THREE-DIMENSIONAL FEW CYCLE OPTICAL PULSES IN OPTICALLY ANISOTROPIC PHOTONIC CARBON NANOTUBE-BASED CRYSTALS INCLUDING NONLINEAR ABSORPTION

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Abstract. This paper considers the propagation of three-dimensional few cycle optical pulses (light bullets) in an optically anisotropic semiconductor carbon nanotube-based spatially-variable refractive index medium (anisotropic photonic crystal). The nonlinear absorption that is described phenomenologically using experimental data as well as the external exciting field are introduced. The pulse shows stable propagation in such a medium and is keeping its energy localized in a limited area. The photonic crystal characteristics (refractive index modulation period and depth) and anisotropy (different velocity components and angle between pulse electric field and carbon nanotube axis) are shown to impact the three-dimensional few cycle optical pulse dynamics.

Key words: few cycle optical pulses, optically anisotropic photonic crystal, carbon nanotube.

1. INTRODUCTION

The exploratory development of interaction of light with matter is long enough under the radar of a large number of research teams. Development efforts on creating optoelectronic, nanoelectronic, and nanophotonic components for optical devices based on materials with specified properties are of particular interest. Different spatially-variable refractive index media can be successfully used as such substances; for example, photonic crystals in which the photonic band gap makes it possible to consider a photonic crystal as an optical filter that transmits photons of certain frequencies [1, 2]. Variable refractive index provides an ideal nonlinear medium for propagation and investigation of electromagnetic solitons, few cycle optical pulses, and light bullets [3]. Few cycle optical pulses are seen as pulses containing 1-5 oscillations of the electric field with duration of several femtoseconds. What is more, the pulse energy remains concentrated in a limited area [4, 5]. Few cycle pulses have a number of
important advantages, such as high radiation directivity, fixed shape, stability against perturbations of parameters and field peak amplitude achievable at which the waveguide material is not destroyed but the nonlinear properties are already on full display [6–15].

For pulses to propagate steadily in a photonic crystal they must exhibit nonlinear properties. Thus, carbon nanotubes can be used as a proper material. It is widely known that carbon nanotubes have unique structures and properties with the latter varying greatly according to shape and geometry [16–19]. However, the carbon nanotube-based medium produces dissipative effects, and therefore, the compensation, or the so-called energy “pumping” is required. Thus, it becomes relevant to consider dissipative effects that real devices cannot do without them. It follows that the treatment of all these parameters stabilizing and destroying a few cycle pulse is a sophisticated problem. Moreover, introduction of medium anisotropic optical properties as well as pulse propagation control are also very attractive. Considering medium anisotropy can lead to different effects, for example, the Zakharov-Benney resonance [20].

Recent articles [21–23] by our research team deal with the propagation of few cycle optical pulses (light bullets) in a spatially-variable refractive index medium. The propagation of one-, two-, and three-dimensional ultrashort pulses and light bullets in variable refractive index media (photonic crystal, Bragg medium) including induced by external fields [24–26] was considered. However, all the previous studies analyzed only single light polarization (the linear one) when the vector of electric field is parallel to carbon nanotube axis.

This article investigates the impact of factors destroying and stabilizing the pulse (nonlinear absorption and pumping by external field), as well as anisotropy of a carbon nanotube-based photonic crystal including birefringence. For this purpose, the system of equations must be supplemented by the summand for the second-order polarization. Besides, it is necessary to factor in different values of velocity components.

2. PHYSICAL MODEL AND BASIC EQUATIONS

As a rule, investigation of carbon nanotube electron structure is carried out by means of the tight-binding method within the framework of π-electron dynamics analysis. The general equation for dispersion law for semiconducting nanotubes is as follows [27, 28]:

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

where \( \gamma_0 \approx 2.7 \text{ eV} \), \( s = 1, 2, \ldots, m \), \( a \) – lattice constant in carbon nanotubes. Note that \( m \) is the number of hexagons along the nanotube circle.
The geometry of the problem implies that the applied electric field is directed at an angle to the carbon nanotube axis with the pulse moving along OZ axis (Fig. 1). Note that since the typical size of carbon nanotubes and the distance between them are much less than the typical size of spatial domain in which the few cycle pulse is localized, we can use the continuum approximation and consider the current to be volume distributed.

