Superlattice Based on Graphene on a Strip Substrate

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A graphene-based superlattice formed due to the periodic modulation of the band gap has been investigated. Such a modulation is possible in graphene deposited on a strip substrate made of silicon oxide and hexagonal boron nitride. The advantages and some possible problems in the superlattice under consideration are discussed. A model describing such a superlattice is proposed and the dispersion relation between the energy and momentum of carriers has been obtained using the transfer matrix method within this model.

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1. INTRODUCTION

Interest in graphene-based superlattices has increased in recent years. Calculations of graphene-based superlattices with periodic rows of vacancies were performed using the molecular dynamics method [1]. Calculations of single-atom-thick superlattices formed by lines of pairs of adsorbed hydrogen atoms on graphene were carried out with the density functional theory [2].

Rippled graphene that can be treated as a superlattice with the one-dimensional periodic potential of ripples was investigated in [3–5]. Superlattices obtained when a periodic electrostatic potential [6–9] or periodically located magnetic barriers [10–13] were applied to graphene were analytically examined.

However, the investigation of the graphene-based superlattice with a periodic electrostatic potential disregarded the fact that the application of the electrostatic potential to a gapless semiconductor (graphene) results in the production of electron–hole pairs and the redistribution of charge: electrons move from the region where the top of the valence band lies above the Fermi level to the region where the bottom of the conduction band lies below the Fermi level. The superlattice becomes a structure consisting of positively charged regions, where the electrostatic potential displacing the Dirac points upward in energy is applied, alternating with negatively charged regions. The strong electrostatic potential of induced charges appears and strongly distorts the initial step electrostatic potential and, therefore, the electronic structure of the superlattice calculated disregarding the electrostatic potential of induced charges.

To avoid the production of electron–hole pairs, a superlattice appearing due to the periodic modulation of the band gap is considered.

A superlattice in the form of the periodic planar heterostructure of graphene nanoribbons between which nanoribbons of hexagonal boron nitride (h-BN) are inserted was previously proposed in [14]. The band structure of such a superlattice was numerically calculated. However, it is very difficult to implement this superlattice even using the advances of modern lithography, because problems inevitably arise with the control of periodicity in the process of the etching of nanoribbons in a graphene sheet and the insertion of h-BN nanoribbons. Moreover, h-BN is an insulator with a band gap of 5.97 eV, which significantly hinders the tunneling of carriers between graphene nanoribbons. Such a heterostructure is most probably a set of quantum wells where the wavefunctions of carriers from neighboring quantum wells almost do not overlap.

In this work, a superlattice formed by a graphene sheet deposited on a strip substrate is proposed. The strip substrate is made of periodically alternating strips of SiO$_2$ (or any other material that does not affect the band structure of graphene) and h-BN, as shown in Fig. 1. The h-BN layers are located so that its hexagonal crystal lattice is under the hexagonal crystal lattice of graphene. Owing to this location, a band gap of 53 meV appears in the band structure of graphene.

![Fig. 1. Graphene on the strip substrate consisting of alternating SiO$_2$ and h-BN strips.](image-url)
The appearing periodic stress field of the substrate can also affect the band structure of the proposed superlattice, but this effect is very small.

2. MODEL DESCRIBING THE SUPERLATTICE

The $x$ and $y$ axes are perpendicular and parallel to the interfaces of h-BN and SiO$_2$ strips, respectively (see Fig. 1). The superlattice is described by the Dirac equation

$$\left( v_F \sigma \hat{p} + \Delta \sigma_z + V \right) \Psi(x,y) = E \Psi(x,y), \quad (1)$$

where $v_F \approx 10^6$ cm/s is the Fermi velocity, $\sigma = (\sigma_x, \sigma_y)$ and $\sigma_z$ are the Pauli matrices, and $\hat{p} = -i \nabla$ is the momentum operator (the system of units with $\hbar = 1$ is used). The half-width of the band gap is periodically modulated:

$$\Delta = \begin{cases} 0, & d(n - 1) < x < -d_{II} + dn, \\ \Delta_0, & -d_{II} + dn < x < dn. \end{cases}$$

where $n$ is an integer enumerating the supercells of the superlattice; $d_I$ and $d_{II}$ are the widths of the SiO$_2$ and h-BN strips, respectively; and $d = d_I + d_{II}$ are the period of the superlattice (the size of the supercell along the $x$ axis). The periodic scalar potential $V$ can appear due to the difference between the energy positions of the middle of the band gap of the gap modification of graphene and conic points of the Brillouin zone of gapless graphene (see Fig. 2):

$$V = \begin{cases} 0, & d(n - 1) < x < -d_{II} + dn, \\ V_0, & -d_{II} + dn < x < dn. \end{cases}$$

