carrier-induced modulation of radiation by a gated graphene

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The modulation of the transmitted (reflected) radiation due to change of interband transitions under variation of carriers concentration by the gate voltage is studied theoretically. The calculations were performed for strongly doped graphene on high-κ (Al₂O₃, HfO₂, AlN, and ZrO₂) or SiO₂ substrates under normal propagation of radiation. We have obtained the modulation depth above 10% depending on wavelength, gate voltage (i.e. carriers concentration), and parameters of substrate. The graphene - dielectric substrate - doped Si (as gate) structures can be used as an effective electrooptical modulator of near-IR and mid-IR radiation for the cases of high-κ and SiO₂ substrates, respectively.

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I. INTRODUCTION

The essential feature of graphene’s optical properties is its substantial interaction with radiation in the wide spectral region, from far-IR up to UV, due to effective interband transitions (see reviews [1]). The enhancement of this response due to interference permits one to make the graphene on dielectric substrate visible [2]. The other example of the exceptional optical properties is the graphene-based saturable absorber for ultrafast lasers in the telecommunication spectral region [3]. Besides this, the carriers contribution modifies essentially the graphene response due to the Pauli blocking effect, when absorption is supressed at \( \hbar \omega / 2 < \varepsilon_F \), where \( \omega \) is the frequency of radiation, \( \varepsilon_F \) is the Fermi energy, see experimental data and discussion in Refs. 4 and 5. Recently, modulation [6] and polarization [7] of IR radiation were observed in the graphene structure integrated with an optical waveguide. The efficiency of modulation can also be enhanced for the case of normal propagation of radiation by the interference effect under an appropriate thickness of substrate, see Figs. 1a and 1b. As a result, an improvement of modulation for transmission and reflection coefficients of the graphene - substrate - gate structure by a gate voltage takes place in contrast to the case of graphene placed on a semi-infinite insulator. [8] In this paper, we perform the calculation of the optical characteristics of such a structure, and we discuss the conditions for realisation of the graphene-based modulator in the near- and mid-IR spectral region.

At low temperatures, or high doping levels, the threshold frequency for the jump of absorption is determined by the condition \( \hbar \omega_{th} = 2 \varepsilon_F \propto \sqrt{n} \), where concentration \( n \) depends linearly on gate voltage, \( V_g \), and is inverse to substrate thickness, \( d \), so that \( n \propto V_g / d \equiv E_\perp \). The dependences of the threshold wavelength \( \lambda_{th} \) on homogeneous field \( E_\perp \) are presented in Fig. 1c for a number of substrates. One can see that the modulation of near-IR radiation (1.55 μm) is possible at \( E_\perp < 3 \text{ MV/cm} \) for the high-κ substrates (Al₂O₃, HfO₂, AlN, and ZrO₂ are examined below), and for SiO₂ substrate the applied field should be twice stronger. The modulation of mid-IR radiation (10.6 μm) can be realised in lower fields, \( E_\perp \approx 1 \text{ MV/cm} \). For the modulation of radiation in the visible spectral range, a field \( E_\perp \) comparable with the breakdown field for the substrate under consideration is needed. The modulation depth can be estimated through the amplitude of the absorption jump on the threshold, equal to 2.3%. For the 5 layer graphene the modulation efficiency can exceed 10%, taking into account that the interference on substrate influences this value. The absorption edge spreads with the increase of temperature (see the real part of dynamic conductivity \( \sigma_\omega \) presented in Fig. 1d), and the modulation efficiency decreases. At room temperature the effective modulation for near-IR radiation only is possible, while the modulation of mid-IR radiation needs cooling to temperatures about 77 K. The efficiency of modulation obtained is comparable to results both in bulk semiconductors and in heterostructures, see Refs. 9 and 10, respectively.

The analysis performed below is organized as follows. In Sect. II we describe the carrier-induced modulation of the response of graphene and evaluate the transmission and reflection coefficients. The efficiency of modulation versus applied field and thickness of substrate is analyzed in Sect. III. Discussion and concluding remarks are given in the last section.

