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Effect of interlayer coupling on the electron spectra of vertical superlattice

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By use of the Green's function method analytical expressions for the dispersion lows of superlattice (SL) consists of two alternating 2D layers are obtained. Weak interlayer coupling regime is analized thoroughly. As the examples, the SLs graphene — h-BN (*1*), AlN — GaN (*2*), Gr — Ni (*3*) and h-BN — Ni (*4*) are considered and analytical electron spectrum characteristics for the corresponding 2D layers are given. It is shown that 1) electron effective masses become havier for the h-BN, AlN, GaN, and Ni layers in all SLs; 2) Fermi velocity becomes lower for the gapless graphene layer in the SL (*1*) and remains constant in the SL (*3*); 3) energy gaps become narrower for the h-BN, AlN and GaN layers in the SLs (*1*) and (*2*) and wider for h-BN layer in the SL (*4*).

Keywords: dispersion low, Fermi velocity, effective mass, graphene-like compound, two-dimensional ferromagnetic metal.

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1. Introduction

The discovery of unique graphene properties has given rise to two research areas: 1) search for new two-dimensional (2D) materials and 2) development of methods for the making of heterojunctions and superlattices (SL) on their basis [1–3]. This activity turned out to be quite successful: at present there are atlases containing many hundreds of theoretically possible 2D-materials [4–7], and different 2DSL formation schemes have been developed [8–10]. In the present paper we suggest a model of the electronic spectrum of vertical 2DSL constructed on the basis of the epitaxial layer theory [11]. Such a scheme allows for obtaining the spectrum characteristics in the analytical form, without implicit consideration of the geometry of interlayer contacts. The main goal of the paper is to answer the question: how does interlayer interaction affect the electronic characteristics of the layers which make up the SL.

The forming 2DSL-monolayers in the present work, in addition to graphene, include graphene-like compounds (GLC) of type A_3B_5 [11,12]. The basis for this is the potential possibility of successful use of the GLC lattice in nanoelectronics similarly to the use of A_3B_5 3D-compounds in microelectronics [13–20]. SLs with ferromagnetic metallic layers, which are of interest for spintronics, are also discussed.

2. Model

Let us begin with the consideration of a set of vertically arranged 2D-sheets. Without considering the sheet interaction, the sheet Green function is $G(\boldsymbol{\kappa}, \omega)$, where ω is the energy variable, $\boldsymbol{\kappa}$ is the wave vector for electron motion in the sheet (x, y) plane. Let us now go to the SL constructed of alternating sheets 1 and 2. Using the Dyson equation [11], for diagonal Green functions $\widetilde{G}_{11}(\boldsymbol{\kappa}_1, k_z; \omega)$ of layers 1 which interact with neighboring layers 2, let us write down a chain of equations

$$\widetilde{G}_{11}(\boldsymbol{\kappa}_1, k_z; \omega) = G_{11}(\boldsymbol{\kappa}_1; \omega) + G_{11}(\boldsymbol{\kappa}_1; \omega)$$

$$\times \sum_{\boldsymbol{\kappa}_2, \boldsymbol{\kappa}_1'} V(\boldsymbol{\kappa}_1, \boldsymbol{\kappa}_2)\left[G_{21}^{>}(\boldsymbol{\kappa}_2, \boldsymbol{\kappa}_1', k_z; \omega) + G_{21}^{<}(\boldsymbol{\kappa}_2, \boldsymbol{\kappa}_1', k_z; \omega)\right],$$

$$G_{21}^{>}(\boldsymbol{\kappa}_2, \boldsymbol{\kappa}_1, k_z; \omega) = G_{22}(\boldsymbol{\kappa}_2; \omega) V(\boldsymbol{\kappa}_2, \boldsymbol{\kappa}_1) \widetilde{G}_{11}(\boldsymbol{\kappa}_1, k_z; \omega)$$

$$\times (1 + e^{2ik_z d}),$$

$$G_{21}^{<}(\boldsymbol{\kappa}_2, \boldsymbol{\kappa}_1, k_z; \omega) = G_{22}(\boldsymbol{\kappa}_2; \omega) V(\boldsymbol{\kappa}_2, \boldsymbol{\kappa}_1) \widetilde{G}_{11}(\boldsymbol{\kappa}_1, k_z; \omega)$$