In order for the superlattice to be a first-type superlattice, the inequality $|V_0| \leq 0$ should be satisfied. The solution of Eq. (1) for the first supercell has the form

$$\Psi(x,y) = \psi_1(x)e^{ik_y y}, \quad 0 < x < d.$$ 

For the $n$th supercell, in view of the periodicity of the superlattice,

$$\psi_n(x) = \psi_1(x + (n - 1)d).$$

In the quantum well region ($0 < x < d_I$), the solution of Eq. (1) is a plane wave

$$\psi_{n}^{(1)}(x) = N_k(\alpha_n^{(1)} b_n^{(1)} e^{ik_1 x} + \lambda_k c_n^{(1)} d_n^{(1)} e^{-ik_1 x}, \quad (2)$$

where $N_k$ is the normalization factor. The substitution of Eq. (2) into Eq. (1) provides the relation between the lower and upper spinor components

$$b_n^{(1)} = \lambda_+ c_n^{(1)}, \quad d_n^{(1)} = -\lambda_- c_n^{(1)}, \quad \lambda_{\pm} = \frac{v_F(k_1 \pm ik_y)}{E}.$$ 

The relation of $E$ with $k_1$ and $k_y$ has the form

$$E = \pm v_F \sqrt{k_1^2 + k_y^2}.$$
It is convenient to represent Eq. (2) in a more compact form [7]:

\[
\psi^{(1)}_n(x) = \Omega_{k_1}(x) \left( \begin{array}{c} a^{(1)}_n \\ c^{(1)}_n \end{array} \right), \\
\Omega_{k_1}(x) = N_{k_1} \left( \begin{array}{cc} 1 & 1 \\ \lambda_+ & -\lambda_- \end{array} \right) e^{ik_1 x \sigma_z}. \tag{3}
\]

When the inequality

\[
\Delta_0^2 + v_F^2 k_y^2 - (E - V_0)^2 \geq 0
\]

is satisfied, the solution of Eq. (1) in the barrier region \((d_1 < x < d)\) has the form

\[
\psi^{(2)}_n(x) = \Omega_{k_2}(x) \left( \begin{array}{c} a^{(2)}_n \\ c^{(2)}_n \end{array} \right), \\
\Omega_{k_2}(x) = N_{k_2} \left( \begin{array}{cc} 1 & 1 \\ -\lambda_- & \lambda_+ \end{array} \right) e^{ik_2 x \sigma_z}, \tag{5}
\]

where

\[
\lambda_{\pm} = \frac{i v_F (k_2 \pm k_y)}{E + \Delta_0 - V_0}, \quad k_2 = \frac{1}{v_F} \sqrt{\Delta_0^2 + v_F^2 k_y^2 - (E - V_0)^2}.
\]

The solution of Eq. (1) in the barrier region under the condition

\[
\Delta_0^2 + v_F^2 k_y^2 - (E - V_0)^2 < 0
\]

is given by Eq. (5) with the change \(k_2 \to i\kappa_2\), i.e., it is oscillating.

The possibility of existing Tamm minibands formed by localized states near the interface between graphene and its gap modification will be considered below. In this case, \(k_1 \to i\kappa_1\) \(k_2\) is real. A necessary condition for existing Tamm states has the form

\[
|k_y| \geq |\kappa_1|;
\]

under this condition, the energy \(E = \pm v_F \sqrt{k_y^2 - \kappa_1^2}\) is real.

3. DERIVATION OF THE DISPERSION RELATION

The dispersion relation is derived using the transfer matrix \((T\) matrix\) method. The \(T\) matrix relates the spinor components for the \(n\)th supercell to the spinor components of the solution of the same type for the \((n+1)\)th supercell. For example, for the solution in the quantum well region,

\[
\left( \begin{array}{c} a_{n+1}^{(1)} \\ c_{n+1}^{(1)} \end{array} \right) = T \left( \begin{array}{c} a_n^{(1)} \\ c_n^{(1)} \end{array} \right). \tag{7}
\]

To determine the \(T\) matrix, the following conditions of the continuity of the solution of the Dirac equation describing the considered superlattice are used:

\[
\Psi^{(1)}_n(d_1 - 0) = \Psi^{(2)}_n(d_1 + 0),
\Psi^{(2)}_n(d - 0) = \Psi^{(1)}_{n+1}(+0).
\]

