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THE EVOLUTION OF FEW CYCLES OPTICAL PULSES IN A DOUBLE-LAYER GRAPHENE – BORON NITRIDE TAKING INTO ACCOUNT NONLINEARITY OF A MEDIUM

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The propagation of ultra-short optical pulses in a thin film created by graphene grown on a boron nitride was considered, taking into account non-linear medium characteristics. Electron conduction in such a system described with a long-wave effective Hamiltonian for the low temperatures media. The electromagnetic field is taken in the framework of classical Maxwell equations. Dependence of the pulse shape on the initial pulse amplitude and the parameters of the linear and nonlinear polarization is shown.

Keywords: Graphene, Boron Nitride, Optical pulse, Nonlinearity.

1. Introduction

Recently, the number of studies on boron nitride-supported graphene has increased [1–8]. Primarily, this is due to graphene's unusual properties [9]. Note that boron nitride has a similar hexagonal lattice to graphene, as well as the fact that the ionic character of interatomic bonds in the hexagonal boron nitride (h-BN) leads to the absence of surface-based 'dangling' covalent bonds and charge trapping [8]. As found in [8], the roughness of graphene on h-BN is much smaller than that of graphene on SiO_2, and charge fluctuations are two orders of magnitude weaker. In general, the electronic characteristics of graphene on h-BN are almost the same as that of free graphene. Thus, to explore graphene on a substrate is much easier and more convenient [8].

The evolution of an ultra-short optical pulse propagating in a double-layer structure of graphene – boron nitride in non-magnetic environments would be revealed taking into account the nonlinear polarization of the medium.

2. Basic equations

We considered a layer of graphene on a substrate of boron nitride. The Hamiltonian we have chosen, in a long-wave approximation, can be written in matrix form as:

$$H(k) = \begin{pmatrix} 0 & k^* & 0 & t \\ k & 0 & 0 & 0 \\ 0 & 0 & \Delta & f^* \\ t & 0 & f & -\Delta \end{pmatrix}, \tag{1}$$

where t is the electron overlap integral between the layers of graphene and boron nitride; Δ is the band gap for boron nitride; $k = v_{FG}(k_x + ik_y)$, v_{FG} – is the Fermi velocity for graphene;

k_x, k_y – are the electron pulse components: $f = v_{FBN}\left(k_x + ik_y\right)$; v_{FBN} – is the Fermi velocity for boron nitride.

The Hamiltonian (1) can be rewritten using a block matrix structure [10]:

$$H\left(k\right) = \begin{pmatrix} 0 & k^* & 0 & t \\ k & 0 & 0 & 0 \\ 0 & 0 & \Delta & f^* \\ t & 0 & f & -\Delta \end{pmatrix} \equiv \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}.$$

In the case of a large band gap in boron nitride compared to the electron's energy, a long-wave approximation can be considered. This makes it possible to write the effective Hamiltonian analogously to bigraphene [10]:

$$H^{eff} \equiv H_{11} - H_{12}H_{22}^{-1}H_{21} = -\frac{1}{t}\begin{pmatrix} \Delta & -\frac{1}{t}f^*k^* \\ -\frac{1}{t}fk & -\frac{1}{t^2}\left|k\right|^2\Delta \end{pmatrix}. \tag{2}$$

The Hamiltonian (2) is easily diagonalized, which gives the electronic spectrum:

$$\varepsilon\left(k_x, k_y\right) = \frac{1}{2}\Delta\left(\left(1 - \frac{v_{fg}^2\left(k_x^2 + k_y^2\right)}{t^2}\right) + \sqrt{\left(1 + \frac{v_{fg}^2\left(k_x^2 + k_y^2\right)}{t^2}\right)^2 + \frac{4v_{fg}^2v_{fnb}^2\left(k_x^2 + k_y^2\right)^2}{\Delta^2t^2}}\right), \tag{3}$$

where v_{FG}, v_{FBN} – the Fermi velocity of electrons for graphene and boron nitride, respectively.

According to quantum-mechanical laws, the presence of an external electric field E, directed along the X axis, the Coulomb gauge can be chosen in the following form: $E = -\frac{1}{c}\frac{\partial A}{\partial t}$. It is necessary to replace the momentum with a generalized momentum: $p \to p - \frac{e}{c}A$ (e is the electron charge). In this case, the effective Hamiltonian (2) can be rewritten as:

$$H = \sum_{p\sigma}\varepsilon\left(p - \frac{e}{c}A(t)\right)a_{p\sigma}^{+}a_{p\sigma}, \tag{4}$$

where $a_{p\sigma}^{+}$, $a_{p\sigma}$ –are the creation and annihilation operators of electrons with quasi-momentum p and spin σ. The vector-potential A is considered as $A = (0, 0, A(x, t))$.