$$\times (1 + e^{-2ik_z d}), \qquad (1)$$

where $V(\boldsymbol{\kappa}_1, \boldsymbol{\kappa}_2)$ is an off-diagonal matrix element which links the states $|\boldsymbol{\kappa}_1\rangle$ and $|\boldsymbol{\kappa}_2\rangle$, k_z is the wave vector for electron motion in the direction of the normal to the (x, y) plane of the z axis, d is the interplanar distance, designations $>$ and $<$ refer to the planes lying above and below the considered plane, respectively. Leaving only the terms with $\boldsymbol{\kappa}_1 = \boldsymbol{\kappa}_1'$ (diagonal approximation) under the sum sign in expression (1) for $\widetilde{G}_{11}(\boldsymbol{\kappa}_1, k_z; \omega)$, we have

$$\widetilde{G}_{11}(\boldsymbol{\kappa}_1, k_z; \omega) = G_{11}(\boldsymbol{\kappa}_1; \omega)/D(\boldsymbol{\kappa}_1, k_z; \omega),$$

$$D(\boldsymbol{\kappa}_1, k_z; \omega) = 1 - 4\cos^2(k_z, d) G_{11}(\boldsymbol{\kappa}_1; \omega)$$

$$\times \sum_{\boldsymbol{\kappa}_2} G_{22}(\boldsymbol{\kappa}_2, k_z; \omega) V(\boldsymbol{\kappa}_1, \boldsymbol{\kappa}_2) V(\boldsymbol{\kappa}_2, \boldsymbol{\kappa}_1). \quad (2)$$

Assuming that

$$\sum_{\boldsymbol{\kappa}_1(\boldsymbol{\kappa}_2)} G_{11(22)}(\boldsymbol{\kappa}_{1,2};\omega)V(\boldsymbol{\kappa}_1,\boldsymbol{\kappa}_2)V(\boldsymbol{\kappa}_2,\boldsymbol{\kappa}_1) = \Sigma_{1(2)}(\omega) \quad (3)$$

and substituting indices 11 and 22 for the layers' diagonal Green functions by indices 1 and 2, we obtain the following expressions for the Green functions of SL

$$\widetilde{G}^{-1}_{1,2}(\boldsymbol{\kappa}_{1,2};\omega) = G^{-1}_{1,2}(\boldsymbol{\kappa}_{1,2};\omega) - 4\cos^2(k_z d)\Sigma_{2,1}(\omega), \quad (4)$$

where $\mathbf{k}_{1,2} = (\boldsymbol{\kappa}_{1,2}, k_z)$. Let us represent the self-energy function $\Sigma_{1(2)}(\omega)$ as the difference $\Lambda_{1(2)}(\omega) - i\Gamma_{1(2)}(\omega)$, where $\Gamma_{1(2)}(\omega)$ and

$$\Lambda_{1,2}(\omega) = \pi^{-1}P\int_{-\infty}^{\infty}\Gamma_{1,2}(\omega')(\omega-\omega')^{-1}d\omega'$$

(P is the symbol of the principal value of the integral) are respectively half-width and shift functions of the band states of layer 2 (1) under the action of layer 1 (2) [11]. Let us assume $\Gamma_{1(2)}(\omega) = \pi V^2\rho_{1,2}(\omega)$, where $\rho_{1,2}(\omega)$ are densities of states of free layers 1 and 2, $V^2 = \langle V(\boldsymbol{\kappa}_1,\boldsymbol{\kappa}_2)V(\boldsymbol{\kappa}_2,\boldsymbol{\kappa}_1)\rangle_{ZB_{1,2}}$ and bracket $\langle\ldots\rangle_{ZB_{1,2}}$ mean averaging by 2D Brillouin zones of layers 1 and 2.

