Optics and Spectroscopy, 2022, Vol. 130, No. 12

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Extremely short pulses in an anisotropic optical medium containing carbon nanotubes with metal conduction

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Received September 14, 2022
Revised September 14, 2022
Accepted September 28, 2022

In this work, we study the interaction of extremely short pulses with a nonlinear anisotropic optical medium with carbon nanotubes (armchair and zigzag type) with metallic conductivity. The dependence of the pulse shape, width, and intensity on the nanotube chirality indices is analyzed. The most appropriate type of carbon nanotubes is substantiated for providing localized propagation of an electromagnetic field in a medium with anisotropic properties.

Keywords: optical anisotropy, extremely short pulse, carbon nanotubes, metallic conduc.

DOI: 10.21883/EOS.2022.12.55246.49-22

Introduction

One of the important problems of nonlinear optics [1] is the study of processes that are associated with the interaction of high-intensity light fields with various materials [2]. It is well known that laser pulses can be controlled by strong external fields (magnetic [3], acoustic [4], electric [5]), as well as by the environment, as such, in which the impulse propagates. Note that as a result of interaction with light, not only the initial properties of matter [6,7] change, but also the characteristics of the electromagnetic pulse itself. Therefore, it is important to use those media whose properties are capable of controlling these characteristics, including having a stabilizing effect on the momentum. From this point of view, media containing carbon nanotubes (CNT) [8] are suitable candidates.

Previously, the authors studied the propagation of extremely short pulses (containing a small number (1-3) of electromagnetic field periods) of various profiles (Gauss, Bessel, Mathieu) in a nonlinear medium with semiconductor-type CNTs [9–11]. The possibility of controlling the localization region of an extremely short optical pulse with the help of parameters of both its initial shape and impurity parameters is shown. The existence of modes of efficient generation for higher harmonics, which are not initially present in the pulse[12], is also demonstrated. Later, the optical anisotropic properties of the medium [13] were taken into account. At the same time, the case of CNTs with metallic conductivity was not considered, which is important from the point of view of applied significance. Note that CNTs of this type do not have a gap in the electron energy spectrum. As a result, there is no division into conduction and valence bands. In the case of „semiconductor CNTs, the low-frequency" part of the wide spectrum of an extremely short pulse causes only a shift in the distribution functions in the valence band (due to - changes in the electron energy in the valence band due to acceleration of the pulse by the electric field). For metallic CNTs, the entire momentum affects all electrons with any (not just in the valence band) energy value.

The existing methods for the synthesis of single-walled CNTs do not allow obtaining CNTs of only a certain conductivity, but some of them make it possible to increase the yield of a given type [14–16], including those with metallic conductivity [17]. Since metal CNTs do not have a band gap, they exhibit a high mobility of charge carriers, as in graphene systems. Note that it is much more difficult to obtain CNTs with metallic properties than those with semiconductor properties. But due to their application in the production of high-performance connecting wires, transparent conductive electrodes, fiber optics, etc. it is important to carry out the controlled growth of CNTs of this type.

Thus, the purpose of this work is to study the influence of the metallic properties of single-walled CNTs placed in an optically anisotropic medium on the characteristics of a three-dimensional electromagnetic pulse as it propagates in such a medium.

Model and basic equations

Consider an array of CNTs immersed in an anisotropic dielectric medium (crystal). The axes of the crystal are aligned with the axes of the Cartesian coordinate system. The CNT axis lies in the XOY plane and forms an angle α with respect to the OX axis. We will investigate the propagation of three-dimensional extremely short electromagnetic pulses in an array of chair-type CNTs (when $m = n$; m and

n i.e. the chirality indices of CNTs), which have metallic properties.

Vector potential is as follows: $\mathbf{A} = \left(A_x(x, y, z, t), A_y(x, y, z, t), 0\right)$, electric current density is $\mathbf{j} = \left(j_x(x, y, z, t),\ j_y(x, y, z, t), 0\right)$.

