Electrically-induced n-i-p junctions in multiple graphene layer structures

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The Fermi energies of electrons and holes and their densities in different graphene layers (GLs) in the n- and p-regions of the electrically induced n-i-p junctions formed in multiple-GL structures are calculated both numerically and using a simplified analytical model. The reverse current associated with the injection of minority carriers through the n- and p-regions in the electrically-induced n-i-p junctions under the reverse bias is calculated as well. It is shown that in the electrically-induced n-i-p junctions with moderate numbers of GLs the reverse current can be substantially suppressed. Hence, multiple-GL structures with such n-i-p junctions can be used in different electron and optoelectronic devices.

I. INTRODUCTION

The possibility to form electrically-induced n-p and n-i-p junctions [1-3] in gated graphene layers (GLs), as well as lateral arrays of graphene nanoribbons and graphene bilayer opens up prospects of creation novel electronic and optoelectronic devices [4-8]. In contrast to GL structures with chemically doped n- and p-region in the GL structures with electrically-induced n-p and n-i-p junctions, there is a possibility of their voltage control. Recent success in fabricating high-quality multiple GLs [9,10] stimulates an interest in different prospective devices in which the utilization of multiple-GL structures (stacks of disoriented GLs) instead of single-GL structures can provide a significant improvement of their performance. Such devices include, in particular, terahertz tunneling transit-time oscillators (similar to that considered in Ref. [2]), lasers with optical and electrical pumping, and high performance interband photodetectors [11-13]. Gated multiple-GL structures can be also used in high-frequency field-effect transistors [14] and other devices (the terahertz frequency multipliers, and plasmonic devices). However the penetration of the electric field (transverse to the GL plane) beyond the topmost GL as well as its screening by electron or hole charges in GLs can substantially limit the influence of the gates (the effect of the quantum capacitance [13]). In this paper, we study the influence of screening in gated multiple-GL structures on the formation and characteristics of n- or p-regions and n-i-p junctions in these structures. We calculate the electron and hole Fermi energies and densities in GLs in the n- and p-regions as functions of the GL index, gate voltage, and temperature. Using these data, we find the voltage and temperature dependences of the reverse current in the n-i-p junctions with different structural parameters.

II. EQUATIONS OF THE MODEL

Let us consider a multiple-GL structure with the side Ohmic contacts to all GLs and two split gates (isolated from GLs) on the top of this structure as shown in Fig. 1(a). Applying the positive ($V_n = V_g > 0$) or negative ($V_p = -V_g < 0$) voltage between the gate and the adjacent contact (gate voltage), one can obtain the electrically-induced n- or p-region. In the single- and multiple-GL structures with two split top gates under the voltages of different polarity, one can create lateral n-p or n-i-p junctions. Generally, the source-drain voltage $V$ can be applied between the side Ohmic contacts to GLs. Depending on the polarity of this voltage, the n-p and n-i-p junctions can be either direct or reverse biased. We assume that the potentials of the first (source) contact and the pertinent gate are $\varphi_s = 0$ and $\varphi_g = V_g > 0$, respectively, and the potentials of another gate and contact (drain) are $\varphi_g = -V_g < 0$ and $\varphi_d = V = 0$ (or $\varphi_d = V \neq 0$). If the slot between the gates $2L_g$
ions and holes, respectively. These densities, taking into account the linear dispersion low for electrons and holes in graphene, are expressed via the electron Fermi energy as

\[
\Sigma_k^\pm = \frac{2}{\pi} \left( \frac{k_B T}{\hbar v_F} \right)^2 \int_0^\infty \frac{d\xi \xi}{1 + \exp(\xi \mp \mu_k/k_B T)}
\]

where \(\Sigma_T = (\pi/6)(k_B T/\hbar v_F)^2\) is the electron and hole density in the intrinsic graphene at the temperature \(T\), \(v_F \approx 10^6\) cm/s is the characteristic velocity of electrons and holes in graphene, and \(\hbar\) and \(k_B\) are the Planck and Boltzmann constants, respectively. Here it is assumed that the electron (hole) energy spectrum is \(\varepsilon = v_Fp\), where \(p\) is the absolute value of the electron momentum. The boundary conditions are assumed to be as follows:

\[
\psi|_{z=-d} = 2 + W_g \frac{d\psi}{dz}|_{z=-d}, \quad \frac{d\psi}{dz}|_{z=k_d+0} = 0.
\]