From now on, we will assume that interlayer interaction V is weak (see below for more detail). The smooth functions $\Gamma_{1,2}(\omega)$ can be neglected on this ground (i.e. we can ignore the finit lifetime of electronic states $\tau_{1,2} \sim \hbar/\Gamma_{1,2}(\omega)$, where $\hbar$ is the reduced Planck constant), while functions $\Lambda_{1,2}(\omega)$, which have logarithmic divergences at the boundaries of continuous spectrum regions (see below), cannot a priori be neglected. Using the made simplification, we get the Green functions

$$\widetilde{G}_{1,2}(\boldsymbol{\kappa}_{1,2};\omega) = (2d/\pi)\int_0^{\pi/2d}\widetilde{G}_{1,2}(\boldsymbol{\kappa}_{1,2},k_z;\omega)dk_z,$$

which characterize the SL layers, in the following form

$$\widetilde{G}_{1,2}(\boldsymbol{\kappa}_{1,2};\omega) = \frac{1+(2/\pi)\mathrm{sgn}\,[A_{1,2}(\boldsymbol{\kappa}_{1,2};\omega)]\arcsin|A_{1,2}(\boldsymbol{\kappa}_{1,2};\omega)|}{\sqrt{1-A^2_{1,2}(\boldsymbol{\kappa}_{1,2};\omega)}} \times \bar{G}_{1,2}(\boldsymbol{\kappa}_{1,2};\omega), \quad (5)$$

where $A_{1,2}(\boldsymbol{\kappa}_{1,2};\omega) = 2\bar{G}_{1,2}(\boldsymbol{\kappa}_{1,2};\omega)\Lambda_{2,1}(\omega)$, $\bar{G}^{-1}_{1,2}(\boldsymbol{\kappa}_{1,2};\omega) = G^{-1}_{1,2}(\boldsymbol{\kappa}_{1,2};\omega) - 2\Lambda_{2,1}(\omega)$. It follows from (4), in particular, that $\widetilde{G}_{1,2}(\boldsymbol{\kappa}_{1,2};\omega) = G_{1,2}(\boldsymbol{\kappa}_{1,2};\omega)$ at $V_{\alpha\beta} = 0$. The electron dispersion laws for SL sheets are determined from the equations $\bar{G}^{-1}_{1,2}(\boldsymbol{\kappa}_{1,2};\omega) = \pm 2\Lambda_{2,1}(\omega)$. These equations provide two groups of bands. We get the following equation at $\bar{G}^{-1}_{1,2}(\boldsymbol{\kappa}_{1,2};\omega) = -2\Lambda_{2,1}(\omega)$

$$G^{-1}_{1,2}(\boldsymbol{\kappa}_{1,2};\omega) = 0, \quad (6)$$

the solutions of which coincide with the bands of free layers 1 and 2. It follows from (5) that the weighting coefficient outside the Green function $\bar{G}_{1,2}(\boldsymbol{\kappa}_{1,2};\omega)$ in this case becomes 0. We get the following equation at $\bar{G}^{-1}_{1,2}(\boldsymbol{\kappa}_{1,2};\omega) = +2\Lambda_{2,1}(\omega)$

$$G^{-1}_{1,2}(\boldsymbol{\kappa}_{1,2};\omega) = 4\Lambda_{2,1}(\omega), \quad (7)$$

which determines the renormalized bands which will hereinafter be called the bands of lattice layers. For subsequent analysis, we must go to specific structures.

3. Superlattices of graphene-like compounds

The Green function for a free binary GLC (per one unit cell atom) is as follows [11]:

$$G_{\mathrm{GLC}}(\boldsymbol{\kappa};\omega) = \Omega/(\Omega - R(\boldsymbol{\kappa}))\big(\Omega + R(\boldsymbol{\kappa})\big). \quad (8)$$

Here $\Omega = \omega - \bar{\varepsilon}$, $R(\boldsymbol{\kappa}) = \sqrt{\Delta^2 + t^2 f^2_{\mathrm{GLC}}(\boldsymbol{\kappa})}$, $\bar{\varepsilon} = (\varepsilon_a + \varepsilon_b)/2$, $\Delta = |\varepsilon_a - \varepsilon_b|/2$, ε_a and ε_b are energies of p-orbitals of atoms A and B which make up the GLC, t is energy of electron transition between neighboring atoms A and B located at distance a from each other,

$$f_{\mathrm{GLC}}(\boldsymbol{\kappa}) = \sqrt{3 + 2\cos(\kappa_x a\sqrt{3}) + 4\cos(\kappa_x a\sqrt{3}/2)\cos(3\kappa_y a/2)}. \quad (9)$$

