Conductivity of a superlattice based on the semi-Dirac crystals

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Abstract. The current-voltage characteristic of a superlattice based on the semi-Dirac crystals has been studied. The case of the absence of a gap between valence and conduction mini-band has been considered. Such a superlattice has been shown to be characterized by both semi-metal and narrow-band semiconductor electrical properties. From the one hand there is the point in the Brillouin zone close to which the depletion of the states occurs without gap opening. From the other hand there is the portion of negative differential conductivity in the current-voltage characteristic. The dependences of longitudinal conductivity and maximum of the current-voltage characteristic on the Fermi energy have been investigated.

1. Introduction

Presently, in physics of the solid-state increased attention of researchers is paid to the electric and optical properties of so-called Dirac and semi-Dirac crystals [1, 2]. The charge carriers of these structures demonstrate a unique dynamics which is peculiar to massless fermions. The class of Dirac materials includes two-dimensional (2D) crystals such as graphene, germanene, silicene, etc. Recently, in the laboratory phosphorene has been obtained [3]. It is referred to the semi-Dirac crystals where electrons have a linear dispersion along one direction, while they have a parabolic energy spectrum and a finite effective mass along the perpendicular direction. Unusual dispersion of carriers for these materials leads to unique transport and optical properties which are intensively studied both experimentally and theoretically [4–6]. So, for example, in [2] topological transitions between the semi-metallic phase and the band insulator had been studied for semi-Dirac crystals.

After graphene-like materials had been obtained researchers focused their attention on the electric and optical properties of Dirac structures with an additional superlattice (SL) potential [7,9]. Firstly, such nanostructures exhibit graphene characteristic properties. Secondly, the presence of SL makes it possible to demonstrate the nonlinear effects associated with a special type of a current-voltage (I-V) characteristic of SL [10]. Namely, it contains the region of negative differential conductivity (NDC) which plays one of the key roles in terahertz (THz) engineering [11,12]. In [13] the dispersion law of new type of SL based on nanostructures with semi-Dirac fermions had been studied. On the one hand the allowed energy bands (mini-bands) of the new type of SL are separated by forbidden bands just as in the case of semiconductor
or graphene SL \[7\]. On the other hand there can be the point in the Brillouin zone close to which the depletion of the states occurs without gap opening. Such a situation is typical for semi-metals.

Below we consider SL based on the semi-Dirac materials with indicated properties. The paper is organized as follows. In the second section we discuss the conditions of the appearing of the region with the depletion of the states in the Brillouin zone. In the third section we calculate the longitudinal I-V characteristic of considered SL. Then we discuss the peculiarities of derived I-V characteristic. The last section is conclusion.

2. Dispersion law within Kronig-Penney model

To find out the dispersion of carriers of SL we use the effective Hamiltonian \[2\] with a periodical modulation of the parameter \(\Delta\) along the axis \(Ox\):

\[
\hat{H} = v_F \hat{p}_x \hat{\sigma}_x + \left(\Delta(x) + \alpha \hat{p}_y^2\right) \hat{\sigma}_y ,
\]

where \(\hat{\sigma}_{x,y}\) are Pauli matrices, \(\Delta(x) = \Delta(x + d)\), \(d\) is SL period, \(\alpha = 1/2m\) and the profile of spatial modulation \(\Delta(x)\) is given by the Kronig-Penney model:

\[
V(x) = \begin{cases} 
\Delta_1, & (n-1)d < x < a + (n-1)d, \\
\Delta_2, & a + (n-1)d < x < nd .
\end{cases}
\]

Here \(n\) is integer, \(d = a + b\), \(\Delta_1 < \Delta_2\), \(a\) and \(b\) are well and barrier widths correspondingly. In \[13\] the dispersion \(\varepsilon(p)\) of carriers in the presence of rectangular modulation \(2\) had been found from the eigenvalue problem \(\hat{H} \psi = \varepsilon \psi\) by means of transfer matrix method. The result reads \((\hbar = 1)\):

\[
\frac{\left(\Delta_1 + \alpha \hat{p}_y^2\right) \left(\Delta_2 + \alpha \hat{p}_y^2\right) - \varepsilon^2}{p_1 p_2 v_F^2} \sin(p_1a) \sin(p_2b) + \cos(p_1a) \cos(p_2b) = \cos(p_x d) ,
\]

where we define

\[
v_{F1,2} = \sqrt{\varepsilon^2 - \left(\Delta_{1,2} + \alpha \hat{p}_y^2\right)^2}.
\]

The energy spectrum of suggested system had been shown in \[13\] to be the number of the allowed mini-bands separated by the forbidden mini-bands. However if \(\Delta_1 < 0\) and \(b \Delta_2 \leq a |\Delta_1|\) then valence mini-band touches conduction mini-band at two Dirac points which exist on the both sides of \(p_y\)-axis origin. The distance between them in \(p\)-space is \(2K\), where

\[
K = \sqrt{\frac{a |\Delta_1| - b \Delta_2}{d}}.
\]

So if \(a |\Delta_1| = b \Delta_2\) then both Dirac Points merge into single one.