Maxwell's equations for polarization of the medium can be written as [11]:

$$\frac{\partial^2\mathbf{E}}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2\mathbf{E}}{\partial t^2} + \frac{4\pi}{c}\frac{\partial\mathbf{j}}{\partial t} = \frac{4\pi}{c^2}\frac{\partial^2\mathbf{P}}{\partial t^2}. \tag{5}$$

Here, we neglect the laser beam diffraction in directions perpendicular to the beam propagation axes. In Eqn. (5), $\mathbf{E}$ is an electric field of light wave, $\mathbf{P} = \alpha\mathbf{E} + \beta\left|\mathbf{E}\right|^2\mathbf{E}$ – is a polarization of the medium, t is a time, c is a speed of light in a vacuum. There is a simple model for the medium nonlinearity when the polarization vector is considered to be parallel to $\mathbf{E}$.

We write the expression for the current density:

$$j_0 = e\sum_{ps}v_s(p - \frac{e}{c}A(t))\left\langle a_{ps}^{+}a_{ps}\right\rangle, \tag{6}$$

where $v_s(p) = \dfrac{\partial \varepsilon_s(p)}{\partial p}$, and brackets denote averaging with the nonequilibrium density matrix $\rho(t)$: $\langle B \rangle = \mathrm{Sp(B(0)\rho(t))}$.

Further, we consider the case of low temperatures, when the sum (6) contributes only a small area in momentum space near the Fermi level. Therefore, we rewrite the expression for the current density in the form:

$$j = e \int\limits_{-\Delta}^{\Delta} \int\limits_{-\Delta}^{\Delta} dp_x dp_y v_y \left(p - \frac{e}{c} A(x,t) \right). \tag{7}$$

The range of pulses integrated in (7) was determined from the particles number equality:

$$\int\limits_{-\Delta}^{\Delta} \int\limits_{-\Delta}^{\Delta} dp_x dp_y = \int\limits_{-\Delta}^{\Delta} \int\limits_{-\Delta}^{\Delta} dp_x dp_y \left\langle a^{+}_{p_x,p_y} a_{p_x,p_y} \right\rangle.$$

3. The results of numerical simulation

Equation (5) was solved numerically using a direct finite-difference cross-like scheme [12]. Steps by time and coordinates were determined using standard conditions of stability, strides of finite-difference scheme were halved serially, until the solution did not change in the eighth sign. The initial conditions were chosen as an ultra short optical pulse consisting of a single oscillation of the zero-width field, respectively, that can be specified by setting the potential **A** as:

$$\begin{gathered} A(x,t) = Q \exp(-(x - vt)^2/\gamma), \\ \gamma = (1 - v^2)^{1/2}, \end{gathered} \tag{8}$$

where Q is the amplitude, v is the initial ultra-short pulse velocity on the sample input. This initial condition corresponds to the fact that the sample is fed an ultra-short pulse, consisting of a single oscillation of the electric field. The values of energy parameters are expressed in Δ units. The resulting evolution of the electromagnetic field propagating along the sample is shown in Fig. 1.

The amplitude of the pulse decreased when the linear polarization of the medium gradually increased. This fact can be interpreted as the pulse spending part of its energy on medium polarization.

The pulse behavior presented in Fig. 1 concerns the presence of dispersion, which leads to a broadening of the optical pulse, as well as non-linearity in the same equation, thus leading to a 'narrowing' of the pulse. The competition between these two terms leads to a deformation of the initial pulse shape and rise to its stable form.

More clearly, the effects associated with nonlinear pulse appear at the front and lead to the formation of additional peaks and the broadening of the pulse which can be explained by an imbalance between dispersion and nonlinearity in the system. This is clearly seen in Fig. 3. The dependence of the electric field pulse on the magnitude of the medium's nonlinear polarization is shown in Fig. 3.

As can be seen in Fig. 3, involving non-linear polarization leads to the appearance of a wave front for the second maximum. As in the case of linear polarization, the initial pulse amplitude decreases, which is to be expected.