Function (9) in the low-energy approximation becomes $f_{\mathrm{GLC}}(\mathbf{q}) = 3a|\mathbf{q}|/2$, where $\mathbf{q} = \mathbf{K} - \boldsymbol{\kappa}$ and $\mathbf{K} = a^{-1}(2\pi/3\sqrt{3}, 2\pi/3)$ is the Dirac point wave vector. Density of states of GLC is as follows

$$\rho_{\mathrm{GLC}}(\Omega) = \begin{cases} 2|\Omega|/\xi^2, & \Delta \le |\Omega| \le \bar{R}, \\ 0, & |\Omega| < \Delta,\ |\Omega| > \bar{R}, \end{cases} \quad (10)$$

where $\xi = \sqrt{2\pi\sqrt{3}}t$ and $\bar{R} = \sqrt{\xi^2 + \Delta^2}$ [11], while the corresponding shift function, according to [21], is equal to

$$\Lambda_{\mathrm{GLC}}(\Omega) = \frac{2V^2}{\xi^2}\,\Omega\ln\left|\frac{\Omega^2 - \Delta^2}{\Omega^2 - R^2}\right|. \quad (11)$$

We must assume that $\Delta = 0$ in order to go to graphene in formulas (8), (10) and (11).

The above-mentioned weakness of the interlayer coupling is determined by condition $(V/\xi)^2 \ll 1$. From here, at $V = t$ we have $(V/\xi)^2 = 1/2\pi\sqrt{3} \sim 0.1$ (covalent bond). Thus, the used approximation by no means reduces to a van der Waals interlayer interaction, for which $V/t \sim 0.1$ and $(V/\xi)^2 \sim 0.01$. Hereinafter the values of energies of transitions between the nearest neighbors for all GLC were determined using the Harrison formulas for the π-bond [22]; for estimates of parameter V, see [23]. It should be noted, however, that the real value of V is to

a large extent determined by the superlattice manufacture technology. Indeed, in case of the absence and presence of misorientation of the lattices of contacting layers, efficient interaction between them, described in our model by the parameter V, differs significantly. Thus, for instance, any misorientation in case of a heterojunction between single-layer graphene (Gr) and hexagonal boron nitride (h-BN) leads to virtually complete disappearance of the gap in the graphene spectrum [24].

Let us begin a consideration of superlattices of graphene-like compounds (SL GLC) with a structure which consists of Gr sheets (hereinafter sheet 1) and h-BN sheets (hereinafter sheet 2). If graphene is considered as gaples [24], we can assume that $\overline{\varepsilon} = \overline{\varepsilon}_1 = \overline{\varepsilon}_2 = 0$ and $\Delta_2 = t$ [25], where, ignoring the insignificant different of values a_1 and a_2, we have adopted $t = t_1 = t_2$. From (7) we obtain

$$\omega\left(1 - \frac{8V^2}{\xi^2}\ln\left|\frac{\omega^2 - t^2}{\omega^2 - t^2 - \xi^2}\right|\right) \mp -\frac{3taq}{2} = 0, \qquad (12)$$

$$\omega^2\left(1 - \frac{8V^2}{\xi^2}\ln\left|\frac{\omega^2}{\omega^2 - \xi^2}\right|\right) - \frac{9t^2(aq)^2}{4} - t^2 = 0, \qquad (13)$$

where equations (12) and (13) refer to the layers of gapless Gr and h-BN, respectively. At $V = 0$ and $q = 0$, we obtain the solution $\omega_0 = 0$ from (12), solutions $\omega_0^{\pm} = \pm t$ — from (13). Then we have the following dispersions in the vicinity of the Dirac point **K**

$$\omega_1^{\pm}(q) \approx \pm 3\eta^2 taq/2,$$

$$\omega_2^{\pm}(q) \approx \pm\eta t\sqrt{1 + (3aq/2)^2},] \qquad (14)$$

where

$$\eta = \left[1 + 8V^2/\xi^2)\ln(2\pi\sqrt{3} - 1)\right]^{-1/2}$$

$$\approx 1/\sqrt{1 + 20(V/\xi)^2}.$$

It follows from (14) that, firstly, the Fermi velocity of electrons in the SL graphene layers is equal to $\tilde{v}_F = \eta^2 v_F < v_F$, where $v_F = 3at/2\hbar$ is the Fermi velocity in free Gr. Secondly, the effective mass of electrons in h-BN lattice layers is equal to $\tilde{m}^* = m^*/\eta > m^*$, where $m^* = 4\hbar^2/9a^2t$ is the effective mass in free h-BN ($m^*/m_e \approx 0.80$ [11], m_e is free electron mass). Thereat, the band gap of the h-BN lattice layer is equal to $\widetilde{E}_g = \eta E_g < E_g$, where $E_g = 2t$ is the band gap in a free h-BN sheet. It should be noted that there is no charge transition between the Gr and h-BN layers in SL due to the symmetric location of bands in relation $\overline{\varepsilon} = 0$.