Further for analytical calculations we put the condition \(a |\Delta_1| = b \Delta_2\) and use the low-energy approximation for the relation \[3\]. As a result we have

\[
\varepsilon(p) = \pm \sqrt{\frac{2v_F^2}{d^2} \left(1 - \cos p_x d\right) + \alpha^2 p_y^4} .
\]

In this section we use the explicit form of the carrier dispersion \[6\] to calculate the density of states (DOS) in valence and conduction bands. The standard formula reads

\[
\rho(\varepsilon_0) = \frac{\partial}{\partial \varepsilon_0} \int \int dp_x dp_y \frac{1}{(2\pi)^2}.
\]
After some transformations we arrive at

\[ \rho(w) = \frac{1}{\pi^2} \sqrt{\frac{2m}{v_F d}} \frac{\partial}{\partial w} \int_0^4 \sqrt{w^2 - \sin^2 \frac{\xi}{2}} \, d\xi, \]  

(8)

where \( w = \epsilon/\Delta_0, \Delta_0 = 2v_F/d, \)

\[ h(w) = \pi \theta(w - 1) + 2\theta(1 - w) \arcsin w, \]

\( \theta(\xi) \) is unit-step function. Result of integration in (8) is represented in Fig. 1. From this figure one can see that there is the region with the depletion of the states in the vicinity of the point with \( \epsilon = 0 \) (solid line). This is the point where valence and conduction mini-bands touch each other without gap opening. Such a situation characterizes the semi-metal state and differs considered SL from both semiconductor SL (for instance, \[14\]) and gapped graphene-based SL \[7\] (dashed line in Fig. 1).

3. Longitudinal I-V characteristic of SL

Let us consider the constant electric field with vector \( \mathbf{E} \) applied along the SL axis \( Ox. \) To calculate the current density being appeared by this field we use the explicit form of the electron spectrum (6) and the \( \tau \)-approximation:

\[ j_x(e) = \int_0^\infty e^{-\xi} d\xi \sum_{\mathbf{p}} V_x (p_x + eE\tau \xi, p_y) f_0 (\epsilon(\mathbf{p})). \]  

(9)

Here \( \tau \) is constant relaxation time, \( V_x = \partial\epsilon/\partial p_x \) is electron group velocity, \( f_0 (\epsilon) \) is equilibrium state function of carriers in the material. We should take into account that at weak fields investigated material has the semi-metallic type of the conductivity due to the absence of the gap between the valence and conduction band. Thus it is necessary to apply the Fermi-Dirac statistics for electrons in conduction mini-band. For extremely low temperatures we have \( f_0 (\epsilon) = \theta(\epsilon_F - \epsilon), \) where \( \epsilon_F \) is Fermi energy. Due to existence of the region of the depletion of the states in the bottom of the conduction band \( \text{Fig. 1} \) it is necessary to ensure the location of Fermi level somewhere inside the valence or conduction band. In opposite case the SL conductivity is zero at zero-temperatures. After some transformations we obtain

\[ j_x = j_0 \int_0^\infty e^{-\xi} d\xi \sum_{s=0,1} (-1)^s \int_0^w \sqrt{\sin^2 \left(h_s (w, y) + \frac{\omega_B \tau \xi}{2} \right) + y^4} \, dy. \]  

(10)
In (10) we have introduced the constant \( j_0 = e \sqrt{m \Delta_0^3/4 \sqrt{2} \pi^2 d} \), Bloch frequency \( \omega_B = e E d \) and the function:

\[
h_s(w, y) = (-1)^s \arcsin \sqrt{w^2 - y^4}.
\]

Further calculations give

\[
j_x = j_0 \sum_{n=1}^{\infty} \frac{nF_n(w) \omega_B \tau}{1 + n^2 \omega_B^2 \tau^2}.
\]

Here we define the following functions:

\[
F_n(w) = -2 \int_{g(w)}^{\sqrt{w}} A_n(\xi) \sin \left(2n \arcsin \sqrt{w^2 - \xi^4}\right) d\xi,
\]

\[
A_n(\xi) = \frac{2\xi \Gamma(3/2)}{\Gamma(n + 3/2)} \Re \left[ \frac{(1 + \xi^4)^{1/4}}{i^n} P_{1/2}^n \left( \frac{1 + 2\xi^4}{2\xi^2 \sqrt{1 + \xi^4}} \right) \right],
\]

where \( \Gamma(\xi) \) is gamma-function, \( P_k^n(\xi) \) is associated Legendre polynomials. The lower limit of integration in (12) is \( g(w) = (w^2 - 1)^{1/4} \theta(w - 1) \). The I-V characteristics have been plotted by use of the result (11). The current density dependences on the electric field intensity are shown in Fig. 2 for different positions of the Fermi level. Here the standard values of the parameters have been used: \( v_F \sim 10^8 \) cm/s, \( d \sim 2 \cdot 10^{-6} \) cm, \( \tau \sim 10^{-12} \) s.