For non-zero electric field components, let's write the wave equation taking into account the transition to a cylindrical coordinate system:

$$\frac{1}{v_x^2}\frac{\partial^2 A_x}{\partial t^2} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial A_x}{\partial r}\right) + \frac{\partial^2 A_x}{\partial z^2} + \frac{1}{r^2}\frac{\partial^2 A_x}{\partial \phi^2} + \frac{4\pi}{c}\, j_x(A_x, A_y),$$

$$\frac{1}{v_y^2}\frac{\partial^2 A_y}{\partial t^2} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial A_y}{\partial r}\right) + \frac{\partial^2 A_y}{\partial z^2} + \frac{1}{r^2}\frac{\partial^2 A_y}{\partial \phi^2} + \frac{4\pi}{c}\, j_y(A_x, A_y),$$

$$v_x = c/n_x, \quad v_y = c/n_y. \tag{1}$$

r, z, ϕ — coordinates in a cylindrical system, n_x, n_y are the refractive indices in the direction x and y respectively, c is the speed of light. Note that we chose a positive crystal [18] as the dielectric. In our geometry, this means that the condition $v_x > v_y$ is satisfied.

Further, we neglect the derivative with respect to the angle due to the fact that the charge accumulation for pulses of the considered duration can be ignored [19] and, as a consequence, one can speak of the preservation of the cylindrical symmetry of the field distribution.

For nanotubes of the $(n,\ m)$ type, the following periodic conditions can be written at the boundary [20]:

$$\sqrt{3}\, n\, k_x a + m\, k_y a = \mathbf{C}_h \mathbf{k} = 2\pi q, \tag{2}$$

where ma defines the translation operation, $\sqrt{3}\, na$ defines rotation operation, a is lattice constant, q iz integer, k is wave vector, $\mathbf{C}_h$ is chiral vector.

The electron dispersion law for chiral nanotubes has the form [20]

$$\varepsilon_q(\mathbf{k}) = \gamma_0 \sqrt{\begin{array}{c} 1 + 4\cos\left(\frac{q\pi}{n} - \frac{m\mathbf{k}a}{2n}\right)\cos\left(\frac{\mathbf{k}a}{2}\right) + \\ + 4\cos^2\left(\frac{q\pi}{n} - \frac{m\mathbf{k}a}{2n}\right) \end{array}}, \tag{3}$$

where $\gamma_0 = 2.7\,\text{eV}$, $\mathbf{k}a$ belongs to the range $[-\pi, \pi]$, $(n,\ m)$ is determined according to equation (2), $a = 3b/2\hbar$, $b = 0.142\,\text{nm}$. Assuming $n = m$, we obtain the dispersion law for chair-type nanotubes.

Note that we do not take into account interband transitions. Therefore, the appearance of the current is due only to electrons in which the branch of the band structure intersects with the Fermi level, which corresponds to a certain value q.

In the limit of low temperatures, the current can be determined according to the formula, the derivation of which for a one-dimensional problem is given in the work [21],

$$\mathbf{j} = e\int_{-\Delta}^{\Delta}\int_{-\Delta}^{\Delta} d\mathbf{k}\, \frac{\partial \varepsilon_q\left(\mathbf{k} - \frac{e}{c}\mathbf{A}\right)}{\partial \mathbf{k}},$$

$$\begin{cases} j_x(A_x, A_y) = e\,\cos\alpha\Bigg(\varepsilon_q\left(\Delta - \dfrac{e}{c}(A_x\cos\alpha + A_y\sin\alpha)\right) \\ \qquad - \varepsilon_q\left(-\Delta - \dfrac{e}{c}(A_x\cos\alpha + A_y\sin\alpha)\right)\Bigg), \\ j_y(A_x, A_y) = e\,\sin\alpha\Bigg(\varepsilon_q\left(\Delta - \dfrac{e}{c}(A_x\cos\alpha + A_y\sin\alpha)\right) \\ \qquad - \varepsilon_q\left(-\Delta - \dfrac{e}{c}(A_x\cos\alpha + A_y\sin\alpha)\right)\Bigg). \end{cases} \tag{4}$$

The momentum integration region is determined from the condition of equality of the number of particles in it and in the first Brillouin zone. And $\Delta = n_0/2$, n_0 is electron concentration, e is electron charge.