The equation for electric field vector potential of three-dimensional few-cycle optical pulse written in the Coulomb gauge \( E = -\frac{\partial A}{\partial t} \) can be calculated as:

\[
\frac{\partial^2 A}{\partial x^2} + \frac{\partial^2 A}{\partial y^2} + \frac{\partial^2 A}{\partial z^2} - \frac{n^2(x, y, z)}{c^2} \frac{\partial^2 A}{\partial t^2} + \frac{1}{c} \frac{\partial A}{\partial t} + \frac{4\pi}{\varepsilon} j(A) - F_1 \left( \frac{\partial A}{\partial t} \right)^3 - \frac{F_2 \frac{\partial A}{\partial t}}{1 + \Delta \left( \frac{\partial A}{\partial t} \right)} = 0, \tag{2}
\]

where \( n(x, y, z) \) is the medium spatially-variable refractive index, \( c \) is the light speed, \( \Gamma \) is the electric field enhancement factor (without linear absorption) [29]; \( F_1, F_2 \) are the nonlinear absorption coefficients (defined from the experiment) [30]; \( \Delta \) is the saturation parameter for nonlinear absorption. The vector-potential may be written as \( A = (A_x(x, y, z, t), A_y(x, y, z, t), 0) \), and \( j = (j_x(x, y, z, t), j_y(x, y, z, t), 0) \) is the electric current density.

Let us represent the current density as the standard expression [31]:

\[ j = \sigma \left( E_0 + \frac{\partial A}{\partial t} \right), \]

where \( \sigma \) is the electric conductivity.
\[ j = 2e \sum_s \int \nu_s(p) f(p,s)dp, \tag{3} \]

where we introduce the group velocity of electrons: \( \nu_s = \frac{\partial E(p)}{\partial p} \), \( f \) is the electron distribution function, and \( e \) is the electron charge. The integration is performed over the first Brillouin zone.

The equation for the electric field vector-potential components in cylindrical coordinate system with the summand depending on the rotation angle neglected can be written as follows \([32, 33]\):

\[
\begin{align*}
\frac{\partial^2 A_x}{\partial z^2} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial A_x}{\partial r} \right) - \frac{n^2(z,r)}{c^2} \frac{\partial^2 A_x}{\partial t^2} + & \\
+ \frac{4en_0y'sa \cdot \sin \alpha}{c} \sum_{q=1} h_x \cos \left( \frac{aeq(A_x \cos \alpha + A_y \sin \alpha)}{c} \right) \frac{aeq}{c} \cdot \phi(t) + & \\
+ \frac{\Gamma}{c} \frac{\partial A_x}{\partial t} - F_1 \left( \frac{\partial A_x}{\partial t} \right)^3 \frac{F_2}{1 + \Delta \left( \frac{\partial A_x}{\partial t} \right)} = 0, & \\
\frac{\partial^2 A_y}{\partial z^2} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial A_y}{\partial r} \right) - \frac{n^2(z,r)}{c^2} \frac{\partial^2 A_y}{\partial t^2} + & \\
+ \frac{4en_0y'sa \cdot \sin \alpha}{c} \sum_{q=1} h_y \cos \left( \frac{aeq(A_x \cos \alpha + A_y \sin \alpha)}{c} \right) \frac{aeq}{c} \cdot \phi(t) + & \\
+ \frac{\Gamma}{c} \frac{\partial A_y}{\partial t} - F_1 \left( \frac{\partial A_y}{\partial t} \right)^3 \frac{F_2}{1 + \Delta \left( \frac{\partial A_y}{\partial t} \right)} = 0, & \\
r = \sqrt{x^2 + y^2}, & \\
h_y = \sum_{q=1} \frac{\exp \left\{ \frac{-\varepsilon_s(p)}{k_B T} \right\}}{2n} \frac{\exp \left[ \frac{-\varepsilon_s(p)}{k_B T} \right]}{1 + \exp \left[ \frac{-\varepsilon_s(p)}{k_B T} \right]} dp,
\end{align*}
\tag{4} \]

