Optik 157 (2018) 521–524

Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.de/ijleo

Original research article

Three-dimensional extremely short optical pulses in the carbon nanotubes medium with polymers

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ARTICLE INFO

Article history:
Received 11 October 2017
Accepted 20 November 2017

Keywords:
Carbon nanotube
Polymers
Extremely short optical pulses

ABSTRACT

In this work, we study the propagation of electromagnetic waves in "zig-zag" carbon nanotubes (CNTs) with polymers. The extremely short optical pulse is selected in the form of two oscillations of the electric field. Based on the Maxwell's equations, the effective equation for the vector potential of the electromagnetic field is obtained. The dependence of the pulse shape on the polymer's concentration is analyzed.

1. Introduction

In recent years, the number of works in the field of extremely short optical pulses (ESOPs) in various media has increased. This is due to the practical applications of these pulses [1–5]. ESOPs are usually called pulses containing 1–3 periods of the electromagnetic field. Such pulses that are localized while retaining their spatiotemporal shape are referred to as "light bullets" [6,7].

At the same time, a huge breakthrough in the physics of nanostructures constantly creates the prerequisites for the discovery of new objects for using from this point of view. One of such objects is carbon nanotube (CNT), whose nonlinear properties have long been intensively studied [8]. Carbon nanotubes are long cylindrical structures ranging in diameter from one to several tens of nanometers and up to several centimeters in length, consisting of one or multiple rolled layers (concentric tubes) of graphene. It is well known, that CNTs are of different types (chiral, "arm-chair", and "zig-zag"). Moreover, the chiral nanotubes in terms of the numbers denoting a variety of ways of graphene sheet rolling into CNT can be either semiconducting or metallic.

The features of the propagation of electromagnetic waves from a small number of oscillations in carbon nanotubes of the "zig-zag" type have been studied in the following works [9–11], where the possibility of the existence of electromagnetic solitons and the dependence of their characteristics on the parameters of CNTs are predicted theoretically. A way beyond the one-dimensional approximation was carried out in [12–14]. The calculations show that there is a possibility for the propagation of stable two-dimensional extremely short pulses, not only through an array of CNTs, but also through a similar array immersed into a Bragg medium with a spatially and periodically varying refractive index.

At the same time, questions related to the peculiarities of the propagation of ESOPs in the array of CNTs with polymers remained outside the scope of the review. These issues are relevant from the point of view of practical applications and require theoretical study. An alliance with CNTs provides new properties of polymer molecules [15,16].

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https://doi.org/10.1016/j.ijleo.2017.11.133
0030-4026/

2. Basic equations and main results

We considered propagation of electromagnetic pulses in array of carbon nanotubes with polymers, wherein the pulse electrical field and the current are along the nanotube axis.

As a rule, the investigation of CNT electron structure is performed in tight-binding simulation within the constraints of the π-electron dynamics analysis. The radius of CNT is considered to be much less than characteristic size of the "light bullet" that allows to neglect the spatial heterogeneity of field in nanotubes. The general dispersion relation for the "zig-zag" (*m*,0) nanotube structure has the following form [17]:

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

where $\gamma_0 \approx 2.7$ eV is the hopping integral, $a = 3b/2\hbar$, $b = 0.142$ nm is a distance between neighboring carbon atoms, (*p*,*s*) is the quasi-momentum, s = 1,2,. . .,*m*.

According to the quantum mechanics rules, in the presence of an external electric field: $E = -\partial A/c\partial t$, pulse should be replaced on the generalized pulse: $p \to p\text{-}eA/c$ (e is the electron charge, c is the light velocity).

The Maxwell's equations in two-dimensional case can be written as [18]:

$$\frac{\partial^2 A}{\partial x^2} + \frac{\partial^2 A}{\partial y^2} - \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} + \frac{4\pi}{c}j_1 + \chi\frac{4\pi}{c}j_2 = 0 \tag{2}$$

here $\boldsymbol{A}$ is the vector-potential of the electric field, $\boldsymbol{j}_1$ and $\boldsymbol{j}_2$ are the contributions to the electric current of carbon nanotubes and polymers, respectively. The factor χ is concentration of the polymers. When there are not polymers − χ=0.

