PLASMON EFFECTS IN A GRAPHENE NANOSTRUCTURE

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I. INTRODUCTION

Plasmons are collective excitations of electrons in solids. The ability to change their properties by an electric field in low-dimensional materials and structures, such as graphene, which makes them promising for the use in a variety of optoelectronic devices, such as sensors, detectors, radiation sources, etc [1]. The interaction between plasmonic oscillations in graphene leads to a strong shift in the absorption spectrum of light in the far- infrared range. Thus, it was experimentally found that the interaction of plasmons in graphene on a dielectric substrate leads to a strong redshift of the absorption spectrum in comparison to the plasmon spectrum in isolated graphene. The absorption spectra of graphene due to the interaction of plasmons cover the far IR range (photon energies from 10 meV to 200 meV), which, in turn, coincides with the vibrational spectra of most biological molecules. This provides the opportunities for the design and manufacture of graphene-based biosensors. In this regard, it's important to simulate plasmon spectra for their use in optoelectronics and biosensorics [2]. Even though plasmon spectra in isolated graphene have already been well studied, for the effective operation of real optoelectronic devices, it is relevant to study plasmon effects in graphene on various substrates, as well as in the composition of nanostructures.

Also, the relevance of plasmon studies is related to the issue of replacing copper interconnects in integrated circuits (ICs). For many years, the reduction in design standards for elements in silicon technology remained sufficient to increase the performance of Ics. Because of this, there was no need for manufacturers to develop devices based on new physical principles or search new materials to replace silicon. However, now everyone agrees that scaling has come to its limit. The need for a further increase in the IC performance forces us to look for new materials with improved electronic properties [3]. Over the past few decades, researchers arrived at the conclusion that it is possible to obtain the surface plasmons on the conductor/dielectric interface with the same frequency as external electromagnetic waves, but with a much shorter wavelength. This will allow to use plasmons in nanostructures to transfer information inside the chip. Plasmonic interconnects would be a real breakthrough in the field of increasing the operating frequencies of Ics. In this regard, a promising direction for solving such kind of problem is the study of plasmon oscillations in the terahertz frequency range and the usage of graphene on a dielectric substrate. However, a plenty of technological and physical problems for the excitation, propagation, and detection of plasmonic oscillations with controlled parameters need to be solved before that.

II. MODEL

To simulate plasmonic effects, a heterostructure that includes graphene on a dielectric substrate with a gate electrode was chosen. First, we calculated the complex dynamic conductivity σ (ω). The dispersion equation for two-dimensional plasmon waves propagating over the surface of a given structure includes the dielectric constants of the environment and the substrate, as well as the dynamic conductivity of graphene. It follows from the dispersion equation that the value of the wavevector and, consequently, the attenuation length of the plasmon wave directly depends on the dynamic conductivity of graphene. In the case of a monatomic graphene layer, the dynamic conductivity is determined by the formulas, generalized in [4], and including the chemical potential of graphene, μ , relaxation time of the electron pulse, τ , ambient temperature, frequency of electromagnetic external radiation, ω (EMR). To determine the propagation coefficients Re (ρ) and absorption *q* of surface plasmon waves, the components of the electric *E* and magnetic *H* fields along the graphene plane *z* were found using Maxwell's equations [3]. The complex propagation coefficient of surface plasmons (ρ) is related to the wave number of the surface plasmon by the relation *q* = Im($\rho\omega/c$). Here *c* is the speed of light. As a result, the equation for the dispersion of surface plasmons was obtained [4]:

$$\sqrt{n^2 - \rho^2} + n^2 \sqrt{1 - \rho^2} + \left(\frac{4\pi}{c\varepsilon_0}\right) \sigma(\omega) \sqrt{n^2 - \rho^2} \sqrt{1 - \rho^2} = 0,$$
(1)

where *n* is the refractive index at the boundary of the medium and graphene, ε_0 is the electrical constant of the vacuum.