Equations (1) - (3) yield

\[
2 - \psi_1 = \Gamma \Phi(\psi_1),
\]

for \(K = 1\),

\[
\frac{d}{W_g}(2 - \psi_1) - \psi_1 + \psi_2 = \frac{d}{W_g} \Gamma \Phi(\psi_1),
\]

\[
\psi_1 - \psi_2 = \Gamma \Phi(\psi_2)
\]

for \(K = 2\), and

\[
\frac{d}{W_g}(2 - \psi_1) - \psi_1 + \psi_2 = \frac{d}{W_g} \Gamma \Phi(\psi_1),
\]

\[
\psi_{k-1} - 2\psi_k + \psi_{k+1} = \frac{d}{W_g} \Gamma \Phi(\psi_k), \quad (2 \leq k \leq K-1),
\]

\[
\psi_{K-1} - \psi_K = \frac{d}{W_g} \Gamma \Phi(\psi_K)
\]

for \(K > 2\). Here

\[
\Phi(\psi) = \frac{12}{\pi^2} \left[ \int_0^\infty \frac{d\xi \xi}{1 + \exp(\xi - U_g \psi)} - \int_0^\infty \frac{d\xi \xi}{1 + \exp(\xi + U_g \psi)} \right],
\]

where \(\Gamma = (8\pi/\varepsilon)(\varepsilon W_g \Sigma_T/V_g) \propto T^2/V_g\) and \(U_g = eV_g/2k_BT\).
III. NUMERICAL RESULTS

Equations (4) - (7) were solved numerically. The results of the calculations are shown in Figs. 2 - 5. In these calculations, we assumed that $\alpha = 4$, $d = 0.35$ nm, and $W_g = 10$ nm.

Figure 2 shows the dependences of the electron Fermi energy

$$\mu_k = \frac{eV_g}{2} \psi_k$$  \hspace{1cm} \text{(8)}

as a function of the GL index $k$ calculated for multiple-GL structures with different number of GLs $K$ at different gate voltages and temperatures. One can see that the Fermi energy steeply decreases with increasing GL index. However, in GLs with not too large $k$, the Fermi energy is larger or about of the thermal energy. As one might expect, the electron Fermi energies in all GLs at $T = 77$ K are somewhat larger than at $T = 300$ K (see also Fig. 5). The obtained values of the electron Fermi energies in topmost GLs are $\mu_1 \approx 92$ meV and $\mu_1 \approx 77$ meV for $V_g = 1000$ mV at $T = 77$ K and $T = 300$ K, respectively.

Figure 3 shows the voltage dependences of the electron Fermi energies in some GLs in multiple-GL structures with different $K$ at $T = 300$ K.

Figure 4 shows the electron densities $\Sigma_k$ in the structures with different number of GLs $K$ at different temperatures. One can see that the calculated electron densities in GLs with sufficiently large indices ($k > 15$ at $T = 77$ K and $T = 300$ K) approach to their values in the intrinsic graphene ($\Sigma_T = 0.59 \times 10^{10}$ cm$^{-2}$ and $8.97 \times 10^{10}$ cm$^{-2}$). The electron densities in GLs in the structures with different $K$ are rather close to each other, particularly, in GLs with small and moderate indices.

Figure 5 presents the Fermi energies in GLs with different indices at different temperatures. One can see from Fig. 5 (as well as from Fig. 2) that the higher $T$ corresponds to lower $\mu_k$. This is due to an increasing dependence of the density of states on the energy and the thermal spread in the electron energies.