It is interesting to compare our results with ab initio calculations of other authors. For instance, the authors of [26] demonstrated that mutual influence of graphene and h-BN layers can be considered as a perturbation, i.e,. it can be considered weak. (This assertion is not given in the text of [26], but it follows from the comparison between Fig. 6, *a, d* and *e*). It has been shown in [27] that h-BN layers induce a gap in graphene in the vicinity of the Dirac point equal to about 0.1 eV. There is no gap in our approach, since the geometric structure of the Gr/h-BN contact is not taken into account and the shift function (11) is identical for both graphene sublattices. It should be noted that much attention is being paid in recent years to moire effects in Gr/h-BN superlattices [28,29].

Let us now consider a SL formed by 2D-layers of AlN (sheet 1) and GaN (sheet 2). Using the results of paper [30] which describes the free layers of these compounds, we assume that $\overline{\varepsilon} = \overline{\varepsilon}_1 = \overline{\varepsilon}_2 = 0$, $\Delta_1 = 2.5\,\text{eV}$, $\Delta_2 = 2.0\,\text{eV}$. Thus, the contact of AlN and GaN layers is a straddling heterojunction [31]. Then the spectra of the AlN and GaN lattice layers in the vicinity of Dirac point **K** are as follows

$$\omega_{1,2}^{\pm}(q_{1,2}) \approx \pm\eta_{1,2}\sqrt{\Delta_{1,2}^2 + (3t_{1,2}a_{1,2}q_{1,2}/2)^2}, \qquad (15)$$

where

$$\eta_{1,2} = \left\{1 + (8V^2/\xi_{2,1}^2)\ln\left[(\xi_{2,1}^2 - \Delta_1^2 - \Delta_2^2)/(\Delta_1^2 - \Delta_2^2)\right]\right\}^{-1/2}.$$

The corresponding effective masses are equal to

$$\tilde{m}_{1,2}^* = m_{1,2}^*/\eta_{1,2} > m_{1,2}^*, \qquad (16)$$

where $m_{1,2}^* = 4\hbar^2\Delta_{1,2}/9a_{1,2}^2t_{12,2}^2$. Since $a_1 = 1.80\,\text{Å}$, $a_2 = 1.88\,\text{Å}$, $t_1 = 1.48\,\text{eV}$, $t_2 = 1.36\,\text{eV}$ [30], we have $m_1^*/m_e = 1.19$ (AlN) and $m_2^*/m_e = 1.04$ (GaN) [31]. We obtain the following for the coefficients $\eta_1 \approx 1/\sqrt{1 + 12(V/\xi_2)^2}$, $\eta_2 \approx 1/\sqrt{1 + 14(V/\xi_1)^2}$, where $\xi_1 \approx 4.9\,\text{eV}$, $\xi_2 \approx 4.5\,\text{eV}$. $\widetilde{E}_{g1,2} = E_{g1,2}/\eta_{1,2} < E_{g1,2}$, where $E_{g1,2} = 2\Delta_{1,2}$. As an example, we give the effective electron masses for 3D-compounds of BN, AlN, GaN with the wurtzite structure, which are correspondingly equal to $m_{\|}^*/m_e = 0.35$ and $m_{\perp}^* = 0.24$, $m^*/m_e = 0.4$, $m^*/m_e = 0.2$ [32]. Thus, effective electron masses in the lattice layers of h-BN, AlN and GaN compounds under an interlayer van der Waals interaction increase by $\sim 5-10\%$, and their band gaps narrow in the same percentage ratio. Graphene layers upon contact with h-BN layers are considered gapless, but the electron Fermi velocity decreases by $\sim 20\%$. It should be noted that SL where one of the components is gapped Gr, the electronic spectrum and density of states of which are described by the same expressions as GLC (h-BN, AlN, GaN), can be considered in a similar way.

4. Superlattices with metallic ferromagnetic layers

A strong interest in magnetic SL (MSL) has arisen due to spintronics problems, and even a new term „spinterface“ was introduced to designate a contact of ferromagnetic and non-magnetic layers (see [23,34] and references therein). Here we will consider MSL formed by graphene or h-BN with 2D ferromagnetic nickel.

