09

Propagation of few cycle pulses in the array of carbon nanotubes with polymers under the constant magnetic field

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The effect of a constant magnetic field on the behavior of few cycle optical pulses in an array of carbon nanotubes with polymers was studied in this research. The main equation describing the propagation of an electromagnetic field in the medium under consideration was obtained on the basis of Maxwell's equations. The dependences of the optical pulse shape on the concentration of the polymer in the medium are obtained.

Keywords: few cycle pulse, cafbon nanotube, magnetic field, polymer.

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Introduction

Investigation of shortest optical pulses propagated in media containing carbon nanotubes, demonstrates unique electrophysical properties of these systems, which disclose huge potential for their practical application in the diversity of semiconductor equipment and electronic nanodevices [1–4]. Spectrum of application of electronic devices, which are based on nanocarbon structures, is rather wide, including nanoengineering, bionanotechnology, nanomedicine, and also nanopharmacology.

Authors from various contents rather closely study dynamics of both unidimensional and two-dimensional and three-dimensional electromagnetic waves propagating in the array of carbon nanostructures. Studies of such media are widely known with application of external electric and magnetic fields [5–8]. Besides, in some papers the authors considered propagation of shortest light pulses in the array of carbon nanotubes with impurities [9–10]. However, despite the active interest of researches in this area, still some issues remain without attention today, which relate to propagation of electromagnetic waves in the array of carbon nanotubes with impurities and applied external electric and magnetic fields.

Apart from the study of nanocarbon structures, polymer nanocomposites conquer more and more attention. Their development is based on fundamental research of physical and chemical processes of material formation and evolution of their structure providing for a wide spectrum of functional properties. Recently carbon nanotubes are often used as a filler, since they are considered to be an ideal reinforcing material for polymers [11]. Carbon nanotubes together with polymers improve mechanical characteristics of the material (stiffness, tensile strength), improve electric conductivity, increase heat conductivity, heat resistance and give new functional properties to nanocomposite. There are different ways to produce stable nanocomposites [12], and also methods of even distribution of carbon nanotubes in a polymer matrix and for efficient transfer of stresses to nanotubes [13].

It is also necessary to note that permanent magnetic field may have considerable effect at behavior of electromagnetic waves since permanent magnetic field may strongly change the single-electron spectrum of the studied task as it was shown in paper [14]. This paper attempts to consider influence of external permanent magnetic field applied in parallel to the axis of nanotubes, at dynamics of 3D shortest optical pulses, propagating in the system of carbon nanotubes with polymers. Solution to the task about propagation of a shortest optical pulse in the case when the permanent magnetic field parallel to the axis of carbon nanotube, is of special interest, since in this case, as presented in [14], single-electron spectrum may not be found precisely, and this causes the need to use numerical methods to identify differences related to presence and absence in the system of permanent magnetic field.

In connection with the above, this research was conducted, and behavior of electromagnetic pulses was analyzed in the considered conditions.

Main calculations

The geometry of the task is such that the permanent magnetic field applied to the studied system in parallel to the electric component of the 3D shortest electromagnetic pulse propagating in the system and matches the axis of carbon nanotubes (axis y). The 3D pulse propagates along the axis z. In its turn, the researched system — is the environment made of carbon nanotubes with polymers. The array considered in the task is heterogeneous, and the type of carbon nanotubes that make this array, — zig-zag $(m, 0)$,