### 4. Analysis of I-V characteristics

From the I-V characteristics represented in Fig. 2, one can see the next peculiarities. There is the region of NDC in I-V characteristic of considered SL. This is the consequence of the narrowness of the conduction band and is manifested for semiconductor SL. Never-the-less investigated structure has the semi-metal properties due to the absence of the gap between valence and
conduction bands and the presence of the depletion of the states in the vicinity of the bottom of the conduction mini-band. The position of maximum of I-V function and its magnitude can be regulated by change of the Fermi energy. These dependences are seen from Fig. 2 to be non-monotonous.

\textbf{Figure 3.} Longitudinal conductivity vs Fermi energy.

To see this fact explicitly the conductivity of SL as function of Fermi energy have been plotted numerically by use of the formula

$$
\sigma = \sigma_0 \sum_{n=1}^{\infty} nF_n(w), \quad (14)
$$

where $\sigma_0 = ed\tau j_0$. The result is shown in Fig. 3. Indeed conductivity $\sigma$ increases with $\varepsilon_F$, passes the maximum and then decreases to zero. Such a behaviour of SL conductivity can be easy explained by DOS dependence on the energy (Fig. 1). At the bottom of the conduction band there is the depletion of the states therefore conductivity is sufficiently low. As the Fermi level rises, it crosses the region of increased DOS (the vicinity of the point $\varepsilon = \Delta_0$). It leads to the increasing of the conductivity. Calculations give that the mobility of charge carriers corresponding to the maximum of conductivity Fig. 3 consists the order $2 \cdot 10^3$ cm$^2$/V·s. This is comparable with that of SiO$_2$-supported graphene [15] and electrolyte-gated graphene [16] (here we use the standard values of the structure parameters indicated at the end of section 3).

Further shifting of the Fermi level gives the decreasing of DOS and as a consequence it yields to decreasing of both the conductivity and the magnitude of I-V characteristic maximum.

Described result gives the possibility of a Bloch generator engineering based on above SL. It is well known that the obstacle of the design of these generators is the existence of low-frequency domain instability in SL, which suppresses THz generation. As had been reported in [11, 17], one of the ways to overcome this instability is to create the situation allowing the control of the position of NDC portion in static I-V characteristic. The possibility of regulating of the position of the maximum in I-V characteristic by changing of the Fermi level location allows us to believe that above difficulty can be overcome by use of SL based on the semi-Dirac materials.

At the end we note that current density (11) and conductivity (14) have been derived from the formula (9) which is based on both Boltzmann kinetic equation and classical equation of motion. Such method is valid if semiclassical limit has been reached. Namely, de Broglie wavelength should be much less than the mean free path of carriers or $\varepsilon_F\tau \gg 1$ ($h = 1$). In opposite case the quantum equations of motion should be applied. Particularly, it had been done in [18] to calculate the optical conductivity of graphene. One can see from Fig. 2 that minimal value of the parameter $\varepsilon_F\tau$ consists the order $20$ ($\Delta_0\tau \sim 10^2$). Thus the condition for the semiclassical approach is quitely justified.

5. Conclusion

The numerical analysis of the I-V characteristic of SL based on the semi-Dirac crystals have shown the following peculiarities. Firstly, there is the region of NDC in I-V characteristic of
considered SL. This is peculiar to semiconductor SL and is the consequence of the narrowness of the conduction band. However investigated structure has the semi-metal properties due to the absence of the gap between valence and conduction band. Secondly, the position of maximum of I-V function can be regulated by change of the Fermi energy. Besides this dependence is non-monotonous. Thirdly, conductivity $\sigma$ of considered SL is determined by the Fermi level location. It increases with Fermi energy, passes the maximum and then decreases to zero.

Thus considered SL is characterized by both semi-metal properties (presence of the region with the depletion of the states at the bottom of the conduction band) and peculiarities of the narrow-band semiconductor (existence of NDC portion in I-V characteristic). The possibility of controlling of the region of NDC gives the opportunity of use of SL based on the semi-Dirac crystals in nanoelectronic engineering.

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