The properties of monoatomic 2D-metals are described in [35], where it is shown, in particular, that a stable

structure in this case is a triangular lattice. Then the Green function of a 2D-ferromagnetic (2DFM) for the spin projection σ can be presented as

$$G^{\sigma 1}_{\mathrm{FM}}(\boldsymbol{\kappa}_m;\omega) = (\omega - \varepsilon^{\sigma}_{\mathrm{FM}}(\boldsymbol{\kappa}_m) + i0^{+})^{-1},$$

where

$$\varepsilon^{\sigma}_{\mathrm{FM}}(\boldsymbol{\kappa}_m) = \varepsilon^{\sigma}_0 - t_m f_{\mathrm{FM}}(\boldsymbol{\kappa}_m),$$

$$f(\boldsymbol{\kappa}_m) = 2\cos(\kappa_{mx}a_m) + 4\cos(\kappa_{mx}a_m/2)\cos(\sqrt{3}\kappa_{my}a_m/2), \quad (17)$$

where t_m is the energy of electron hopping between the nearest atoms located at distance a_m [36]. Near the bottom of the σ-subband

$$\varepsilon^{\sigma}_{\mathrm{FM}}(\mathbf{q}) \approx \varepsilon_{0\sigma} - 6t_m + 3t_m q^2_m a^2_m/2,$$

where $\mathbf{q}_m = \mathbf{K}_m - \boldsymbol{\kappa}_m$ and $\mathbf{K}_m = a^{-1}_m(2\pi/2, 2\pi/\sqrt{3})$, so that the effective mass of an electron of free 2DFM is equal to $m_{\mathrm{FM}} = \hbar^2/6t_m a^2_m$. Though an analytical expression for the density of states is known [36,37], we will here opt for an approximation already used in our paper [38] dedicated to the epitaxial Gr formed on an FM metal substrate.

Let us represent the 2DFM density of states as

$$\rho^{\sigma}_{\mathrm{FM}}(\omega) = \begin{cases} 5/W_d, & |\omega - \varepsilon_{0\sigma}| \le W_d/2, \\ 0, & |\omega - \varepsilon_{0\sigma}| > W_d/2, \end{cases} \quad (18)$$

where W_d is width of the d-band, $\omega_{)\sigma}$ is the energy of the σ-subband center. Such a density of states corresponds to the Stoner magnetism [39] in the Friedel model [40]. Assuming that $\Gamma = 5\pi V^2/W_d$, we can easily demonstrate that

$$\Lambda^{\sigma}_{\mathrm{FM}}(\omega) = (\Gamma/\pi)\ln\left|\frac{\omega - \varepsilon_{0\sigma} + W_d/2}{\omega - \varepsilon_{0\sigma} - W_d/2}\right|. \quad (19)$$

The number of electrons in the $d\sigma$-state is equal to

$$N^{\sigma}_{\mathrm{FM}} = 5(E_F - \varepsilon_{0\sigma} + W_d/2)/W_d, \quad (20)$$

where E_F is the Fermi level. Hereinafter Ni will be considered as 2DFM. Rounding off the data of [40] according to occupation numbers of massive nickel (see Table 2.1 in [40]), i.e. assuming that $N^{\uparrow}_{\mathrm{met}}(\mathrm{Ni}) = 5$, $N^{\downarrow}_{\mathrm{met}}(\mathrm{Ni}) = 4$, we obtain $E_F - \varepsilon_{0\uparrow} = 0.5W_d$ and $E_F - \varepsilon_{0\downarrow} = 0.3W_d$. Since the experimental value is $W_d(\mathrm{Ni}) = 5.4\,\mathrm{eV}$ [36] and $W_d = 9t_m$ [36], we obtain $T_m = 0.6\,\mathrm{eV}$. Two circumstances should be noted here. Firstly, as demonstrated in [35], the characteristics of 2D- and 3D-metals are close. Secondly, it was shown in [41] that magnetizations on the surface and in the bulk of massive nickel samples are virtually the same. It is this that gives us the ground to use the results of [39,40] for 3DFM to describe 2DFM.