IV. ANALYTICAL MODEL

At not too low gate voltages when $U_g \gg 1$, one can assume that in a number of GLs the electrons under the gate are degenerate, i.e., $\mu_k \gg k_B T$, and the contribution of holes (nondegenerate) can be disregarded, hence, from Eq. (7) we obtain

$$\Phi(\psi) \approx \frac{6}{\pi^2} U_g^2 \psi^2. \hspace{1cm} \text{(9)}$$

In this case, for a single-GL structure ($K = 1$), Eq. (4) yields

$$2 - \psi_1 \approx \frac{6}{\pi^2} U_g^2 \psi_1^2, \hspace{1cm} \text{(10)}$$
where $\mu$ obtain tron Fermi energy in a GL (in a single-GL structure), we solving Eq. (10) and considering Eq. (8), for the electron density is shared between the topmost GL and underlying the fact that in multiple-GL structures the electron densities is disregarded. This can be attributed to exaggerated because the temperature spread in the electron energies is markedly larger than those calculated for the topmost GLs in multiple-GL structures (although it is somewhat can neglect the discreteness of the structure and replace the summation in Eq. (1) by the integration. As a result, following Ref. [13], one can arrive at

$$\frac{d^2\psi}{dz^2} = 0 \quad (-W_g < z < 0, \; z > z_K), \quad (12)$$

$$\frac{d^2\psi}{dz^2} = \frac{\Gamma}{dW_g}\Phi(\psi) \quad (0 < z < z_K). \quad (13)$$

In this case, considering Eq. (7), we arrive at

$$\frac{d^2\psi}{dz^2} = \frac{\psi^2}{L_s^2} \quad (14)$$

with the characteristic screening length

$$L_s = \frac{\pi \sqrt{dW_g}}{\sqrt{6}U_g} = \frac{\hbar v_F}{2e^2V_g} \propto V_g^{-1/2}. \quad (15)$$

The boundary conditions for Eq. (14) are

$$\psi|_{z=0} = 2 + W_g \frac{d\psi}{dz}|_{z=-0}, \quad \frac{d\psi}{dz}|_{z=z_K+0} = 0, \quad (16)$$

In multiple-GL structures with a large number of GLs ($K \gg 1$), one can extend the coordinate of the lowest GL to infinity and set $d\psi/dz|_{z=\infty} = 0$ with $\psi|_{\infty} = 0$. Solving Eq. (14) with the latter boundary conditions, we arrive at

$$\psi = \frac{1}{(C + z/\sqrt{6L_s})^3}, \quad (17)$$

where $C$ satisfies the following equation:

$$C^3 - C/2 = (W_g/\sqrt{6L_s}), \quad (18)$$

Since in reality $W_g \gg \sqrt{6L_s}$, one obtains $C \simeq (W_g/\sqrt{6L_s})^{1/3} \propto V_g^{1/6}$.

Taking into account Eq. (8), Eq. (17) yields

$$\mu_k \simeq \frac{eV_g}{2[C + (k - 1)d/\sqrt{6L_s}]^2} = \mu_1 a_k. \quad (19)$$

Here

$$\mu_1 = \frac{eV_g}{2C^2} \propto \left(\frac{V_g}{W_g}\right)^{2/3} \quad (20)$$

is the Fermi energy of electrons in the topmost GL in the n-section (holes in the p-section),

$$a_k = [1 + (k - 1)\gamma]^{-2}, \quad (21)$$

and

$$\gamma = \frac{d}{\sqrt{6L_s}C} \propto \frac{d}{W_g^{1/3}L_s^{2/3}} \propto \left(\frac{V_g}{W_g}\right)^{1/3}. \quad (22)$$

Solving Eq. (10) and considering Eq. (8), for the electron Fermi energy in a GL (in a single-GL structure), we obtain

$$\mu_1 \simeq \frac{\mu_g}{eV_g} \sqrt{1 - \frac{\mu_g}{eV_g}}, \quad (11)$$

where $\mu_g = \hbar v_F \sqrt{\alpha V_g/4eW_g}$. For the same parameters as those used in Figs. 2-4, $\mu_1 \simeq 150$ meV. Such a value is markedly larger than those calculated for the topmost GLs in multiple-GL structures (although it is somewhat exaggerated because the temperature spread in the electron energies is disregarded). This can be attributed to the fact that in multiple-GL structures the electron density is shared between the topmost GL and underlying GLs resulting in lower Fermi energies in all of them.