where \( n_0 \) is the electron density; \( a_{sq} \) are the Fourier series expansion coefficients of the electron dispersion law \([34]\); \( k_B \) is the Boltzmann constant; \( T \) is the temperature.
The summand \( \varphi(t) \) is the empirical correction for current density in both collisionless and relaxation time approximations [35]. Note that the derivation of the basic equations is the same as that in Refs. [32, 33] excluding the fact that the electrons of carbon nanotubes are exposed to the sum of electrical field projections onto the nanotube axis that lie along \( x \) and \( y \) axes of medium. In this case, it is this electric field that changes the electron quasi momentum. Therefore, the current generated in carbon nanotube should be factored in as current summand in relevant Maxwell equations for \( x \) and \( y \) components of electric field. Projecting the occurring current onto axes, then we get the equations written above.

Since the few cycle pulse field is heterogeneous when propagating in carbon nanotube-based photonic crystal, there may be a heterogeneous current and it can lead the charge to accumulate in some region. However, earlier calculations [36] have shown that the charge-storage effect for femtosecond pulses can be neglected. As a consequence, it can be considered that a cylindrical symmetry is retained in the field distribution and therefore the derivative with respect to the angle can be neglected. It should be noted that as coefficients \( b_q \) decrease with the increase in \( q \) we can factor in as few as the first fifteen nonvanishing summands [37] and we obtain the generalized sin-Gordon equation [15].

The initial conditions for the electric field vector-potential of the three-dimensional few cycle optical pulse (5) and of the refractive index of optically anisotropic photonic crystal (6) are as follows:

\[
A_{1, k=0} = A_{0 x} \cdot \exp\left(-\frac{r^2}{\gamma_r^2}\right) \cdot \exp\left(-\frac{z^2}{\gamma_z^2}\right);
\]

\[
\frac{dA_x}{dt}\bigg|_{t=0} = A_{0 x} \cdot \frac{2uz}{\gamma_z^2} \cdot \exp\left(-\frac{r^2}{\gamma_r^2}\right) \cdot \exp\left(-\frac{z^2}{\gamma_z^2}\right); \tag{5}
\]

\[
A_y|_{t=0} = 0; \quad \frac{dA_y}{dt}|_{t=0} = 0.
\]

\[
n(z, r) = 1 + \mu \cos\left(\frac{2\pi z}{\chi}\right), \tag{6}
\]

where \( \gamma_z, \gamma_r \) are the parameters determining the pulse width along \( z \) and \( r \) axes, respectively, \( t_0 \) is the initial time, \( u \) is the initial pulse velocity when entering the medium, \( \mu \) is the refractive index modulation depth, and \( \chi \) is the refractive index modulation period.
3. NUMERICAL SIMULATION RESULTS

The equation under investigation (4) was numerically solved with the Standard Leapfrog explicit difference scheme [38]. The investigated system parameters in the process of numerical simulation were selected as follows [33]: \( m = 13 \) is the number of hexagons along the nanotube perimeter, \( T = 293 \text{ K} \), the relaxation time in carbon nanotube is approximately equal to \( 10^{-11} \text{ s} \), the pulse duration is about \( 10^{-14} \text{ s} \), and \( F_1 = F_2 = 0.01 \) are the nonlinear absorption coefficients.

The evolution of electromagnetic field pulse propagating in optically anisotropic carbon nanotube-based photonic crystal with nonlinear absorption and amplification factored in is represented in Fig. 2 with the values of optically anisotropic photonic crystal parameters (\( \mu = 0.25 \) is the refractive index modulation depth, \( \chi = 2.5 \text{ } \mu\text{m} \) is the refractive index modulation period), the values of anisotropic parameters (\( \alpha = \pi/3 \) is the angle between the carbon nanotube axis and the electric field vector of the pulse, \( v_x/c = 0.9, \ v_y/c = 0.5 \) are the pulse velocities along crystallographic axes).

Figure 2 shows that the pulse keeps its energy localized in a limited area. The change in pulse amplitude does not exceed 10\%, but its shape is modified. After the pulse passes through the medium electric oscillations appear. Thus, we can say that there is a stable propagation of the pulse and a balance between factors that stabilize (pumping by external field, photonic crystal nonlinearity) and destruct the pulse (nonlinear absorption, dispersion and diffraction spreading). The dispersion spreading along the sample axis is neutralized by carbon nanotube medium nonlinearity due to the non-parabolic dispersion law for electrons localized at conduction band.