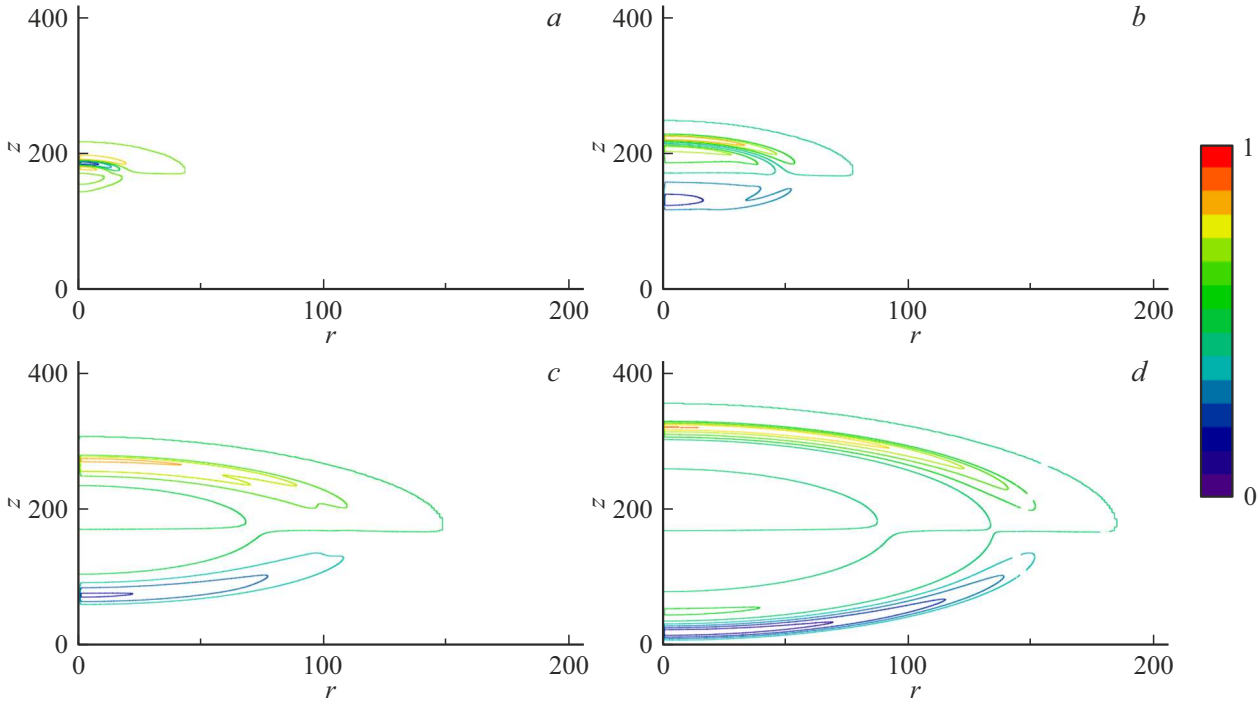

Figure 1. Intensity of three-dimensional optical pulse $I(r, z, t) = E^2(r, z, t)$: (a) initial form of pulse $t = 2 \cdot 10^{-12}$ s; (b) $t = 6 \cdot 10^{-12}$ s; (c) $t = 1.2 \cdot 10^{-11}$ s; (d) $t = 1.8 \cdot 10^{-11}$ s; $\Phi/\Phi_0 = \pi/2$; $v/c = 0.93$. Values specified in the figure are given in non-dimensional values. Color gradation corresponds to the intensity of electric field $I/I_{\max}$.

where m — is the number of hexagons along the nanotube circumference.

The electronic structure of carbon nanotubes was investigated by us as approximation of strong connection within analysis of dynamics of π-electrons. The law of dispersion of carbon nanotube electrons with applied permanent magnetic field, the intensity vector of which is parallel to the axis of the nanotube, is [14]:

$$\varepsilon_s(k_x, k_z, H) = \pm\gamma \times \sqrt{1+4\cos\left(\frac{\sqrt{3}ak_x}{2}\right)\cos\left(\frac{3ak_z}{2}\right)+4\cos^2\left(\frac{\sqrt{3}ak_x}{2}\right)}, \quad (1)$$

where $a = 1.4$ Å, $\gamma \approx 2.7$ eV, $k_x = \frac{2\pi}{\sqrt{3}am}\left(s + \frac{\Phi}{\Phi_0}\right)$, k_z — wave vector along the axis of the tube, Φ — magnetic flux through the cross section of the tube, $\Phi_0 = \frac{\hbar c}{e}$, $s = 1, 2, \ldots, m$.