Let us write the standard expression for the density of current:

$$j = e\sum_{ps\sigma} v_s(p - \frac{e}{c}A(t))\langle C^+_{ps\omega}C_{ps\sigma}\rangle, \tag{3}$$

where $v_s(p) = \partial\varepsilon_s(p)/\partial p$, where the brackets denote averaging with the non-equilibrium density matrix ρ(*t*): <*B*> = *Sp*(*B*(0) ρ(*t*). C$^+$, C are the birth/annihilation operators. After expanding $\varepsilon_s(p)$ into Fourier series and summing up with respect to *s* and *p* we obtain an effective equation for the vector-potential:

$$\begin{aligned}
&\frac{\partial^2 A}{\partial x^2} + \frac{\partial^2 A}{\partial y^2} - \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} + \frac{4en_0}{c}\sum_{q=1}^{\infty} qb_q sin\left(\frac{qaeA}{c}\right) + \frac{4en_0\chi}{c}sin(a_{pol}eA/c) = 0\\
&b_q = \sum_s a_{sq}\int dpcos(apq)\frac{exp(-\varepsilon_s(p)/kT)}{1 + exp(-\varepsilon_s(p)/kT)}
\end{aligned} \tag{4}$$

here a_{pol} is the carbon–carbon bond length in polymers, n_0 is the electron concentration in CNTs, and χn_0 is the electron concentration in polymers. Due to the decrease of the coefficients b_q with increasing *q* in the sum, the first 15 non-vanishing terms can be limited in Eq. (5), and the double sine-Gordon equation [19] widely used in applications but not integrable by the inverse scattering method is obtained. For polymers, the dispersion law is limited to one term in the sum (4).

It three-dimensional case in cylindrical system, Eq. (2) can be written as:

$$A_{tt} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial A}{\partial r}\right) + \frac{\partial^2 A}{\partial z^2} + \frac{1}{r^2}\frac{\partial^2 A}{\partial\varphi^2} + 4e\pi n_0\sum_{k=1}^{\infty} kB_k sin\left(\frac{kaeA}{c}\right) + 4e\pi n_0\chi sin(a_{pol}eA/c) = 0 \tag{5}$$

According to the arguments from [20], we can conclude that the effect of charge accumulation in a given system can be neglected.

Eqs. (2) and (5) were solved numerically using the direct difference scheme "cross-type". [21]. Time and coordinate steps were determined from the standard stability conditions. Difference scheme steps where iteratively decreased twice until the solution be came unchanged in the eighth decimal place. The initial condition for 2D (6a) and 3d case (6b) have the form:

$$\begin{aligned}
&A(y,0) = Q\cdot exp\left(-y^2/\gamma_y\right) exp\left(-x^2/\gamma_x\right),\\
&\frac{dA(y,0)}{dt} = \frac{2yv_y}{\gamma_y}Qexp\left(-y^2/\gamma_y\right) exp\left(-x^2/\gamma_x\right)
\end{aligned} \tag{6a}$$

$$\begin{aligned}
&A(z,r,0) = Q\cdot exp\left(-(z-z_0)^2/\gamma_z\right) exp\left(-r^2/\gamma_r\right)\\
&\frac{dA(z,r,0)}{dt} = 2Q\frac{(z-z_0)\,v_z}{\gamma_z}exp\left(-(z-z_0)^2/\gamma_z\right) exp\left(-r^2/\gamma_r\right)
\end{aligned} \tag{6b}$$

here *Q* is the pulse amplitude, v_l is the pulse initial velocity directed along *l*, γ_l determines the pulse width along *l*; *r* is the radius, z_0 is the initial coordinate of the pulse center.

The evolution of the electromagnetic field during its propagation through each sample in 2D case is shown in Fig. 1.