As an example of MSL, we will consider a structure consisting of gapless Gr (sheet 1) and 2D-nickel layers (sheet 2). Such a structure has been formed [42] and has been rather well studied by now [43–45]. As in [35], we will assume that the Gr and 2D Ni work functions are equal, thus the interlayer charge transition is excluded. Equation (7) is now transformed into

$$\left[G^{\sigma}_{\mathrm{Gr}}(\boldsymbol{\kappa}_{1,2};\omega)\right]^{-1} = 4\Lambda^{\sigma}_{\mathrm{FM}}(\omega),$$

$$\left[G^{\sigma}_{\mathrm{FM}}(\boldsymbol{\kappa}_{1,2};\omega)\right]^{-1} = 4\Lambda_{\mathrm{Gr}}(\omega), \quad (21)$$

from which we obtain the following for the Gr and Ni lattice layers respectively

$$\omega - \frac{8\Gamma}{\pi}\ln\left|\frac{\omega - \varepsilon_{0\sigma} + W_d/2}{\omega - \varepsilon_{0\sigma} - W_d/2}\right| \mp \frac{3ta_1q_1}{2} = 0, \quad (22)$$

$$\omega\left(1 - \frac{8V^2}{\xi^2}\ln\left|\frac{\omega^2}{\omega^2 - \xi^2}\right|\right) - \varepsilon_{0\sigma} + 6t_m - \frac{3t_m(a_m q_m)^2}{2} = 0. \quad (23)$$

It follows from (22) that Gr bands depend on the spin induced by 2D Ni layers. This is a manifestation of the so-called proximity effect. The electron Fermi velocity does not change and remains equal to $v_F = 3at/2\hbar$. The spin-dependent effective mass for 2D Ni lattice layers is equal to

$$\tilde{m}^{\sigma}_{\mathrm{FM}} \approx m_{\mathrm{FM}}/\eta_{n\sigma} > m_{\mathrm{FM}}, \quad (24)$$

where $\eta_{m\sigma} = \left[1 + (8V^2/\xi^2)\ln(\xi^2 - \omega^2_{0\sigma})/\omega^2_{\sigma 0}\right]^{-1}$, $\omega_{0\sigma} = \varepsilon_{0\sigma} - 6t_m$. Since $\varepsilon_{0\uparrow} = -2.70\,\mathrm{eV}$, $\omega_{0\uparrow} = -6.30\,\mathrm{eV}$ and $\varepsilon_{0\downarrow} = -1.62\,\mathrm{eV}$, $\omega_{0\uparrow} = -5.22\,\mathrm{eV}$, we have $\eta_{m\uparrow} \approx [1 + 0.1(V/\xi)^2]^{-1}$ and $\eta_{m\downarrow} \approx [1 + 3(V/\xi)^2]^{-1}$. Thus, the electron effective mass in nickel lattice layers in case of a van der Waals bond with graphene layers is almost the same as in isolated layers. It should be noted that the notion of dependence of effective carrier mass on its spin is used rather for a long time and widely (see, for instance, [46–50]). An energy-dependent effective mass can be also introduced [51].

Now let h-BN act as sheets 1 (see [45]). Then we have the following equations

$$\omega^2 - \frac{8\omega\Gamma}{\pi}\ln\left|\frac{\omega - \varepsilon_{0\sigma} + W_d/2}{\omega - \varepsilon_{0\sigma} - W_d/2}\right| - \frac{9t^2(aq)^2}{4} - t^2 = 0, \quad (25)$$

$$\omega\left(1 - \frac{8V^2}{\xi^2}\ln\left|\frac{\omega^2 - t^2}{\omega^2 - t^2 - \xi^2}\right|\right) - \varepsilon_{0\sigma} + 6t_m - \frac{3t_M(a_m q_m)^2}{2} = 0. \quad (26)$$