Solving equation (1) with respect to ρ , it becomes possible to find the propagation coefficient Re(ρ) and the absorption coefficient Im($\rho\omega/c$), which is the plasmon spectrum. In the case when the refractive index of the medium *n* is equal to 1, Eq. (1) is simplified and analytically resolved for ρ .

To determine the chemical potential in graphene μ , which value self-consistently depends on the gate voltage V_g , the dielectric capacitance, and the charge carrier concentration in graphene, an integral expression for the charge carrier concentration is used depending on the value of the chemical potential and

the electrostatic equation for the graphene/dielectric/gate electrode heterostructure [5]. The electrostatic equation includes the chemical potential of graphene, the charge carrier concentration, the dielectric capacitance, the quantum capacitance of graphene, and the capacitance of the graphene/dielectric interface.

The integral expression for the charge carrier concentration in graphene depends on the chemical potential and is determined by the density of states in graphene and the Fermi-Dirac statistics. The electrostatic equation for the considered heterostructure is determined as follows [5]:

$$eV_g = \mu + \frac{e^2 n_s}{c_{ox}} + \frac{c_{it}}{c_{ox}} \mu, \tag{2}$$

where $n_s(\mu)$ is the charge carrier concentration in graphene; C_{ox} is the capacitance per unit area of the gate insulator, C_{it} is the capacitance per unit area of the interface states.

III. RESULTS AND DISCURSSION

The calculations of the transmission and absorption coefficients, as well as the values of the wavevector of plasmons, have been conducted. Frequency dependences of the propagation coefficient are obtained for different values of the gate voltage for different materials of the gate insulator at temperatures of 77 and 300 K. It is shown that its value can both increase with frequency and change nonmonotonically in the frequency range 1-20 THz. Monotonic dependences of the propagation coefficient were obtained in the range of 1-12 THz at values of the chemical potential of graphene 0.01-0.02 eV and the refractive index at the medium/graphene interface *n*=1-3. In this case, the value of the propagation coefficient increases with frequency up to values of 5-40 with increasing *n*. For a non-monotonic dependence, the maximum value of the propagation coefficient corresponds to the value Re(ρ) = 10-14, and the frequency at which the peaks are observed lies in the range of 7-16 THz, depending on the capacitance of the dielectric and the potential of the gate electrode. These parameters varied in the range $C_{ox} = 1-5 \ \mu F/m^2$, $V_g = 0.02-0.12 \ V$. Moreover, with an increase in the potential of the gate electrode, the maximum shifts towards an increase in frequency.

The frequency dependences of the absorption coefficient are obtained for different values of the gate voltage for different materials of the gate dielectric at temperatures of 77 and 300 K. It is shown that its value varies non-monotonically in a given frequency range, taking both positive and negative values with varying C_{ox} and V_g in the same ranges as indicated above. A significant change in the absorption coefficient is observed at a frequency of more than 5 THz. Its negative value reaches a value of $-3 \cdot 10^5$ cm⁻¹ at a frequency of 13 THz and then, with an increase in the frequency of EMR, it sharply increases and takes positive values up to $4 \cdot 10^5$ cm⁻¹. The obtained results indicate that, depending on the ratio of the parameters of the nanostructure and the frequency of the EMR, the modes of both absorption of EMR and its amplification due to plasmon oscillations can be realized.

The frequency dependences of the wavevector of plasmon oscillations were obtained at various gate voltages V_g for various materials of the gate insulator at a temperature of 77-300 K. Surface plasmons with a wavevector $q \sim 10^5$ cm⁻¹, which corresponds to a wavelength of $\lambda \sim 1 \,\mu\text{m}$ or less, are in the considered frequency range of EMR. The decrease in the wavelength of plasmon oscillations in graphene in the terahertz frequency range is due to the strong localization of plasmons in graphene.

IV. CONCLUSIONS

Simulations of the frequency dependences of the propagation and absorption coefficients of EMR by a graphene heterostructure were modeled. The regularities of influence of the electrophysical parameters of the heterostructure on the amplification of plasmon oscillations and a decrease in their wavelength to 1 μ m and less have been established.

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