Considering multiple-GL structure with large $K$, one can neglect the discreteness of the structure and replace

![FIG. 4: Electron density vs GL index in multiple GL-structures with different number of GLs ($K = 10$ and $K = 50$) at different temperatures and $V_g = 1000$ mV.](image)

![FIG. 5: Comparison of the $\mu_k$ vs $k$ dependences calculated for different temperatures using numerical and simplified analytical (solid line) models.](image)
Setting \( d = 0.35 \) nm, \( W_g = 10 \) nm, \( \alpha = 4 \), and \( V_g = 1 \) V, one can obtain \( L_s \approx 0.44 \) nm. \( C \approx 2.14 \), \( \mu_1 \approx 109 \) meV, and \( \gamma \approx 0.153 \). The \( \mu_k \) versus \( k \) dependence obtained using our simplified analytical model, i.e., given by Eqs. (15) and (17) is shown by a solid line in Fig. 5.

Equations (9) - (22) are valid when \( \mu_k > k_B T \), i.e., at sufficiently large \( V_g \) or and sufficiently small \( T \). Since the Fermi energy (at fixed electron density) decreases with increasing temperature, the above formulas of our simplified (idealistic) model yield somewhat exaggerated values of this energy [compare the dependences in Fig. 5 obtained numerically using Eqs. (4) - (7) and that found analytically using Eqs. (19) - (22)].

V. THE REVERSE CURRENT

The current across the n-i-p junctions under their reverse bias (\( V < 0 \), see Fig. 2(c)) is an important characteristic of such junctions [10]. In particular, this current can substantially affect the performance of the terahertz tunneling transit-time oscillators and interband photodetectors [3, 13]. This current is associated with the thermogeneration and tunneling generation of the electron-hole pairs in the i-region. A significant contribution to this current can be provided by the injection of minority carriers (holes in the n-region and electrons in the p-region). Such an injection current in the \( k \)-th GL is determined by the height of the barrier for the minority carrier which, in turn, is determined by the Fermi energy \( \mu_k \) of the majority carrier. The latter, as shown above, depends on the gate voltage and the GL index. As a result, the reverse current can be presented as

\[
J = J_i + J_{th} + J_{tunn},
\]

(23)

where the injection current (which is assumed to be of the thermionic origin) is given by

\[
J_i = \frac{2eV_F}{\pi^2} \left( \frac{k_B T}{\hbar v_F} \right)^2 \int_{-\pi/2}^{\pi/2} d\theta \cos \theta \\
\times \sum_{k=1}^{K} \int_0^{\infty} \frac{d\xi}{1 + \exp(\xi + \mu_k/k_B T)}
\]

\[
= \frac{24eV_F \Sigma_T}{\pi^3} \sum_{k=1}^{K} \int_0^{\infty} \frac{d\xi}{1 + \exp(\xi + \mu_k/k_B T)}
\]

\[
= \frac{12J_T}{\pi^2} \sum_{k=1}^{K} \int_0^{\infty} \frac{d\xi}{1 + \exp(\xi + \mu_k/k_B T)}
\]

(24)

with \( J_T = 2eV_F \Sigma_T / \pi \). At \( T = 77 - 300 \) K, \( J_T \approx 0.06 - 0.9 \) A/cm. Deriving Eq. (24), we have taken into account that the distribution function of holes which enter the n-region overcoming the barrier in the \( k \)-th GL with the height \( \mu_k \) is \( f_k^{p_i} \approx \{1 + \exp[(\mu_k + \mu_f)/k_B T]\}^{-1} \). Similar formula is valid for electrons in the p-region. The factor 2 appears in Eq. (24) due to the contribution of both holes and electrons. Equation (24) is valid when the bias voltage is not too small: \( eV > k_B T \). At \( V \to 0 \) one has \( J_i \to 0 \) (as well as \( J_{th} \) and \( J_{tunn} \)). Scattering of holes in the n-region and electrons in the p-region resulting in returning of portions of them back to the contacts leads to some decrease in \( J_i \).