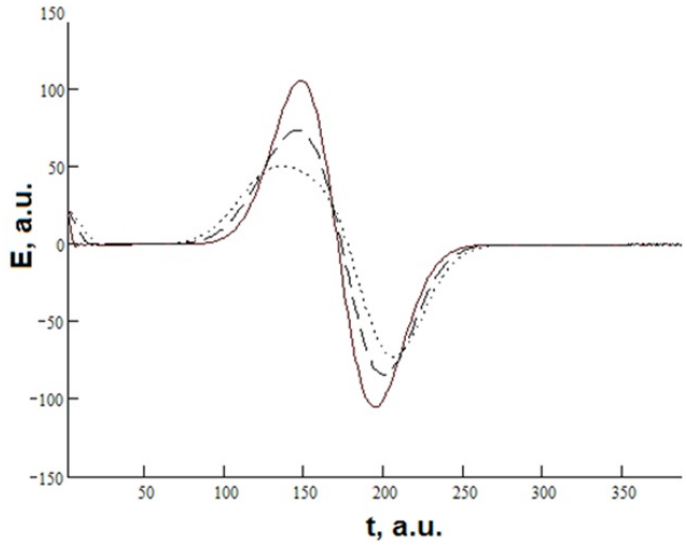

FIG. 1. Time dependence of the electric field: a) solid line – $\alpha = 0.0$; b) dotted line – $\alpha = 0.3$; c) dashed line – $\alpha = 0.5$, the nonlinear polarization is absent. Time, a.u. is time $3 \cdot 10^{-16}$ s.; electric field a.u. is 10^7 V/m

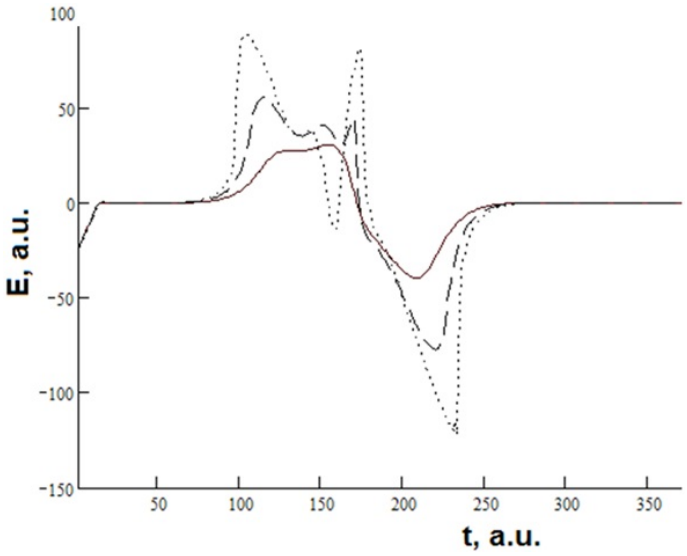

FIG. 2. Time dependence of the pulse form for different cases of pulse amplitude value: a) solid line – $Q = 2$; b) dotted line – $Q = 3$; c) dashed line – $Q = 5$. Time and electric field a.u. as in Fig. 1

4. Conclusion

As follows from the obtained results, the stable ultra-short optical pulses can undergo propagation in hexagonal boron nitride-supported graphene in a medium with nonlinear polarization.

By increasing the initial pulse amplitude, the wave front is broadened, and there is a second pulse of lower intensity. This effect may be useful in the development of hybrid devices based on the effect of light interaction with graphene electrons.

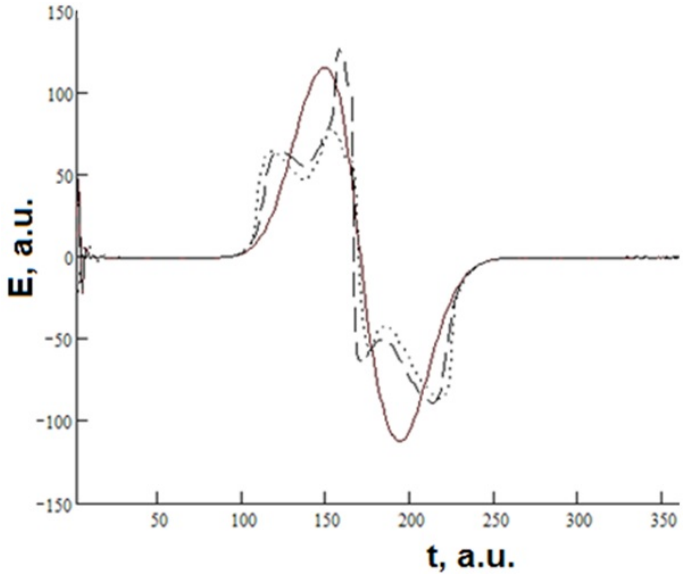

FIG. 3. Time dependence of the electric field on time taking into account the nonlinear polarization of the medium: a) solid line – $\beta = 0.03$; b) dotted line – $\beta = 0.4$; c) dashed line – $\beta = 0.6$ the dispersion is almost zero, $\alpha = 0.01$. Time and electric field a.u. as in Fig.1

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