These conditions provide the equalities

\[
\left( \begin{array}{c} a^{(2)}_n \\ c^{(2)}_n \end{array} \right) = \Omega_{k_2}^{-1}(d) \Omega_{k_1}(d) \left( \begin{array}{c} a^{(1)}_n \\ c^{(1)}_n \end{array} \right), \\
\left( \begin{array}{c} a^{(1)}_{n+1} \\ c^{(1)}_{n+1} \end{array} \right) = \Omega_{k_1}^{-1}(0) \Omega_{k_2}(d) \left( \begin{array}{c} a^{(2)}_n \\ c^{(2)}_n \end{array} \right). \tag{8}
\]

According to definition (7) of the \(T\) matrix and the last two equalities\(^1\),

\[
T = \Omega_{k_2}^{-1}(0) \Omega_{k_2}(d) \Omega_{k_1}^{-1}(d) \Omega_{k_1}(d). \tag{9}
\]

The substitution of Eqs. (3) and (5) with the corresponding arguments into Eq. (8) yields the expressions

\[
T_{11} = \alpha e^{ik_1 d} \left[ (\lambda_+ + \tilde{\lambda}_+)(\lambda_+ + \tilde{\lambda}_-) e^{-k_2 d} - (\lambda_- + \tilde{\lambda}_-)(\lambda_+ - \tilde{\lambda}_+) e^{k_2 d} \right],
T_{12} = 2 \alpha e^{-ik_1 d} \left[ (\lambda_+ + \tilde{\lambda}_+)(\lambda_- - \tilde{\lambda}_-) sh(k_2 d), \right],
T_{21} = T_{12}, \quad T_{22} = T_{11}^*.
\]

The last two relations in Eqs. (9) are the general properties of the \(T\) matrix.

The derivation of the dispersion relation with the use of the \(T\) matrix is briefly as follows.

Let \(N = L/d\) be the number of supercells in the entire superlattice, where \(L\) is the length of the superlattice along the \(x\) axis, i.e., the direction of the application of the periodic potential. The Born–Karman cyclic boundary conditions for the superlattice have the form

\[
\Psi^{(1)}_N(x) = \Psi^{(2)}_1(x).
\]

At the same time,

\[
\Psi^{(1,2)}_N(x) = T^N \Psi^{(1,2)}_1(x),
\]

from which, \(T^N = I\), where \(I\) is the \(2 \times 2\) unit matrix.

It is convenient to diagonalize the \(T\) matrix by means of the transition matrix \(S\):

\[
T_d = S T S^{-1} = \left( \begin{array}{cc} \lambda_1 & 0 \\ 0 & \lambda_2 \end{array} \right),
\]

where \(\lambda_{1,2}\) are the eigenvalues of the \(T\) matrix and have the property \(\lambda_2 = \lambda_1^\ast\). According to \(T^N_d = I\)

\[
\lambda_1 = e^{2\pi i n/N}, \quad -N/2 < n \leq N/2.
\]

In view of the property \(TrT = TrT_d\) and in terms of the notation \(k_z = 2\pi n/L\) \((\pi/d < k_z \leq \pi/d)\), the dispersion relation is obtained in the form

\[
TrT = 2 \cos(k_z d). \tag{10}
\]

\(^{1}\)Note that the cyclic permutations of the factors of \(T\) matrices are possible in the definition of the \(T\) matrix; these permutations do not change the dispersion relation (10). This can be verified by comparing Eq. (8) with Eq. (23) in [7].
Taking into account the last relation in Eqs. (9), Eq. (10) can also be written in the form
\[ \text{Re} T_{11} = \cos(k_x d). \]

Dispersion relation (10) under condition (4) gives the equation
\[
\frac{v_F^2 k_1^2 - v_F^2 k_2^2 + V_0^2 - \Delta_0^2}{2v_F^2 k_1 k_2} \sin(k_2 d_{II}) \sin(k_1 d_I) + \cosh(k_2 d_{II}) \cos(k_1 d_I) = \cos(k_x d) .
\]

(11)

According to this equation, the passage to the single-band limit is performed by two methods: first, \( V_0 = \Delta_0 \) (the quantum well only for electrons) and, second, \( V_0 = -\Delta_0 \) (the quantum well only for holes). The result of the passage coincides with the known nonrelativistic dispersion relation (see, e.g., [22]), although the expressions for \( k_1, k_2 \), and \( E \) are different.