The system of equations (1) taking into account (4) was solved using numerical simulation methods. The initial conditions were chosen in the following form:

$$A_x = U_0 \exp\left(-\left(\frac{z}{l_z}\right)^2\right)\exp\left(-\frac{x^2 + y^2}{l_r^2}\right),$$

$$\frac{d}{dt}A_x = \frac{2v_0 U_0}{l_z^2}\exp\left(-\left(\frac{z}{l_z}\right)^2\right)\exp\left(-\frac{x^2 + y^2}{l_r^2}\right), \tag{5}$$

where U_0 ia pulse amplitude at $t = 0$, l_z, l_r determine the longitudinal and transverse pulse widths, v_0 i- pulse velocity at the initial time along the OZ axis.

Results and discussion

In the future, we will calculate the field intensity, which for two components is determined according to the formulas

$$I_x = \frac{1}{c^2}\left(\frac{\partial A_x}{\partial t}\right)^2, \quad I_y = \frac{1}{c^2}\left(\frac{\partial A_y}{\partial t}\right)^2. \tag{6}$$

The evolutionary pattern the case of chair-type CNTs is shown in Fig. 1.

It can be seen from Fig. 1 that the pulse experiences dispersive spreading, which is related to the allowance for the second field component. Note the division of the main pulse into several pulses that preserve the localization region.

Next, let's make a comparison with the case considered earlier for semiconductor CNTs of the zigzag [22] type, as

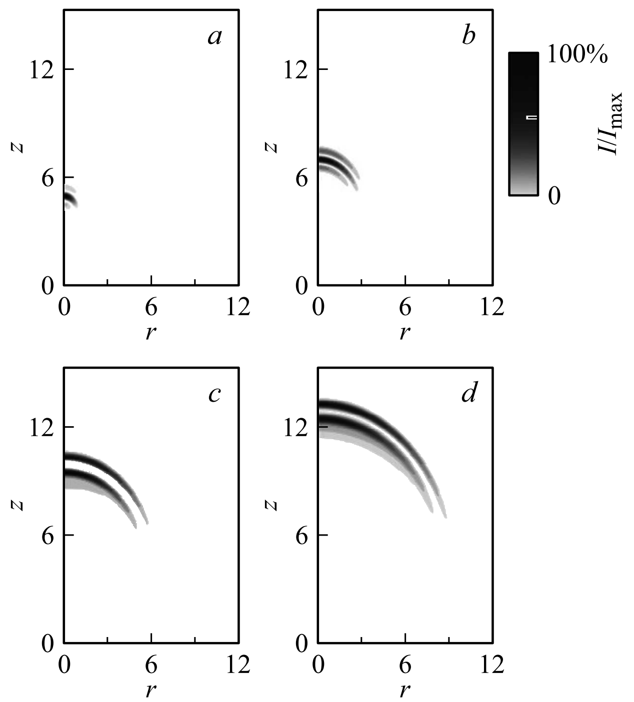

Figure 1. Evolution of the intensity of the x- component of momentum in a medium with CNT (6,6): (a) $t = 1.0$; (b) $t = 4.0$; (c) $t = 7.0$; (d) $t = 9.0$. The unit along the axes r and z corresponds to $2 \cdot 10^{-5}$ m, and along the time is- 10^{-14} s. I_{max} is maximum field intensity.

well as for zigzag tubes with metallic conductivity (n, 0), when n is a multiple of 3 (Fig. 2). To compare metallic CNTs, we choose (6.6) and (9.0) tubes with similar diameters.

It can be seen that the type of achiral CNTs (armchair or zigzag) affects the field strength for both components. Moreover, for zigzag tubes (solid and dashed lines), the intensity is several times higher than for armchair tubes. This is due to the fact that zigzag CNTs at a multiple of n 3 have a very small band gap and are essentially semimetals [23], therefore, they have lower conductivity compared to armchair nanotubes.

Despite the significant growth of the y-component, which was absent at the initial moment of time, it does not exceed the corresponding x-component of the field. It also follows from the figures that the spreading of the pulse in the longitudinal direction for chair-type CNTs is less than for zigzag tubes, for which the appearance of a „tail" behind the main pulse is also observed. Thus, from the point of view of preserving the region in which the extremely short optical pulse is localized, CNTs of the armchair type are more preferable.

The dependence of the transverse pulse width L for the field components x and y is shown in Fig. 3. As the width we consider the distance at which the intensity of the electromagnetic field decreases by 2 times.