II. BASIC EQUATIONS

The response of a doped graphene sheet on probe radiation is described by the two-dimensional dynamic conductivity \( \sigma_\omega \). In the colisionless approximation, when \( \omega \) exceeds any relaxation rate, the real and imaginary parts of \( \sigma_\omega \) are given by the expressions:

\[
\text{Re} \sigma_\omega \approx \frac{e^2}{4\hbar}(1 - f_{ep,\omega} - f_{hp,\omega}),
\]

\[
\text{Im} \sigma_\omega \approx \frac{e^2}{4\hbar}f_{ep,\omega}
\]
The in-plane electric field in a doped graphene - high-k substrate - heavily doped Si structure \((V_g = \text{gate voltage})\). Normal propagation of incident (\(in\)), reflected (\(r\)), and transmitted (\(t\)) radiation through the graphene placed over substrate of thickness \(d\) on doped Si \((\epsilon_s = \epsilon, \epsilon_r, \epsilon_0\) are the corresponding dielectric permittivities). Threshold wavelengths \(\lambda_{th}\) versus transverse field \(E_z\) for different substrates: SiO\(_2\) (1), AlN (2), Al\(_2\)O\(_3\) (3), and HNO\(_2\) (4) (the results for ZrO\(_2\) are similar to curve (4)). Dashed line is correspondent to the telecommunication wavelength, 1.55 \(\mu\)m. Spectral dependences of \(\text{R}_{\sigma\omega}\) and \(\text{Im}_{\sigma\omega}\) (solid and dotted curves) at room temperature for concentrations: 10\(^{12}\) cm\(^{-2}\) (1), 2 \(\times\) 10\(^{12}\) cm\(^{-2}\) (2), 4 \(\times\) 10\(^{12}\) cm\(^{-2}\) (3).

\[
\text{Im}_{\sigma\omega} \approx \ddot{\sigma}_{\omega} - \frac{e^2}{4\hbar p_{\omega}} \mathcal{P} \int_0^\infty \frac{dp^2}{p_{\omega}^2 - p^2} (f_{sp} + f_{hp}).
\]

In a doped graphene, when \(E_{\pm}\) is strong enough, the Pauli blocking factor in \(\text{R}_{\sigma\omega}\) is written through electron and hole distribution functions, \(f_{e,h,p}\), taken at \(p_{\omega} = \hbar \omega/(2v)\), where \(v = 10^8\) cm/s is the velocity of quasiparticles. Mention, that in the absence of carriers \(\text{R}_{\sigma\omega}\) does not depend on any material parameters. In the imaginary part of \(\sigma_{\omega}\) we eliminate the contribution of the non-doped graphene \(\ddot{\sigma}_{\omega}\), see Refs. 12 and 13, and the carriers contribution is connected with \(\text{R}_{\sigma\omega}\) through the Kramers-Kronig relation, where \(\mathcal{P}\) means the principal value of integral. The response of N-layer epitaxial graphene \([14]\) is described by the total conductivity \(N\sigma_{\omega}\).

We restrict ourselves to the geometry of normal propagation of the incident (\(in\)), reflected (\(r\)), and transient (\(t\)) waves through the structure "N-layer graphene - dielectric substrate - doped Si", as it is shown in Fig. 1a. The in-plane electric field \(E(z)\) \(\exp(-i\omega t)\) is governed by the wave equation: \([11, 13]\)

\[
\frac{d^2E(z)}{dz^2} + \epsilon_{\omega}(z) \left(\frac{\omega}{c}\right)^2 E(z) = 0,
\]

where \(z \neq 0\) and the permittivity \(\epsilon_{\omega}(z)\) is equal to the constant \(\epsilon_s\) in the substrate layer with the thickness \(d\) (at \(0 < z < d\)), while in the thick Si the dispersion \(\epsilon_{\omega}\) should be taken into account, see Ref. 15. The boundary conditions at \(N\)-layer graphene, where \(z \to 0\), takes the form

\[
\left.\frac{dE(z)}{dz}\right|_{z=0}^{+0} + i\frac{4\pi\omega}{c^2} N\sigma_{\omega} E(z = 0) = 0, \quad \left.E(z)\right|_{z=0}^{+0} = 0.
\]

These expressions contain the contribution of surface current, proportional to \(N\sigma_{\omega}\), that determines the jump of \([dE(z)/dz]\), while \(E(z)\) is continuous. At the substrate-Si interface we use the two conditions of continuity:

\[
\left.\frac{dE(z)}{dz}\right|_{z=0}^{d+0} = 0, \quad \left.E(z)\right|_{z=0}^{d+0} = 0.
\]

Outside of the graphene sheet the solution of electrodynamic problem (2)-(4) should be written in the form

\[
E(z) = \begin{cases} 
E_{in} e^{ik_{\omega} z} + E_r e^{-ik_{\omega} z} & z < 0 \\
E_{+} e^{ik_{\omega} z} + E_{-} e^{-ik_{\omega} z} & 0 < z < d \\
E_{d} e^{ik_{\omega} z} & d < z
\end{cases}.
\] (5)

