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Influence of Fermi velocity engineering on electronic and optical properties of graphene superlattices

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ABSTRACT

In this paper, using Kronig–Penney model, the electronic states in graphene-based superlattices with various substrates and considering exact electron Fermi velocity values are investigated. The analysis of our results clearly indicates that the difference between Fermi velocity values of gaped and gapless graphene regions determines the patency rate of band gap. Also, using transfer matrix method (TMM) the absorbance spectrum of mentioned structures is calculated. The more important result is that the absorbance of these structures is significantly near zero.

Graphene, a two-dimensional material with a monolayer honeycomb lattice of carbon atoms, displays very interesting properties. In this perfect two-dimensional system, electrons have a linear relation between energy and momentum, so its band structure has no energy gap. As a consequence, Dirac electrons become massless, and thus behave like massless relativistic particles [1] and lead the observation of a number of very interesting electronic properties such as the chiral behavior, the quantum Hall effect [2,3], ambipolar electric field effect [4] and transport via relativistic Dirac fermions [5], frequency-dependent conductivity [6] and so on.

Besides, graphene exhibits unique electrical [7], mechanical [8,9] and chemical [10,11] properties. These features suggest that graphene could replace other materials in existing applications. Hence, the fabrication of graphene-based optoelectronic devices is of interest and significance from scientific and engineering viewpoints. However, problems associated with absence of a band gap, which basically means that graphene electrical conductivity cannot be switched off completely, is one of the main obstacles to using this material in device applications.

Therefore, the challenge for device developers is to create an improved version of graphene that has a band gap. Several schemes have been explored – such as applying an electric field, adding chemical impurities or modifying the structure of graphene. On the other hand, as has been shown, the gap can be induced by substrate or strain engineering as well as by deposition or adsorption of molecules on a graphene layer [12]. Generally speaking, for manipulating the electronic structure of materials, semiconducting and metallic superlattice structures are now commonly used [13]. Recently, the interest of researchers was concentrated on the study of graphene-based superlattices (SLs) [14–20]. In this field, the investigations have been done for electron behaviors in graphene superlattices (GSLs), associated with different types of periodic potential: Kronig–Penney [21–23], muffin-tin [24,25], and cosine [26].

As has been shown, the most reasonable and simple model of the superlattice on the base of graphene is substrate engineering. For example, in [27] the model superlattice on the base of graphene placed on the substrate, consisted of periodically interchanged strips of different dielectrics, is investigated. As we know, the interaction between graphene and the substrate may lead energy band gap opening in the graphene energy spectrum. In the spectrums of graphene on silicon carbide substrate and graphene on hexagonal boron nitride there are an energy gap about 0.26 eV [28] and 53 meV, respectively [29]. On the other hand, graphene placed on the quartz substrate doesn't have the band gap in its energy spectrum [27]. The alternation of strips of gap and gapless modification of this material creates a set of potential barriers for charge carriers.

In this study, the graphene superlattices are formed by periodically altering strips. These strips include quartz (i.e. the material that doesn't have effect on the graphene band structure) and h-BN

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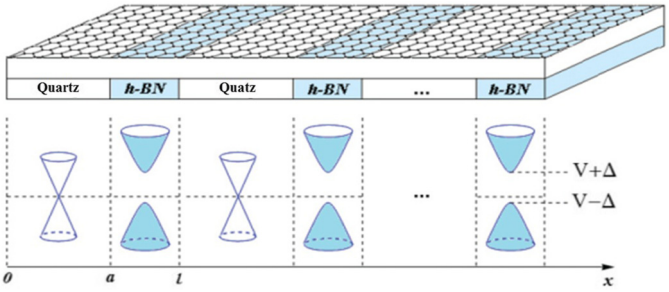

Fig. 1. Graphene layer on the striped substrate composed of quartz and hexagonal boron nitride.

or SiC (i.e. materials that have significant effect on the graphene band structure).

Despite other work that they neglect the effect of Fermi velocity on electronic band structures, by supposing same Fermi velocities in both graphene fractions [30,31], in our model, for more detailed investigation, the exact Fermi velocity amounts of graphene on each substrate are considered.

The outline of this paper is the following. In Section 2, based on Kronig–Penney model and transfer matrix method (TMM), and by regarding exact Fermi velocities for graphene on each substrate and using two component bases, the electronic band structures of two different graphene superlattices and also the transmittance, reflectance and absorbance of these structures are investigated. Finally, in Section 3, our conclusion is summarized.

We consider a one-dimensional graphene superlattice with period of "L" that in which the gap and band shift are only position-dependent. Such structures can be obtained, e.g., on the base of graphene deposited on a strip substrate combined from quartz and h-BN or quartz and SiC (see Fig. 1).