It can be seen from Fig. 3 that the excited y-component broadens more (curves *3* and *4*) than the x-component (curves *1* and *2*). In this case, the CNT type does not significantly affect the transverse width pulse.

Conclusion

As a result of the study, the following was established.

1. The intensity and width of the pulse make it possible to judge the degree of influence of the properties (metal or semiconductor) of CNTs contained in an optically anisotropic medium.

2. The use of CNTs of a certain type makes it possible to control the spatial and energy characteristics of an extremely short pulse. In particular, the use of armchair type CNTs makes it possible to obtain a smaller longitudinal pulse width.

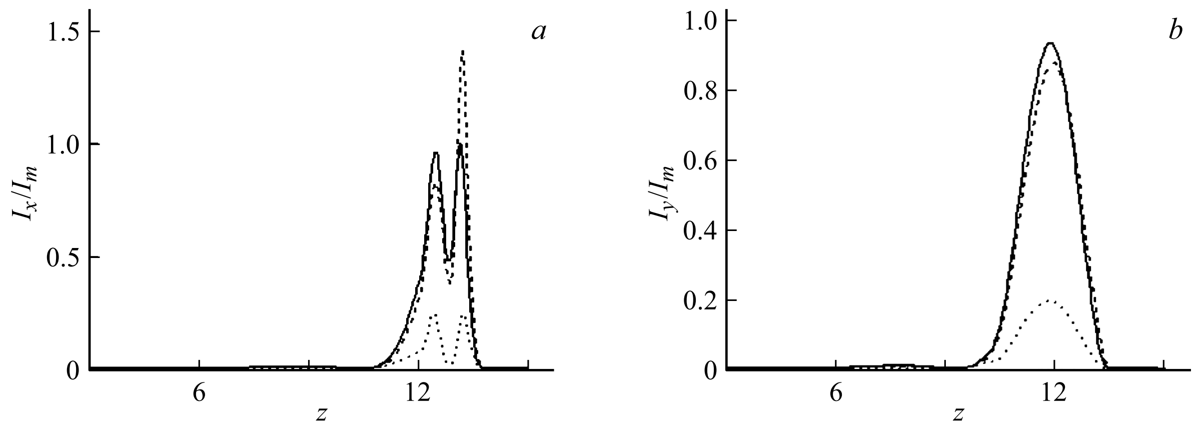

Figure 2. Dependence of the intensity of the electric field of the pulse on the longitudinal coordinate z ($t = 9.0$), slices are presented at $r = 0$: (a) for the x-component of the field, (b) for the y-field component. The solid curve corresponds to CNT (13.0), the dotted line is CNT (6.6), the dashed line is CNT(9.0). I_m -is maximum intensity value of the x- field component for UN (13,0).

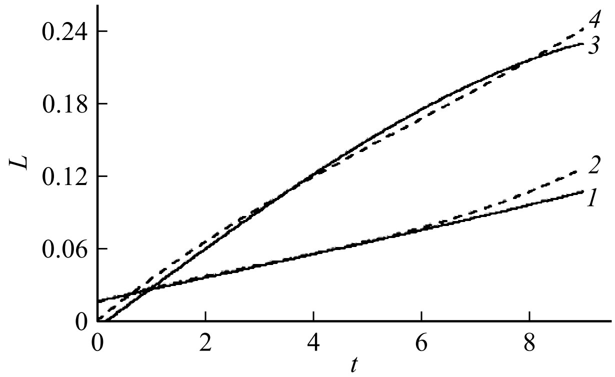

Figure 3. Pulse width versus time: curves *1* and *2* — for the x-field components, curves *3* and *4* — for y-field components. Solid curves correspond to CNTs of the armchair (6.6) type, dashed correspond to CNTs of the zigzag (9.0) type. Unit in time corresponds to 10^{-14} s, in axis L — $2 \cdot 10^{-5}$ m.

3. It is shown that chair CNTs are more promising than zigzag ones for localized pulse propagation in an optically anisotropic medium.

Funding

This work was supported by the Ministry of Education and Science of the Russian Federation, the Council for Grants of the President of the Russian Federation, grant № MD-3173.2021.1.2.

Conflict of interest

The authors declare that they have no conflict of interest.

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