Figure 3 below shows the Fourier spectra for amplitude and intensity of the three-dimensional few cycle optical pulse in an anisotropic photonic crystal. The values of parameters are similar to those set for Fig. 2.

One relative unit in Fig. 3 is equal to the frequency at which the maximum of the Fourier spectrum of the pulse is halved at the initial moment of time.

The problem under consideration is strongly nonlinear for two reasons: the first one is the carbon nanotube system response nonlinearity and the second reason is the absorption coefficient nonlinearity. This is most pronounced at the spectrum evolution. Figure 3 shows that first the spectrum is enriched due to interaction with the varying refractive index medium and then the higher harmonics are effectively generated. Note that we can observe harmonics higher than the third one as well. This makes such systems most advanced in constructing wide-spectrum pulse generation devices.

Figure 4 shows the dependence of the pulse on parameters of anisotropic carbon nanotube-based photonic crystal (depth and period of refractive index modulation). The point of time for which the comparison is made at is 10 ps.
Fig. 2 – a) Dynamics of three-dimensional few cycle optical pulse in anisotropic carbon nanotube-based photonic crystal at fixed points of time: 5, 10, and 15 ps; b) longitudinal shears of the pulse under $r = 0$.

Fig. 3 – Fourier spectra of three-dimensional few cycle optical pulses in anisotropic photonic crystal at fixed points of time: 5, 10, and 15 ps.
The increase in refractive index parameters of anisotropic carbon nanotube-based photonic crystal influences primarily the group velocity of the pulse wave packet and the shape thereof. As the modulation period increases, the pulse speed increases due to reduced interference processes in photonic crystal sites (Fig. 4B). Thus, it appears possible to control the pulse velocity by varying the refractive index parameters of the carbon nanotube-based photonic crystal, which is a relevant result applicable in practice. In contrast, the refractive index modulation depth has a significant impact on the shape of few cycle optical pulse and its amplitude, which decreases with increase in $\mu$ (Fig. 4A). The derived results have been repeatedly proved by the authors in earlier researches [25, 26].

Fig. 4 – The longitudinal shears of three-dimensional few cycle optical pulse in optically anisotropic carbon nanotube-based photonic crystal at different values of the photonic crystal parameters under $r = 0$: A) at refractive index modulation depth equal 0.25, 0.5, 0.75; B) at refractive index modulation period equal 5, 7.5, 10 $\mu$m.
Figure 5 shows the influence of optical anisotropic photonic crystal (positive or negative) on the pulse propagation dynamics.

It should be noted that the photonic crystal type has a great impact on the group velocity of the pulse wave packet. This follows from the fact that in the case of positive crystal ($v_x > v_y$, Fig. 5 (top, left panel)) the pulse propagates faster than in the case of negative crystal ($v_x < v_y$, Fig. 5 (top, right panel)).

Fig. 5 – Coordinate dependence of three-dimensional electric field $E_x$ for the point of time 10 ps: positive crystal (top, left panel), negative crystal (top, right panel); the longitudinal section under $r = 0$ (bottom panel).
4. CONCLUSIONS

The following conclusions can be drawn from the investigation of three-dimensional few cycle optical pulse evolution in optically anisotropic carbon nanotube-based photonic crystal with nonlinear absorbing and pumping by external electric field factored in:

1. The three-dimensional few cycle optical pulse propagates steadily in optically anisotropic carbon nanotube-based photonic crystal under the influence of nonlinear absorbing and pumping by external electric field. The shape of the pulse undergoes minor changes; after it passes, a tail area is formed.

2. The anisotropic photonic crystal refractive index modulation period and depth have an impact on the shape and group velocity of few cycle optical pulses.

3. It was found that the type of carbon nanotube-based photonic crystal (either positive or negative) has a strong effect on both the group velocity of the pulse wave packet and its shape.

The listed statements are of great practical importance since it becomes possible to control both shape and speed and reduce the region of pulse energy localization, i.e., to stabilize the pulse.

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