It follows from (25) that the bands of the h-BN layers under the impact of the Ni layers are split into σ-subbands (proximity effect). Substituting the logarithm in (25) by $L^{\sigma}_{\pm}(\varepsilon_{0\sigma}) = \ln\left|(\pm t - \varepsilon_{0\sigma} + W_d/2)/(\pm t - \varepsilon_{0\sigma} - W_d/2)\right|$, we will obtain the following solution

$$\omega^{\sigma}_{\pm}(\mathbf{q}) = \left(4\Gamma L^{\sigma}_{\pm}(\varepsilon_{0\sigma})/\pi\right) \pm R^{\sigma}_{\pm}(\mathbf{q}), \quad (27)$$

where $R^{\sigma}_{\pm}(\mathbf{q}) = \left[\left(4\Gamma L^{\sigma}_{\pm}(\varepsilon_{0\sigma})/\pi\right)^2 + t^2 + (3ta\mathbf{q}/2)^2\right]^{1/2}$, the subscripts of function $L^{\sigma}_{\pm}(\varepsilon_{0\sigma})$ correspond to the signs

before t and summands $R^{\sigma}_{\pm}(\mathbf{q})$. Effective electron masses in h-BN and Ni layers are respectively equal to

$$\tilde{m}^{\sigma}_{\mathrm{GLC}} = m^*/\eta^{\sigma}_{\mathrm{GLC}} > m^*, \ \tilde{m}^{\sigma}_{\mathrm{FM}} = m_{\mathrm{FM}}/\eta^{\sigma}_{m} > m_{\mathrm{FM}}, \quad (28)$$

where

$$\eta^{\sigma}_{\mathrm{GLC}} = [1 + (4\Gamma L^{\sigma}_{+}/t)^2]^{-1.2}, \quad m^* = 4\hbar^2/9a^2t,$$

$$\eta^{\sigma}_{m} = [1 + (8V^2/\xi^2)L^{\sigma}_{m}(\omega_{0\sigma})]^{-1}, \quad m^* = 4\hbar^2/9a^2t,$$

$$L^{\sigma}_{m} = \ln[(\xi^2 - \omega^2_{0\sigma} - t^2)/(\omega^2_{0\sigma} - t^2)]^{-1}.$$

Since $L^{\uparrow}_{+} = 1.1$ and $L^{\downarrow}_{+} = 1.4$, estimates for lattice layers of h-BN give $\eta^{\uparrow}_{\mathrm{GLC}} \sim 1/\sqrt{1 + 2V^2/t_m t}$ and $\eta^{\downarrow}_{\mathrm{GLC}} \sim 1/\sqrt{1 + 3V^2/t_m t}$. It should be noted that at $t_m \sim t$ the $V^2/t_m t \sim ratio is 2\pi\sqrt{3}(V/\xi)^2$. $V^2/t_m t \sim 0.1$ under a van der Waals interlayer interaction, so that the effective masses increase by 20–30%. Then, as distinct from graphene-like SL, we have $\tilde{E}^{\sigma}_{g} = E_g/\eta^{\sigma}_{\mathrm{GLC}} > E_g$, i.e. there is a considerable increase of the band gap. For Ni lattice layers we have $L^{\uparrow}_{m} = 0.15$ and $L^{\downarrow}_{m} = 0.80$, from which we obtain $\eta^{\uparrow}_{m} \sim [1 + (V/\xi)^2]^{-1}$ and $\eta^{\downarrow}_{m} \sim [1 + 6(V/\xi)^2]^{-1}$, which corresponds to a slight increase of the effective mass. An SL formed by gap Gr and 2D Ni can be considered in a similar way.

5. Conclusion

In the present paper we have considered 2DSL graphene — h-BN, AlN — GaN, Gr — Ni and h-BN — Ni. Effective masses of electrons in h-BN, AlN and GaN layers increase in all the considered cases; the electron Fermi velocity for gapless graphene decreases. An interlayer interaction in the first two cases leads to a narrowing of the GLC band gaps. The electron Fermi velocity in graphene layers in Gr — Ni and h-BN — Ni lattices is the same as in free graphene. The effective electron mass in nickel layers in the Gr — Ni lattice increases, but very slightly. The effective electron mass and band gap of the h-BN layer considerably increase in case of the h-BN — Ni lattice.

Unfortunately, we did not find any data in the literature to compare with the obtained results. The fact is that all the papers available to us considered the vertical transport only. We have estimated the characteristics of an electron moving in the constituent 2DSL-layers.

So, we have suggested a relative simple scheme (ignoring the contact geometry) for estimating the mutual influence of 2DSL components on the electronic spectrum of the layers which make up the given lattice. In a similar way, graphane [52], fluorographene [53] or, broader, compounds of type h-AB — C [54] can be considered as 2DSL components. Moreover, the suggested scheme allows for a rather easy description of 2DSL composed of three, four etc. types of 2D-compounds.

Conflict of interest

The author declares that he has no conflict of interest.

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