In Maxwell equations the external electric field shall be written with account of Coulomb calibration: $\mathbf{E} = -1/c \cdot \partial\mathbf{A}/\partial t$, and pulse q shall be replaced with generalized pulse: $q \to q - eA/c$ (here e — electron charge, c — light speed), and we will get Maxwell equations in the following form for a 3D case [15,16]:

$$\frac{\varepsilon}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2} - \frac{\partial^2\mathbf{A}}{\partial x^2} - \frac{\partial^2\mathbf{A}}{\partial y^2} - \frac{\partial^2\mathbf{A}}{\partial z^2} - \frac{4\pi}{c}\mathbf{j}_1 - \frac{4\pi}{c}\mathbf{j}_2 = 0, \quad (2)$$

where $\mathbf{A}$ — vector-potential of electric field, which is written as $\mathbf{A} = \big(0, A(x, y, z, t), 0\big)$. Such presentation corresponds to the fact that electromagnetic field is polarized along the axis of carbon nanotubes. The investigated environment at the same time does not rotate polarization, nanotubes are oriented in the same manner, which makes it possible for us to neglect effects related to the action of the magnetic field of electromagnetic wave. Here $\mathbf{j}_1$ — is current density for carbon nanotubes, and current density for polymers is set by value $\mathbf{j}_2$. In equation (2), following from Maxwell equation, parameter ε — is dielectric permeability of environment with carbon nanotubes, defining the speed of propagation of linear electromagnetic waves in this environment. We believe that the array of carbon nanotubes is built into a dielectric matrix, and the resulting effective coefficient of dielectric permeability of the system was believed to be equal to 4, and frequency dispersion of this parameter under such conditions was not estimated [17].

We further use standard expression for current density for the considered system of electrons of carbon nanotubes [18]:

$$j_1 = e\sum_{ps} v_s\left(p - \frac{e}{c}A(t)\right)\langle C_{ps}^{+}C_{ps}\rangle. \quad (3)$$

Here $v_s(p) = \frac{\partial\varepsilon_s(p)}{\partial p}$, C_{ps}^{+}, C_{ps} corresponds to operators of creation and destruction of excitations with quasi momentum (p, s), angular brackets note averaging with unbalanced density matrix $\rho(t)$: $\langle B\rangle = Sp\big(B(0)\rho(t)\big)$. If we take into account the fact that $[C_{ps}^{+}C_{ps}, H] = 0$, then from