If inequality (6) is satisfied, the change \( k_2 \rightarrow i\kappa_2 \) should be made in Eq. (11):
\[
\frac{-v_F^2 \kappa_2^2 - v_F^2 k_2^2 + V_0^2 - \Delta_0^2}{2v_F^2 k_1 \kappa_2} \sin(\kappa_2 d_{II}) \sin(k_1 d_I) + \cosh(\kappa_2 d_{II}) \cos(k_1 d_I) = \cos(k_x d) .
\]

(12)

For Tamm minibands, the change \( k_1 \rightarrow i\kappa_1 \) should be made in Eq. (11):
\[
\frac{v_F^2 k_2^2 + v_F^2 \kappa_1^2 + V_0^2 - \Delta_0^2}{2v_F^2 \kappa_1 k_2} \sinh(k_2 d_{II}) \sinh(\kappa_1 d_I) + \cosh(k_2 d_{II}) \cosh(\kappa_1 d_I) = \cos(k_x d) .
\]

(13)

Equation (13) has the solution only under the condition
\[ v_F^2 k_2^2 + v_F^2 \kappa_1^2 + V_0^2 - \Delta_0^2 < 0 . \]

However, this inequality is never satisfied; correspondingly, the Tamm minibands are absent in the superlattice under consideration.

4. RESULTS OF THE NUMERICAL CALCULATION

The numerical calculations of the dependence of the energy on \( k_x \) were performed for two values \( k_y = 0 \) and \( 0.1 \text{ nm}^{-1} \) at \( V_0 = 0 \) (see Fig. 3). The energy of carriers is assumed to be low, \( |E| \lesssim 1 \text{ eV} \), because the Dirac dispersion relation for carriers and, correspondingly, Dirac equation (1) are invalid for high energies.

The electron minibands are separated from hole minibands by a band gap, which increases with \( |k_y| \). For \( d_I = d_{II} \) at \( k_y = 0 \), it is \( E_g \approx 10-30 \text{ meV} \) when \( d=10—100 \text{ nm} \). In this case, the solution of Eq. (11) is transformed to the solution of Eq. (12). The band gap can increase strongly when \( d_{II} \) increases with respect to \( d_I \): \( E_g \gtrsim 100 \text{ meV} \), i.e., is several times larger than \( 2\Delta_0 \).

The width of the minibands decreases with an increase in the period of the superlattice \( d \). The dependence of the width of the minibands on \( V_0 \) was also examined. The widths of the electron and hole minibands increase and decrease, respectively, at \( V_0 > 0 \) and vice versa at \( V_0 < 0 \).

Fig. 3. Numerically calculated dependence of the energy on \( k_x \) for two \( k_y \) values and two superlattice periods \( d \). The dispersion curves for the superlattices with \( d_I = (\text{solid lines}) \ d_{II}, \ (\text{dashed lines}) \ d_{II}/2, \) and (dotted lines) \( 2d_{II} \).
5. POSSIBLE APPLICATIONS OF THE SUPERLATTICE

The described superlattice can be used as a field-effect transistor (FET) where the substrate serves as a gate. The ratio of the current through the superlattice to the current through the gate at a substrate thickness of about 10 nm can reach \( \sim 10^6 \) as for FET based on graphene nanoribbons [23]. The main advantage of the considered superlattice is the absence of the effect of the scattering of carriers on the edges of a nanoribbon on their mobility. The mobility of the carriers in gapless graphene reaches \( \mu_0 = 2 \times 10^6 \text{cm}^2/(\text{V s}) \) [24, 25]. However, the mobility of carriers in FET based on the graphene nanoribbon with a width of \( w \sim 3 \text{ nm} \) is three orders of magnitude smaller than \( \mu_0 \). The cause of such a strong decrease is possibly the scattering of carriers at the edges of graphene nanoribbons. The mean free path between two acts of the scattering of carriers at the edges of graphene nanoribbons. The mean free path between two acts of the scattering of carriers at the edges of the graphene nanoribbon \( \lambda_{edge} \propto w/P \), where \( P \) is the probability of backscattering [23]. For sufficiently good edges, \( P < 1 \). The problem of scattering on edges is absent for the proposed superlattice; for this reason, the mobility of the carriers in the superlattice is expected to be \( \sim \mu_0 \) in the absence of the problems with the periodicity of the potential. At the same time, a sufficiently large \( E_g \) value, which provides the operation of FET at room temperature, can be reached.

If an Au film is deposited on the lower side of the substrate and graphene is optically pumped, the superlattice can be used as a terahertz laser similar to a terahertz laser based on gapless graphene [26]. In this case, terahertz radiation will be emitted from the regions of the SiO\(_2\) substrate.

6. CONCLUSIONS

A model describing such a superlattice based on graphene on a strip substrate has been proposed. The dispersion relation has been derived, which is transferred to the known nonrelativistic dispersion relation in the passage to the single-band limit. The numerical calculations have been performed for a pair of the nearest electron and hole minibands using the derived dispersion relation. Possible applications of the superlattice as a transistor or a terahertz laser have been pointed out.

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