The temperature dependences of the reverse current associated with the injection from the n- and p-region calculated using Eq. (24) (with the quantities \( \mu_k \) shown in Fig. 5) are presented in Fig. 6. As one might expect, the reverse current sharply increases with the temperature and the number of GL. The latter is due to relatively low energy barriers for minority carriers in the n- and p-regions in GLs with large indices. For comparison, the injection current in a single-GL structure calculated using Eq. (24) with Eq. (8), is given by

\[
J_i^S = \frac{12J_T}{\pi^2} \int_0^{\infty} \frac{d\xi}{1 + \exp(\xi + \mu_1/k_B T)}
\]

\[
\approx \frac{12J_T}{\pi^2} \exp \left( -\frac{\hbar v_F \sqrt{\gamma V_g / 8eW_2}}{k_B T} \right).
\]

(25)

At the same parameters as above and \( T = 300 \) K, Eq. (25) yields \( J_i^S \approx 0.01 \) A/cm.

When \( K \gg \gamma^{-1} \sqrt{\mu_1/k_B T} \), the main contributions to the reverse current is associated with GLs with large indices (in which the barriers are very low), so that one obtains

\[
J_i \lesssim KJ_T.
\]

(26)

As follows from Eq. (26), the injection current (and, therefore, the net reverse current) can be fairly large due to the “shortcut” by GLs with large indices (placed deep below the gate).
Since the thermogeneration is associated primarily with the absorption of optical phonons [17], the pertinent rate $g_{th}$ is independent of the electric field in the i-region, but it is proportional to the i-section length $2l$ ($l \lesssim L_g$). The contribution of the thermogeneration to the reverse current can be presented as

$$J_{th} = 4K_{el}g_{th},$$  \hspace{1cm} (27)$$

The quantity $g_{th}$ as a function of the temperature was calculated in Ref. [17]. Equations (24) - (27) are valid if $2l < l_R$, where $l_R$ is the recombination length. In the situations when the bias voltage between the side contacts is not too small (as it should be, for instance, in GL-based interband photodetectors), the recombination length is fairly long. Indeed, assuming that the recombination time $\tau_R \approx 5 \times 10^{-10}$ s [17] and $v_0 > v_F/2 = 5 \times 10^7$ cm/s [18], respectively, one obtains $l_R \approx 250 \mu$m.

Assuming that $2l = 10 \mu$m with $g_{th} = 10^{13}$ cm$^{-2}$s$^{-1}$ and $g_{th} = 10^{21}$ cm$^{-2}$s$^{-1}$ at $T = 77$ K and $T = 300$ K, respectively [17], we obtain $J_{th} \approx 3.2 \times (10^{-9} - 10^{-1})$ A/cm. One can see that the thermogeneration contribution to the reverse current is much smaller than the injection contribution at lower temperatures, while it can be substantial at $T = 300$ K in the n-i-p structures with long i-region.

The tunneling generation can significantly contribute to the reverse current at elevated electric fields in the i-region, i.e., in relatively short GL structures at elevated bias voltages [1-3]. This current can be calculated using the following formula which follows from the expression for the tunneling probability in GLs [1, 2] (see, for instance [3]):

$$J_{tunn} = \frac{e v_F \left( \frac{e V}{2 l_2 v_F} \right)^{3/2}}{\pi^2 l^2} \propto V^{3/2} l^{1/2}.$$  \hspace{1cm} (28)$$

Depending on the n-i-p junction applications, the quantities $V$ and $l$ should be chosen to provide either domination of tunneling current (as in tunneling transit-time oscillators [4]) or its suppression (as in the interband photodetectors [13]).

VI. CONCLUSIONS

We calculated the dependences of the Fermi energies and densities of electrons and holes in the n- and p-regions of the electrically induced n-i-p junctions formed in multiple-GL structures on the GL indices, gate voltage, temperature, and the structural parameters. Using the obtained values of the Fermi energies and, hence, of the heights of potential barriers for minority carriers in the n- and p-regions, we found the temperature dependences of the reverse injection current for multiple-GL structures with different numbers of GLs. It was shown that the formation of effective electrically-induced n- and p-regions and n-i-p junctions, i.e., the n-i-p junctions with suppressed reverse currents in multiple-GL structures with several GLs is possible. The utilization of the electrically-induced n-i-p junctions in multiple-GL structures in different devices, such as terahertz tunneling transit-time oscillators, lasers, high performance interband photodetectors, and some others might provide an enhancement of the device performance (an increase in output power and responsivity) and widening of their functionality (owing to the possibility of the gate-voltage control).

Acknowledgments

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