Here the amplitudes for \(in\)- and \(r\)-waves \((z < 0)\), \(t\)-wave \((z > d)\), and for the field \(E_{\pm}\) in the dielectric substrate \((0 < z < d)\) are introduced. In Eq.(5) the wave vectors \(k_{\omega} = \omega/c\) (to the left), \(\tilde{k}_{\omega} = \sqrt{\epsilon_{\omega}/c}\) (to the right), and \(k_{\omega} = \sqrt{\epsilon_{\omega}/c}\) (in the dielectric substrate) are introduced as well. Using the boundary conditions (3) and (4) we get the system of linear equations for the amplitudes above. The solution of such a system determines the transition and reflection coefficients, \(T_{\omega}\) and \(R_{\omega}\), according to

\[T_{\omega} = \frac{\sqrt{\epsilon_{\omega}} |E_{in}|^2}{|E_{in}|^2}, \quad R_{\omega} = \frac{|E_r|^2}{|E_{in}|^2}.
\] (6)

According to energy conservation law, which connects \(T_{\omega}\) and \(R_{\omega}\) with the relative absorption coefficient \(\xi_{\omega}\), one obtains:

\[T_{\omega} + R_{\omega} + \xi_{\omega} = 1.
\] (7)

As a result, variations of \(T_{\omega}\) and \(R_{\omega}\) are correlated due to the Pauli blocking effect which leads to a jump of \(\xi_{\omega}\).

The direct expressions for the transmission and reflection coefficients take form

\[T_{\omega} = \frac{A_{\omega}}{|A_{\omega}(+)|^2}, \quad R_{\omega} = \frac{|A_{\omega}(\mp)|^2}{|A_{\omega}(+)|^2}.
\] (8)

where \(A_{\omega}(\pm)\) are expressed through the dynamic conductivity and the structure parameters according to

\[A_{\omega}(\pm) = \sqrt{\epsilon_{\omega}} \cos k_{\omega} d - i \sqrt{\epsilon_{\omega}} \sin k_{\omega} d \quad \text{or} \quad \left(\frac{4\pi\sigma_{\omega}}{c} \pm 1\right) \left(\cos k_{\omega} d - i \sqrt{\epsilon_{\omega}} \sin k_{\omega} d\right).
\] (9)
In the case $\epsilon_\omega = \epsilon_s$ the oscillating factors eliminate from (9), and Eqs. (8) are in agreement with the previous results. Taking into consideration the interference on the substrate, when $\epsilon_\omega \neq \epsilon_s$, the spectral dependences of $T_\omega$ and $R_\omega$ are determined by carriers concentration (through variations of $E_\perp$ or $V_g$), the dielectric substrate thickness $d$, and the permittivities $\varepsilon_s$ and $\varepsilon_\omega$. We have neglected a weak absorption in Si and used $\varepsilon_s$ for SiO$_2$ and high-$\kappa$ dielectrics from Refs. 15 and 16, respectively.

III. RESULTS

Performing the numerical integration in Eq. (1) and using Eqs. (8, 9) one obtains the transmission and reflection coefficients. Below we analyze the dependences of $T_\omega$ and $R_\omega$ on the applied field $E_\perp$, which determines the carriers concentration, for the substrates of various thickness on the base of high-$\kappa$ dielectrics or SiO$_2$. The computations were performed for near-IR and mid-IR spectral regions ($\lambda$ = 1.55 $\mu$m and 10.6 $\mu$m).

A. High-$\kappa$ substrates

We examine first the modulation of the telecommunication range radiation, $\lambda$ = 1.55 $\mu$m, by the structures of 5-layer graphene on high-$\kappa$ substrate at room temperature. Figures 2(a) and 2(b) show the contour plots of $T$ and $R$ versus $E_\perp$ and $d$ for the case of Al$_2$O$_3$ substrate.

One can see, that the change of $T$ versus $E_\perp$ is $\sim$ 10% near the transmission maximum, and the modification of $T$ by interference can be as large as 0.3 if $d$ is in the range 0.1 - 0.5 $\mu$m. Similarly, the change of $R$ versus $E_\perp$ does not exceed several %, while the modification of $R$ versus $d$ can be of 0.3 order. The maximum of $T$ corresponds the minimum of $R$ and vice versa.