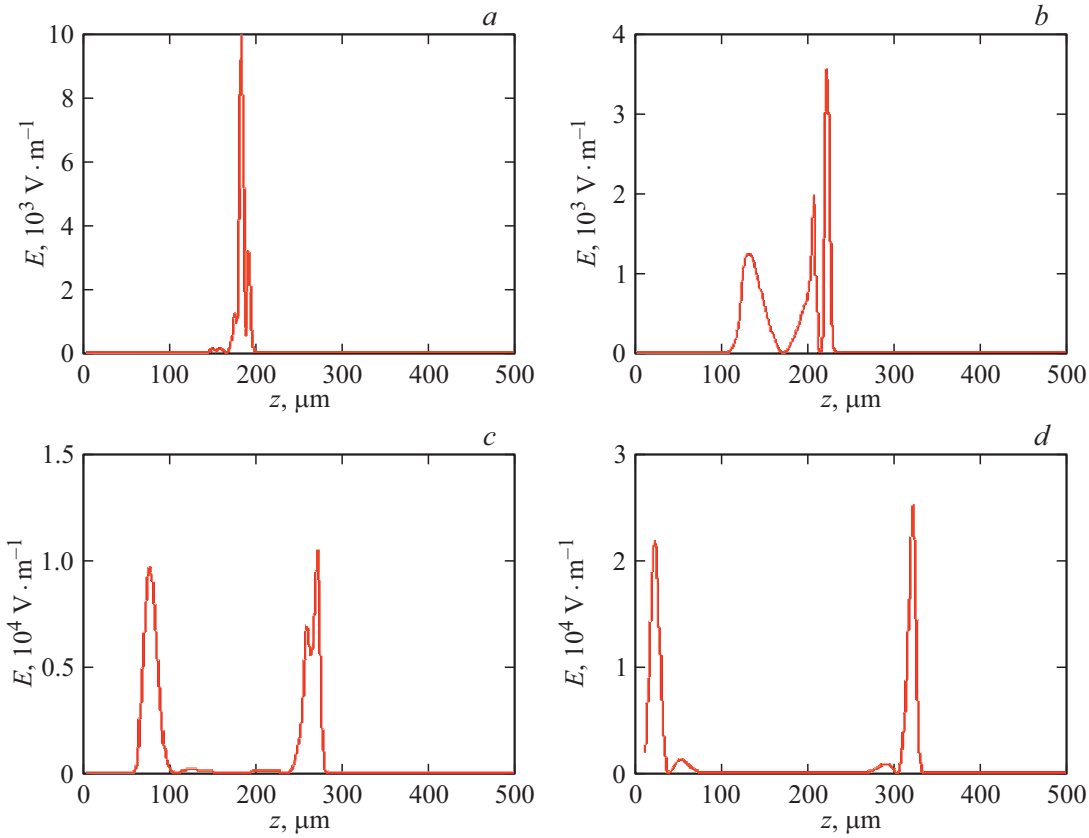

Figure 2. Sections showing pulse energy concentrated in the low region near the axis of pulse propagation and passing through the certain point of the axis z at different moments of time (a) $t = 2 \cdot 10^{-12}$ s; (b) $t = 6 \cdot 10^{-12}$ s; (c) $t = 1.2 \cdot 10^{-11}$ s; (d) $t = 1.8 \cdot 10^{-11}$ s; $\Phi/\Phi_0 = \pi/2$; $v/c = 0.93$. The axis of ordinates — intensity of the electric component.

equations of movement for the density matrix one can get that $\langle C^+_{ps} C_{ps} \rangle = \langle C^+_{ps} C_{ps} \rangle_0$, besides $\langle B \rangle_0 = Sp\big(B(0)\rho(0)\big)$, $\rho_0 = \exp(-H/kT)/Sp\big(\exp(-H/kT)\big)$, where k — Boltzmann?s constant, T — temperature.

Calculation of current $\mathbf{j}_2$ for polymers is carried out similarly to calculation of current for the system of quantum dots with hopping conductivity [19]. With account of such model justified in detail in [20], the expression for current is written as

$$j_2 = e \sum_{ps\sigma} v_s \left(p - \frac{e}{c} A(t) \right) \langle C^+_{ps\sigma} C_{ps\sigma} \rangle, \qquad (4)$$

where $C^+_{ps\sigma}$, $C_{ps\sigma}$ correspond to polymer electron creation and destruction operators.

Let us present electron dispersion law (1) as Fourier?s series, and we will get an effective equation for vector-potential $\mathbf{A}$:

$$\frac{\partial^2 \mathbf{A}}{\partial x^2} + \frac{\partial^2 \mathbf{A}}{\partial y^2} + \frac{\partial^2 \mathbf{A}}{\partial z^2} - \frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} + \frac{4en_0}{c} \sum_{q=1}^{\infty} q b_q \sin\left(\frac{qaeA}{c} \right)$$

$$+ \frac{4en_{pol}}{c} \sin\left(\frac{a_{pol} eA}{c} \right) = 0,$$

$$b_q = \sum_s a_{sq} \int dp \cos(apq) \frac{\exp\big(-\varepsilon_s(p)/kT\big)}{1 + \exp\big(-\varepsilon_s(p)/kT\big)}, \qquad (5)$$

where $\varepsilon_s(p)$ — law of electron dispersion in carbon nanotubes, a_{pol} — length of carbon–carbon link in polymers, n_{pol} — concentration of polymer (in absence of polymer we accept $n_{pol} = 0$), n_0 — concentration of electrons in carbon nanotubes.

Integration is carried out within the first Brillouin zone. As a result of decrement of coefficients b_q with growth q in the sum in equation (5) one may be limited to the first fifteen nonvanishing summands and get generalized equation sine–Gordon [21] widely used in applications, but not integrated by inverse scattering method. Expression of dispersion law for polymers is limited to one summand in the sum in equation (5).

In 3D case and with account of transition to cylindrical system of coordinates, equation (5) will be written as

$$A_{tt} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \mathbf{A}}{\partial r} \right) + \frac{\partial^2 \mathbf{A}}{\partial z^2} + \frac{1}{r^2} \frac{\partial^2 \mathbf{A}}{\partial \phi^2}$$

$$+ 4\pi j_1(\mathbf{A}) + 4\pi j_2(\mathbf{A}). \qquad (6)$$

Following discussions in papers [22,23], charge accumulation effect in this system may be neglected.

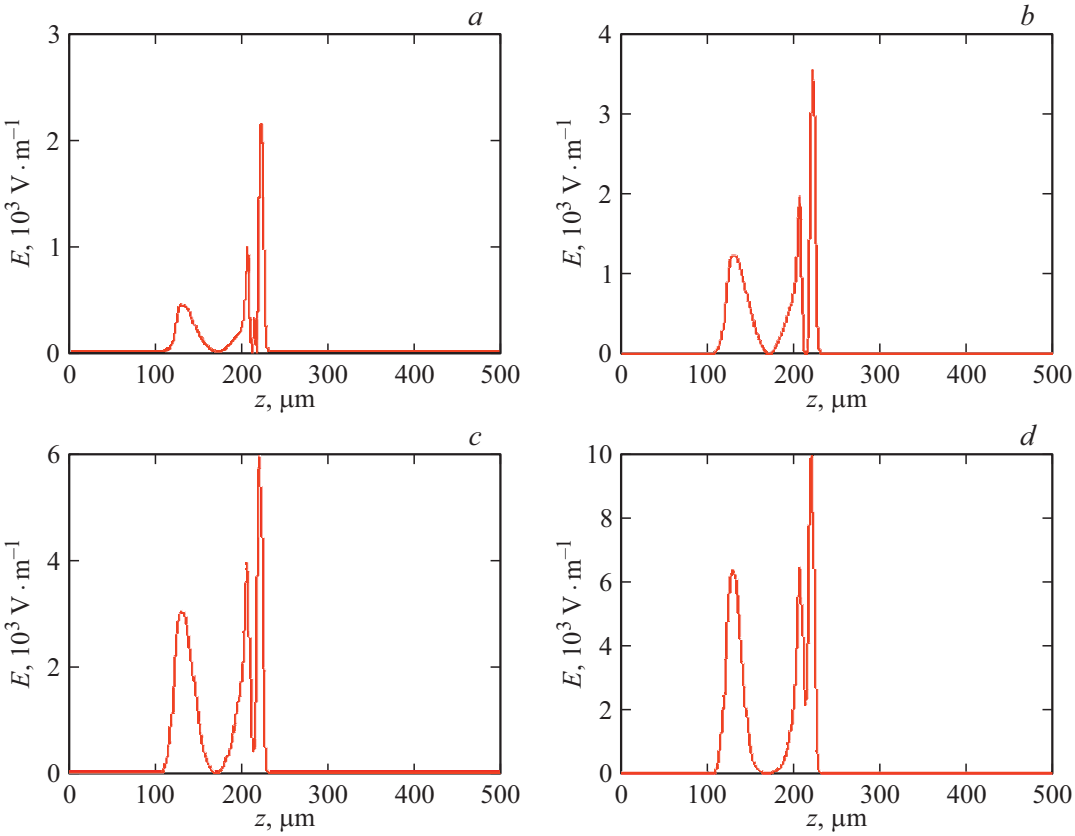

Figure 3. Sections passing through a certain point of the axis z and showing the energy concentrated in the small region near the axis of propagation of the pulse, for different values n_{pol}/n_0: (a) $n_{pol}/n_0 = 1$; (b) $n_{pol}/n_0 = 2$; (c) $n_{pol}/n_0 = 3$; (d) $n_{pol}/n_0 = 4$; $\Phi/\Phi_0 = \pi/2$; $v/c = 0.93$; $t = 6 \cdot 10^{-12}$ s. The axis of ordinates: intensity of the electric component.

Results of the numerical experiment

For numerical solution to equation (6) a method was used, which was based on finite-difference scheme of cross type [24]. Steps by time and coordinate were defined from standard conditions of stability. The difference scheme step was reduced by half in series, until the solution would change in 8-th significant sign. The following initial conditions were chosen for the 3D case:

$$A(z, r, 0) = Q \exp\left(-\frac{(z - z_0)^2}{\gamma_z}\right) \exp\left(-\frac{r^2}{\gamma_r}\right),$$

$$\frac{dA(z, r, 0)}{dt} = 2Q - \frac{(z - z_0)v_z}{\gamma_z} \exp\left(-\frac{(z - z_0)^2}{\gamma_z}\right) \times \exp\left(-\frac{r^2}{\gamma_r}\right). \quad (7)$$

Here Q — pulse amplitude, v_z — initial speed of amplitude in direction z, parameter γ_z sets pulse width in direction z; r — radius, z_0 — initial displacement of pulse center. The evolutionary variable here is time. For numerical modeling the light speed is accepted as one.

Visualization of electromagnetic field propagation in the studied specimen in 3D case is shown in fig. 1.

For more detailed study of the pulse propagation pattern in the system of carbon nanotubes with polymers, sections of electric field intensity were made near the axis z at different moments of time. Fig. 2 shows sections of electric field intensity near the axis z, in other words, these are sections showing pulse energy concentrated in the low region near the axis of pulse propagation and passing through the certain point of the axis z at different moments of time.

From fig. 1 and 2 one can see that first the 3D pulse propagates in the specimen, not changing its shape, then as propagation time increases, it spreads in the specimen and decomposes. Such pulse behavior is explained by impact of non-integrated summands in (5), which cause appearance of a certain tail after the pulse, and its surface area is approximately equal to zero. This may be explained by approximated compliance with the theorem of areas, that is why disturbances added by the non-integrated part of equation (5), do not change the total area under the pulse. Besides, pulse amplitude increase is also noted at long times as a result of electric field dispersion in the environment of carbon nanotubes.

Light field intensity sections near the axis z for various values of polymer concentration in the studied environment are shown in fig. 3.

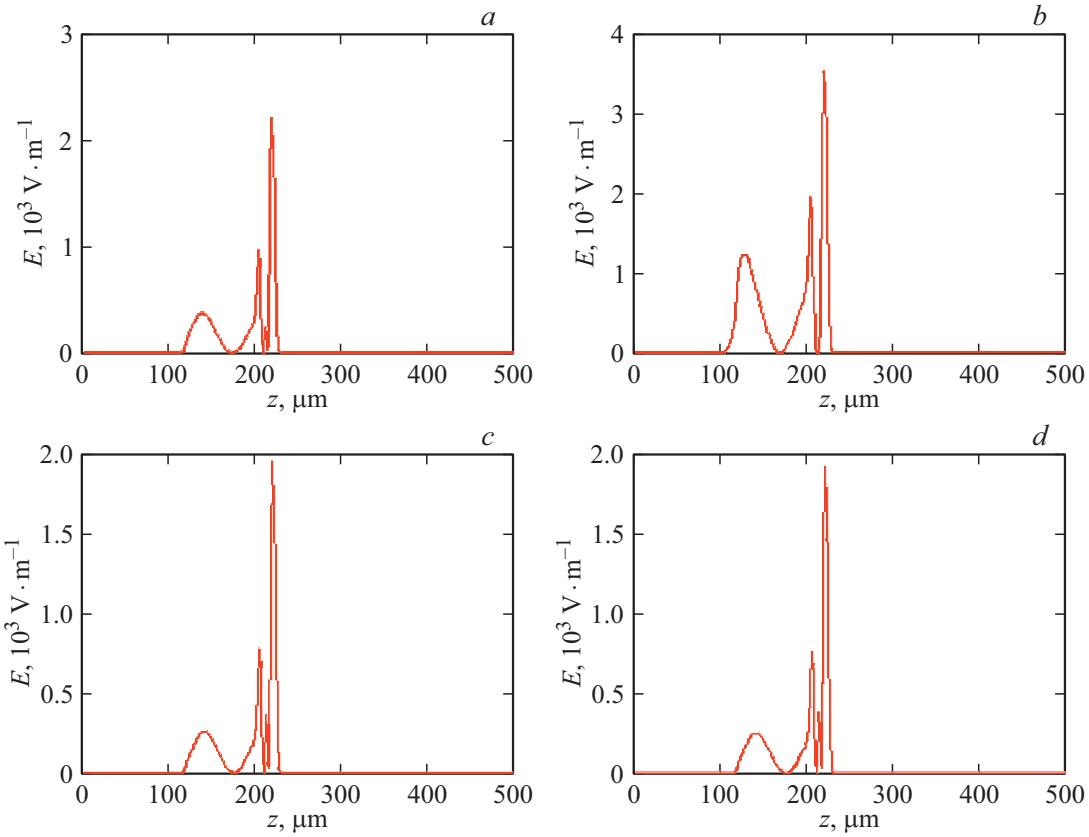

Figure 4. Sections passing through a certain point of the axis z and showing the energy concentrated in the small region near the axis of pulse propagation, for different values of the applied magnetic field: (a) $\Phi/\Phi_0 = \pi/4$; (b) $\Phi/\Phi_0 = \pi/2$; (c) $\Phi/\Phi_0 = 3\pi/4$; (d) $\Phi/\Phi_0 = \pi$; $v/c = 0.93$; $t = 6 \cdot 10^{-12}$ s. The axis of ordinates — intensity of the electric component.

In fig. 3 we see pulse spread, its decomposition into components, and increase of amplitude with changed concentration of polymers. Therefore, we observe that increased polymer concentration causes energy rise not in the pulse front, but in the pulse parts downstream. This may be related to inertia of polymer response and subsequent re-radiation of energy by it.

Fig. 4 shows how permanent magnetic field impacts dynamics of 3D shortest pulse propagation in the system of carbon nanotubes containing polymers.

From presented fig. 4 one can see that pulse energy is concentrated in a limited area, when magnetic field is applied. This fact may be related to achieving balance of electromagnetic field dispersion and non-linearity of the environment containing carbon nanotubes and polymers. Besides, the experiment established numerically that maximum amplitude of the studied pulse is achieved with magnetic field value of $\Phi/\Phi_0 = \pi/2$.

Conclusion

To conclude the completed study, let us word the main conclusions.

1. As time of 3D shortest pulse propagation increases in the specimen made of carbon nanotubes and polymers, the amplitude of this pulse rises, which is caused by electric field dispersion in the environment of carbon nanotubes. This fact makes it possible to use this environment in devices for amplification of such pulses.

2. Nature of pulse propagation to a large extent depends on concentration of polymers that defines the nature of oscillations in „the tail“ and is responsible for energy redistribution among the main pulse and the „reflected one“.

3. Appearance of „the tail“ downstream the shortest pulses may be used in applications to generate terahertz pulses.

4. If external magnetic field value is $\Phi/\Phi_0 = \pi/2$, its impact at propagation of the shortest pulse in the system of carbon nanotubes is most significant.

Conflict of interest

The authors declare that they have no conflict of interest.

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