The Kronig–Penney model is applied for investigation of graphene superlattices performance. In the vicinity of the K point of the Brillouin zone, the superlattice electronic structure can be described by the Dirac-like equation:

$$\hat{H}\psi(x,y) = E\psi(x,y) \tag{1}$$

H is the Hamiltonian operator and defined as below,

$$\hat{H} = v_f(x)\hat{\mathbf{P}}\hat{\boldsymbol{\sigma}} + V(x)\hat{I} + \Delta(x)\hat{\sigma}_z \tag{2}$$

Here, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ and σ_z are the Pauli matrices, and $\mathbf{P} = (p_x, p_y) = (-i\hbar\frac{\partial}{\partial x}, -i\hbar\frac{\partial}{\partial y})$ is the momentum operator. In our study, the potential V defines the shift of the forbidden band center in the gapped graphene with respect to the Dirac point in the gapless graphene [27,32] (see Fig. 1). Besides, the half-width of the band gap have periodically modulated by Δ. Generally speaking, we have

$$\text{For } 0 \le x < a: \quad \Delta(x) = \Delta \text{ and } V(x) = V. \tag{3}$$

$$\text{For } a \le x < l: \quad \Delta(x) = V(x) = 0. \tag{4}$$

As it mentioned in [33], the Fermi velocity is one of the key concepts in the study of a material and it bears information on a variety of fundamental properties. Due to the graphene lattice structure and its Fermi energy position, the low-energy electronic excitations of this material are described by an effective field theory that is Lorentz invariant [34]. Lorentz invariant theories are characterized by an effective velocity. Because of this, an increase of electron–electron interactions induces an increase of the Fermi velocity. In this paper, we follow the trend of [33] to control electron–electron interactions and the Fermi velocity of graphene using dielectrics. Hence, based on the results of [33], it is obvious that the Fermi velocity can differ in graphene modification placed on different substrates.

Table 1
Fermi velocity (v_f) and dielectric constant (ε) of graphene on each substrate.

Substrate	$v_f(\times 10^6)$ m/s	ε
SiC	1.15 ± 0.02	7.26 ± 0.02
h-BN	1.49 ± 0.08	4.22 ± 0.01
Quartz	2.49 ± 0.30	1.80 ± 0.02

Despite other work that they neglect the dependence v_f on 'x' supposing same v_f in both graphene fractions [31], in our model, to obtain exact results, we consider the dependence of v_f on 'x'. For this purpose we use the Fermi velocity as listed in Table 1 [33].

Because of the translation invariance in the y direction, we expect that wavefunction satisfies the following equation,

$$\psi(x,y) = e^{ik_y y}\psi(x) \tag{5}$$

The above Hamiltonian acts on smooth envelope functions for two triangular sublattices in monolayer graphene. Therefore, from Eq. (1), we obtain

$$i\frac{\partial\psi_A(x)}{\partial x} - ik_y\psi_A(x) = \frac{V(x) - E - \Delta(x)}{\hbar v_f(x)}\psi_B(x) \tag{6}$$

$$i\frac{\partial\psi_B(x)}{\partial x} + ik_y\psi_B(x) = \frac{V(x) - E + \Delta(x)}{\hbar v_f(x)}\psi_A(x) \tag{7}$$

Eqs. (6) and (7), yield

$$i\frac{d\psi}{dx} = \hat{h}(x)\psi(x) \tag{8}$$

where $\hat{h}(x)$ is defined as below

$$\hat{h}(x) = \begin{pmatrix} ik_y & \frac{V(x)-E-\Delta(x)}{\hbar v_f(x)} \\ \frac{V(x)-E+\Delta(x)}{\hbar v_f(x)} & -ik_y \end{pmatrix} \tag{9}$$

The simple solution of this equation can be

$$\psi(x) = \exp\left[-i(x - x_0)\hat{h}\right]\psi(x_0) \tag{10}$$

Here, it is assumed that x, x_0 belong to the space-homogeneous region.

The wavefunction of this superlattice structure is a Bloch function and using its transfer matrix, it is possible to obtain an expression for the dispersion relation

$$\cos(kl) = \cos\big((l-a)Q_x\big)\cos(aK_x) + \frac{EV - (\hbar^2 v'_f v'' k_x^2)}{K_x Q_x(\hbar^2 v'_f v''_f)}\sin\big((l-a)Q_x\big)\sin(aK_x) \tag{11}$$

where $K_x = \sqrt{\frac{E^2}{(\hbar v'_f)^2} - k_y^2}$, $Q_x = \sqrt{\frac{(V-E)^2-\Delta^2}{(\hbar v''_f)^2} - k_y^2}$ and $k_x = \sqrt{\frac{E^2}{\hbar^2 v'_f v''_f} - k_y^2}$.

A similar equation for the allowed energies was obtained also in [31] via neglecting the dependence v_f on x supposing same v_f in both graphene fractions.

The dispersion relation (Eq. (11)) shows that simultaneous variation of $E \to -E$ and $V \to -V$ doesn't have any effect on this equation. So, we only investigate the effects of positive relative band shift V. Simulation results show that the miniband structures have strong dependence on the system parameters.

The numerical calculations of energy dependence on k were performed for three values $V = 0$, 26.8 and 43.2 meV at $\Delta = 29.5$ meV, $k_y = 0$, $L = 80$ nm and $a = L/2$ (see Fig. 2). It can be

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