![FIG. 2: (Color online) (a) Contour plot of transmission coefficient of graphene over Al$_2$O$_3$ substrate as a function of applied field $E_\perp$ and thickness $d$. (b) The same for reflection coefficient.](image)

![FIG. 3: (Color online) Transmissivity $T$ at wavelength 1.55 $\mu$m versus $E_\perp$ for different substrates: (a) Al$_2$O$_3$, (b) HfO$_2$, (c) AlN, and (d) ZrO$_2$. Curves 1 - 5 are correspondent to the thicknesses $d$ = 0.08, 0.12, 0.16, 0.2, and 0.24 $\mu$m.](image)

![FIG. 4: (Color online) Reflectivity $R$ at wavelength 1.55 $\mu$m versus $E_\perp$ for the same substrates as in Fig. 3(a-d). Curves 1 - 5 are correspondent to the thicknesses $d$ = 0.28, 0.32, 0.36, 0.4 and 0.44 $\mu$m.](image)

Gate-voltage-induced modification of transmission is presented in Fig. 3 for different high-$\kappa$ substrates at sev-
eral thicknesses near the maximum of $T$. Similar dependences for $R$ are presented in Fig. 4 near the reflection maximum, corresponding to the greater thicknesses. Besides the essential dependence on thickness, $T$ and $R$ depend also on high-frequency and static permittivity of the materials under consideration. Therefore, the effective modulation for Al$_2$O$_3$ and AlN occurs in the range $E_{\perp} \sim$ 8 - 12 MV/cm, and for HfO$_2$ and ZrO$_2$ the weaker fields $E_{\perp} \sim$ 4 - 6 MV/cm are needed. The modulation depth for transmission exceeds in several times the modulation depth for reflection. The effective modulation interval, corresponding the region of the jump in absorption, becomes narrower with the decrease of temperature.

B. SiO$_2$ substrate

Now we are going to examine the structures "graphene - SiO$_2$ - Si", where the permittivities are smaller. Therefore the effective modulation for transmission of near-IR radiation takes place at $E_{\perp} \sim$ 25 - 35 MV/cm, see Fig. 5(a), i.e. it needs stronger fields than the threshold of single-layer graphene on SiO$_2$ substrate $\sim$ 6 MV/cm, see Fig. 1(b). The modulation of $R$ in the same range of fields does not exceed several percents, see Fig. 5(b). It should be noted, that these fields $E_{\perp}$ are of the same order of values, as a breakdown field, therefore a possibility of modulation in this case needs a special verification.

The effective modulation of transmission (over 5%, see Fig. 6(a)) takes place in mid-IR spectral region, for $\lambda = 10.6 \, \mu m$. The applied field in this case does not exceed 2 MV/cm, but the substrate thickness should be greater because of the increase of $\lambda$. The corresponding modulation of reflection does not exceed several percents as well, see Fig. 6(b).

For the single layer graphene the modulation depth obviously cannot be greater, than 2.3%. However, this modulation of transmission occurs for much lower fields, than in the previous cases under examination, 200 kV/cm, and the jump region becomes rather narrow with the decrease of temperature, see Figs. 7a, b.

IV. CONCLUDING REMARKS

The results obtained clearly demonstrate the possibility for realization of the modulator for telecommunication spectral range (\sim 1.5 \, \mu m) on the base of multilayer graphene, placed over high-$\kappa$ substrate. The effective modulation can be realized in this case for the applied fields \sim 5 MV/cm, while for the case of SiO$_2$ substrate the field should be \sim 20 MV/cm comparable to a breakdown value. The modulation depth for multi-layer ($N = 5$-10) graphene can be as large as 10-20\% (\sim 2\% per one layer). The same efficiency of modulation for the mid-IR radiation (\sim 10.6 \, \mu m) can be realized for the applied fields not stronger than 2 MV/cm for the low temperature region.

The consideration performed takes into account the contribution of interband transitions, described by the complex dynamic conductivity, and the radiation interference on the structure "vacuum - graphene - substrate - doped Si" for the case of normal propagation of radiation. The modulation is determined by the Pauli blocking effect under the change of the carriers concentration by the gate voltage, therefore the time of modulation is governed by the recombination time of the excess concentration of carriers, or by the time of injection from contacts.

Next, we discuss the assumptions used in our calcu-
lations, which are rather standart ones. The dynamic conductivity of the carriers in the spectral region under examination is described properly with the use of the linear dispersion law of carriers in graphene. The phenomenological description of the dispersion of $\text{Im} \sigma$ due to the transitions from the valence band (see Refs. 12 and 13) does not change the results essentially due to the smallness of its contribution for the spectral range under consideration. The study of the declined propagation of radiation is more complicated, and the modulation efficiency in this case decreases. Moreover, the modulation efficiency can also be reduced in mid-IR range due to the absorption of radiation in the doped Si. It should be noted, that modulation of electron concentration in the gate gives a weak contribution to IR response and can be neglected in comparison to the Pauli blocking effect in graphene.

In conclusion, the results obtained should stimulate the experimental study of the electrooptical modulation of the near-IR radiation by the structure of multilayer graphene over high-$\kappa$ dielectric substrate at room temperature and high gate voltages (concentrations). For the mid-IR spectral region the effective modulation can be realized at low temperatures.

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