport properties of a silicene nanoribbon have been studied. Also, the Klein tunneling of *pn* and *npn* junctions made from silicene has been investigated [16]. In the semiconductor context there are basically a large number of works on the tunneling, which have resulted in the "obvious" declaration that the electronic properties of semiconductor superlattice are different from those calculated in a single-barrier junction. In the graphene superlattices, a new Dirac point is found which corresponds to the zero averaged wave number inside the 1D periodic potentials.

With the advent of more sensitive characterization techniques, it has become evident that not only are semiconductor interfaces almost never ideal, but that this unintentional disorder in real samples has discernible spectroscopic and transport consequences that should be taken into account by theory. Disorder in the superlattices can be classified in two: (i) lateral and (ii) vertical categories. Vertical disorder, studied in this paper, is along the superlattice growth direction in the form of discrete layer-thickness fluctuations. The electronic properties of semiconductor superlattices in the presence of disorder have been studied by several groups [17–21]. The transition hitting massless particles in a clean [22] or disordered [23,24] graphene-based superlattice structure has been studied. It is shown that the conductivity of the system depends on the superlattice structural parameters. Importantly, all the electronic states are localized in the thermodynamic limit for a semiconductor superlattice in the presence of white-noise disorder [25]. Also, it is investigated that how the conductance of graphene superlattice junctions is affected by structural white noise and compared the conductances with those calculated for disordered semiconductor superlattice. In this paper we study the conductance of Dirac fermions in clean and disordered silicene superlattices. We show that the number of resonance picks increases with increasing the number of superlattice barriers. This behavior also appears in graphene. We calculate analytically the transmission probability and describe the reason of the appearance of the resonance picks. Also, the effect of onsite potential difference Δ_z is investigated on the transmission probability. We plot the conductance of the system as a function of potential height and show that it has an oscillatory behavior. Finally, we consider the effect of barriers disorder that maybe generated because of the random nature of experimental technique on the conductance of the silicene superlattice.

The rest of this paper is organized as follows. In Section 2, we describe the transfer matrix method and calculate the transmission probability of Dirac fermions in the ordered silicene superlattice and Section 3 gives the numerical and theoretical results. The conclusions are summarized in Section 4.

2. Model and method

Consider a system of superlattice *p–n* junctions in the independent carrier model at zero temperature and in the absence of carrier–phonon interactions. The Hamiltonian of silicene in the continuum model in the vicinity of the K and K' points can be written as [16]

$$\hat{H_0} = \hbar v_f (k_x \tau_x - k_x \tau_x \eta_z) - \Delta_{SO} \tau_z \sigma_z \eta_z + \Delta_z \tau_z, \tag{1}$$

where $\eta_i = \pm 1$ for the inequivalent the K and K' valleys, τ_i is the sublattice (A and B sites) pseudospin, k_i is an envelope function momentum operator, $\sigma_i = \pm 1$ is the pauli matrices for the spin, where i=x, y and z, and v_f is the Fermi velocity. Δ_{SO} denotes the intrinsic spin–orbit coupling constant. And also, Δ_z is the onsite potential difference between A and B sublattices, which is tunable by an electric field applied perpendicular to the plane.

We consider superlattice *p–n* junctions in a silicene based structure. The system consists of two kinds of monolayer silicene strip with different potentials alternately. Due to the difference of Fermi energy and band structure between two silicene strips, the potential profile of the system is the multiple quantum well structure which is given by

$$V(x) = \begin{cases} V_0, & \text{if } L_{2i-1} < |x| < L_{2i}; \\ 0, & \text{otherwise}, \end{cases} \tag{2}$$

where x_{2i} is the position of barriers' center. In this system the thickness of wells and barriers are d_W and d_B respectively. The model is similar to the potential of semiconductor superlattices that has been used by other groups [21].

The total Hamiltonian of a Dirac carrier in a special geometry is written as $H = H_0 + V(x)$, where $V(x)$ is the silicene-based superlattice potential which is described above. The growth direction is taken to be the x-axis which is designed as the superlattice axis. To solve the transport problem in a silicene superlattice, we assume that the incident electron propagates at angle Φ along the x-axis with energy E across the barriers, in such a way that the Fermi level lies in the conduction band outside the barrier and the valence band inside it. Throughout the paper, we consider the electronic states with energy below the barrier energy ($\Delta < E < V_0 - \Delta$) called Klein zone, which are the most interesting ones to study quantum confinement effects. In order to neglect the strip edges, we assume that the width of the silicene strip is much larger than d_B. Hereafter, we focus only on the K point ($\eta_z = 1$). The same analysis is applicable to the K' point.

In order to analyze the transport problem in a monolayer silicene superlattice, we assume that the electrons are incident at an angle Φ, with respect to the x-axis. The general solutions of the Dirac Hamiltonian can be expressed as:

$$\psi_1(x) = a_i e^{iK_i x} \begin{pmatrix} \hbar v_f k_{i+} \\ E_i \end{pmatrix} + b_i e^{-iK_i x} \begin{pmatrix} -\hbar v_f k_{i-} \\ E_i \end{pmatrix} \tag{3}$$

where

$$s_i = \mathrm{sgn}(E_0 - V(x)), \quad k_y = k \sin(\varphi), \tag{4}$$

$$K_i = \begin{cases} k_x = k \cos(\varphi_i) & \text{for well} \\ k_x' = \dfrac{1}{\hbar v_f} \sqrt{(E - V_0)^2 - (\Delta)^2 - (\hbar v_f k_y)^2} & \text{for barrier} \end{cases} \tag{5}$$

$$E_i = \begin{cases} E_w = E + \Delta & \text{for well} \\ E_b = E + \Delta - V_0 & \text{for barrier} \end{cases} \tag{6}$$

and $\Delta = \eta \sigma \Delta_{SO} - \Delta_z$.

In order to calculate the transmission coefficients, we use the transfer matrix method [21] as follows:

$$\begin{pmatrix} 1 \\ r \end{pmatrix} = A \begin{pmatrix} t \\ 0 \end{pmatrix}, \tag{7}$$

where A is the transfer matrix. We apply the continuity of the wave function at the boundaries and we can calculate the transmission coefficient from the expression: