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Extremely short optical pulses in a thin polymer film with carbon nanotubes

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ABSTRACT In this work, we study the dynamics of electromagnetic radiation in a thin polymer film containing carbon nanotubes. Maxwell's equations are supplemented with a term that takes into account the presence of polymers in the medium. The dependence of the spatial-energy characteristics of the optical pulse on the polymer concentration is revealed.

KEYWORDS optical pulses, polymer film, carbon nanotubes

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1. Introduction

Propagation of multidimensional localized structures in optical and waveguide media is of great interest to researchers from the point of view of both fundamental and applied science [1–5]. The first work on the extremely short pulses propagation in a medium with carbon nanotubes (CNTs) [6] was published in 2006 [7]. Since that time the number of publications on this topic has been steadily growing. Many interesting patterns and effects were discovered. Among them, the stabilizing properties of nanotubes, the influence of external electric and magnetic fields, as well as the acoustic field, are presented. The dependence of the pulse characteristics on the properties of the medium, including the anisotropic optical medium, was analyzed [8, 9].

In the present paper, we study the evolution of an extremely short optical pulse during its scattering on a thin film, which is a composite of a polymer with CNTs [10]. We use previously developed model [11], which was modified taking into account the polymer in the medium.

When the pulse is scattered by a thin film (i.e., with a thickness comparable to the characteristic size of the pulse), there are many new effects. As shown in Ref. [12, 13], even in the case of weak fields, analog of differentiation and integration of the extremely short optical pulse is possible. Of course, it is necessary to generalize such effects to the case of strong fields. We consider this case in the present work.

2. Basic equations

We consider the interaction of an extremely short pulse with a thin polymer film containing semiconductor carbon nanotubes of the zigzag type. We place the film in the path of the pulse in such a way that the electric field of the pulse is directed along the axis of the nanotubes (y-axis). We assume that all nanotubes are oriented in the same way and are located at the same distance from each other, forming a homogeneous bulk. The distances between neighboring nanotubes are large compared to their diameter. This specific assumption allows us to neglect the interaction between CNTs.

It is known that the electron dispersion law for carbon nanotubes of type (m, 0) can be written as [14]:

$$\varepsilon\left(p,s\right)=\pm\gamma_0\sqrt{1+4\cos\left(ap\right)\cos\left(\frac{\pi s}{m}\right)+4\cos^2\left(\frac{\pi s}{m}\right)}, \tag{1}$$

where $\gamma\approx 2.7$ eV, p is the electron quasi-momentum, $a=3b/2\hbar$, $b=0.142$ nm is the distance between adjacent carbon atoms.

The wave equation for vector-potential $\mathbf{A}$ has the following form:

$$\frac{1}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2}=\frac{\partial^2\mathbf{A}}{\partial x^2}+\frac{\partial^2\mathbf{A}}{\partial y^2}+\frac{\partial^2\mathbf{A}}{\partial z^2}+\frac{4\pi}{c}\mathbf{j}\left(\mathbf{A}\right)\Big(\Phi\left(z_0-z\right)-\Phi\left(z_0+h-z\right)\Big), \tag{2}$$

here Φ is the Heaviside function, h is the thickness of the polymer film with CNTs, z_0 is the location of the edge of the thin film from the side of the traveling pulse, $\mathbf{j}$ is the electric current density.

Since the thin film is a composite of a polymer with carbon nanotubes, the current density consists of two components: $\mathbf{j_1}$, $\mathbf{j_2}$ – contributions to the electric current of carbon nanotubes and polymers, respectively.

Let us take into account that the field is directed along the y axis, then the vector potential has the form: $\mathbf{A} = (0, A(x^2 + y^2, z, t), 0)$. The expression for the projection of the current density $\mathbf{j_1}$ onto CNT axis can be written as follows:

$$\begin{aligned} j_1(A) &= -en_0\gamma_0 a \sum_q B_q \sin\left(\frac{aeA}{c}q\right), \\ B_q &= \sum_s \frac{q}{\gamma_0} a_{sq} \int\limits_{BZ} \frac{\exp\left(-\varepsilon(p,s)/k_BT\right)}{1+\exp\left(-\varepsilon(p,s)/k_BT\right)} \cos\left(q\cdot p'\right)\, dp', \end{aligned} \tag{3}$$

where n_0 is the electron concentration in CNT array, $k_B = 1.380649 \cdot 10^{-23}$ J·K^{-1}, T is the temperature, BZ is the first Brillouin zone, a_{sq} are the coefficients of spectrum expansion (1) in the Fourier series. The calculation of the current j_2 is carried out similarly to the calculation of the current for a system of quantum dots with hopping conductivity [15]. This model is described in details and justified in [16].

Finally, the equation for the vector potential of the electric field component takes the following form in the cylindrical coordinate system:

$$\frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial A}{\partial r}\right) + \frac{\partial^2 A}{\partial z^2} + \frac{1}{r^2}\frac{\partial^2 A}{\partial \phi^2} + \frac{4\pi}{c}\Big(j_1(A) + j_2(A)\Big)\Big(\Phi(z_0 - z) - \Phi(z_0 + h - z)\Big). \tag{4}$$

Here (r, z, φ) are the coordinates in the cylindrical system, so that $r^2 = x^2 + y^2$, $\tan\varphi = y/x$.

In the general case, when the extremely short pulse propagates through a CNT array, due to the inhomogeneity of the pulse field, current inhomogeneity may arise. So, it can lead to charge accumulation in some area. However, previous calculations [17] showed that this effect for femtosecond pulses can be neglected. As a result, we can assume that cylindrical symmetry in the field distribution is preserved. Based on this, we believe that, due to the cylindrical symmetry, the derivative with respect to angle is equal to zero. In this case, we obtain an effective equation for the components of the vector potential in the cylindrical coordinate system:

$$\begin{aligned} &\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial A_1}{\partial r}\right) + \frac{\partial^2 A_1}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2 A_1}{\partial t^2} + \frac{4en_0\gamma_0 a}{c}\times \\ &\qquad\times\left[\sum_{q=1}^{\infty} B_q \sin\left(\frac{aeq}{c}A\right) + \chi\cdot\sin\left(\frac{a_{POL}e}{c}A\right)\right]\cdot\Big(\Phi(z_0 - z) - \Phi(z_0 + h - z)\Big) = 0. \end{aligned} \tag{5}$$

Here $\chi \cdot n_0$ is the electron concentration in polymer, a_{POL} is the polymer C–C bond length.

3. Numerical modeling and discussion

To solve the resulting equation (5), we use a cross-type numerical scheme with standard stability conditions [18]. The initial condition is chosen in the Gaussian form:

$$\begin{aligned} A\left(r^2, z, 0\right) &= A_0 \cdot \exp\left(-\frac{z^2}{l_z^2}\right)\exp\left(-\frac{r^2}{l_r^2}\right), \\ \frac{dA\left(r^2, z, 0\right)}{dt} &= 2\cdot u\cdot\frac{z}{l_r^2}\cdot A_0\cdot\exp\left(-\frac{z^2}{l_z^2}\right)\exp\left(-\frac{r^2}{l_r^2}\right). \end{aligned} \tag{6}$$

Here A_0 is the pulse amplitude, l_r, l_z are the pulse width along the directions r and z, correspondingly, u is the initial pulse velocity along z-axis.

The evolution of the pulse is shown in Fig. 1.

Note that the pulse is divided into several peaks of different amplitudes when scattered by a thin polymer film with carbon nanotubes, while maintaining the region of its localization.

The pulse intensity for different film thicknesses h and different initial velocity is shown in Fig. 2. According to Fig. 2, we can conclude that the shape of the extremely short optical pulse is greatly influenced by both the pulse velocity and the thickness of the composite film. Note that the greater the initial pulse velocity, the more local maxima are formed. For a better understanding of what exactly happens to the spatial-energy characteristics of an electromagnetic wave, let us construct slices at $r = 0$, which are shown in Fig. 3.

It can be seen from Fig. 3 that for the initial velocity of the pulse $u = 0.95$, there is a larger number of additional peaks compared to the case of $u = 0.9$. The lower the speed, the longer the pulse interacts with the polymer film and stronger localization is observed. That is, the effects of nonlinearity of the medium act for a longer time and a balance between dispersion and nonlinearity has time to be established, which leads to conservation of the pulse energy in a smaller region of space, i.e. its stabilization. The film thickness has the greatest influence on the pulse intensity.

The dependence of the shape of an extremely short optical pulse on the polymer concentration is shown in Fig. 4.

The polymer concentration in a thin film does not affect the spatial localization of the pulse, but manifests itself in a change in its shape and amplitude.

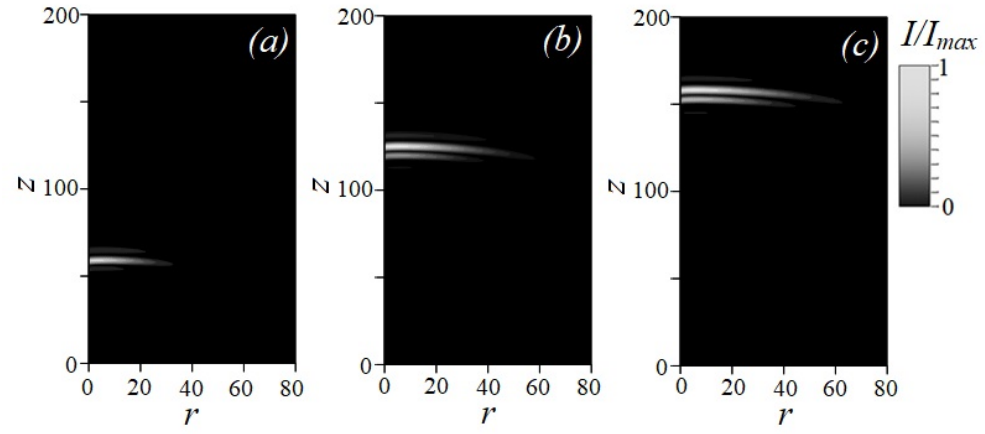

FIG. 1. Dynamics of the pulse propagation after passing through a thin polymer film with CNTs: a) $t = 7$; b) $t = 11$; c) $t = 13$. The film is located between $z = 0$ and $z = 50$. The time unit corresponds to 10^{-13} s, the unit corresponds to coordinates r, z – 1.2 μm. $I_{\max}$ is the maximum intensity value for each moment of time.

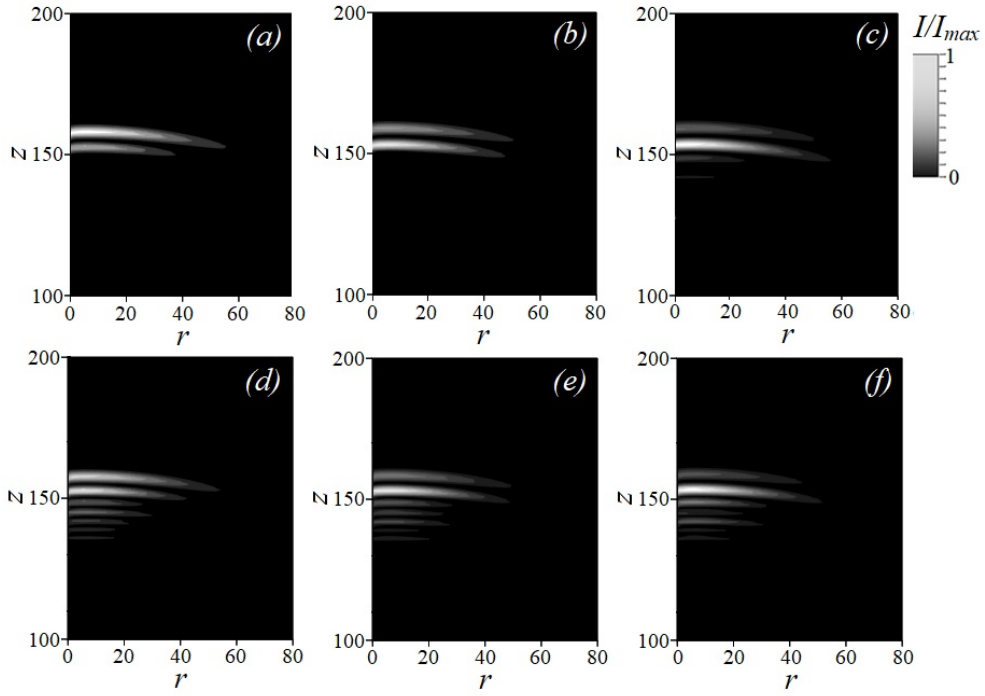

FIG. 2. Pulse intensity after passing through thin polymer film with CNTs at $t = 13$ for different film thickness: (*a, d*) 50; (*b, e*) 80; (*c, f*) 100. The film starts at position $z = 0$. Figures (*a-c*) $u = 0.9$; (*d-f*) $u = 0.95$ (in units of the speed of light). The time unit corresponds to 10^{-13} s, the unit corresponds to coordinates r, z – 1.2 μm. $I_{\max}$ is the maximum intensity value for each row of patterns (for each velocity value).

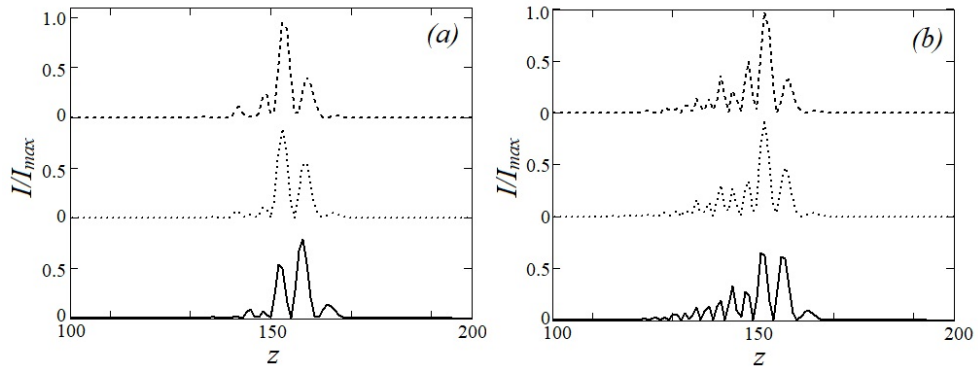

FIG. 3. Pulse intensity after passing through thin polymer film with CNTs at $t = 13$ for different film thickness (slices at $r = 0$): a) $u = 0.9$; b) $u = 0.95$. The solid curve corresponds to $h = 50$; the dotted curve – $h = 80$; the dashed curve – $h = 100$. The film starts at position $z = 0$. The time unit corresponds to 10^{-13} s, the unit along z-axis corresponds to 1.2 μm. $I_{\max}$ is the maximum intensity value for velocity value.

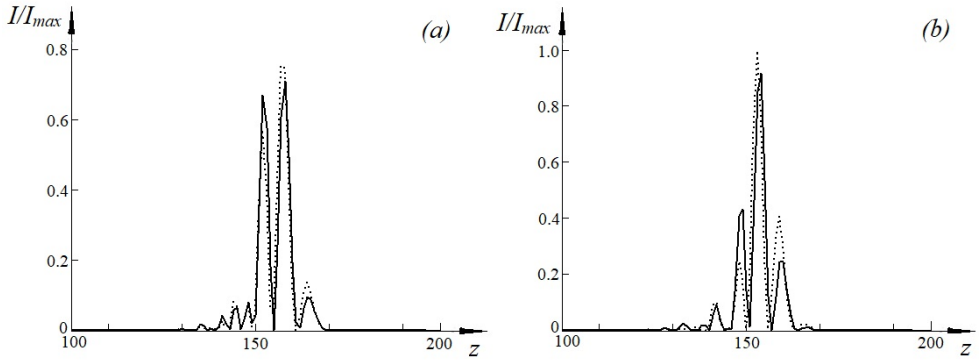

FIG. 4. Pulse intensity after passing through thin polymer film with CNTs at $t = 13$ for different film thickness (slices at $r = 0$, $u = 0.9$): a) $h = 50$; b) $h = 100$. The film starts at position $z = 0$. The solid curved corresponds to $\chi = 0.1$; the dotted curve – $\chi = 0.8$. The time unit corresponds to 10^{-13} s, the unit along z-axis corresponds to 1.2 μm. $I_{\max}$ is the maximum intensity value for all figures.

4. Conclusion

(1) The model for the passage of an extremely short optical pulse through a thin polymer film with carbon nanotubes has been constructed.
(2) The thickness of the polymer film with CNTs allows one to control the shape and intensity of the pulse.
(3) The localization area of an extremely short optical pulse when passing through a polymer film can be controlled using the initial velocity of the pulse.
(4) When a short-duration electromagnetic pulse is scattered by a composite film, the generation of higher harmonics is possible.

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