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Original article

Two-dimensional non-topological solutions of Maxwell's equations in a medium of strained carbon nanotubes with impurities

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ABSTRACT In this work, we investigate the few-cycle optical pulses with Gauss and Bessel profile in strained carbon nanotubes with impurities. We consider a multi-level impurity in which the energy levels are well separated from the conduction and valence bands of carbon nanotubes. The effect of the impurity parameters on the electromagnetic pulse is analyzed. Also, we investigate the influence of the value of the mechanical stretching on the few-cycle pulse shape.

KEYWORDS carbon nanotubes, impurities, mechanical tension, few-cycle pulse

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1. Introduction

Few-cycle optical pulses have a great practical potential in the development of nonlinear optics devices [1, 2]. Such pulses include those that contain only a few oscillations of the electromagnetic field. Pulses with Gaussian [3] and Bessel [4] cross sections are of great interest. The first (Gaussian beam) is most commonly used in lasers. The second has a number of unusual properties, one of which is diffractionlessness [5].

Note that the medium in which pulse propagates has a great influence on its behavior. From this point of view, media containing carbon nanotubes [6] are very attractive due to their stabilizing effect, including on pulses with the Bessel cross section [7]. It should be said, that the presence of impurities in CNTs has a significant effect on the pulse evolution, which is shown in many works [8, 9]. There are several models for accounting for the impurities. The simplest of them is the Anderson model [10], which takes into account only the hybridization of electronic subsystems. Another is the strong electron-electron model [11], in which the Fermi velocity depends on the electron energy in a logarithmic manner. And, the third model considered in this work is the multi-level impurity model [12], in which transitions between the CNT conduction band and impurity levels are possible.

At the same time, the question related to the influence of a strong acoustic field remains unexplored. In Ref. [13] the authors study the effect of external deformations in the one-dimensional case. In this work, we study the dynamics of 2D few-cycle optical pulse in a dielectric medium with impurity CNTs under the action of an acoustic field.

2. Model and basic equations

The electron spectrum for zigzag carbon nanotubes $(n, 0)$, taking into account the impurity $\varepsilon_{imp}(p, s)$, has the following form [12]:

$$\begin{gathered}\varepsilon_{imp}(p,s) = 0.5\left(R + Q + \sqrt{(R-Q)^2 - 4\left(2D\cdot\Delta(p,s) - \Delta(p,s)^2 - D^2\right)}\right),\\ R = -\sum_{j=1}^{4}\frac{|\alpha_{1,j}|^2}{W_j},\quad Q = -\sum_{j=1}^{4}\frac{|\alpha_{2,j}|^2}{W_j},\quad D = \sum_{j=1}^{4}\frac{\alpha_{1,j}\alpha_{2,j}^*}{W_j}.\end{gathered} \tag{1}$$

Here R, Q determine the transitions of an electron between impurity levels and sublattices of nanotubes, D describes interlattice transitions in CNTs, W_j is the energy of an electron localized at the j-th impurity level, $\alpha_{i,j}$ is the quantity equals to the hopping integral related to the concentration of impurities between the site of the sublattice of the nanotube i and the impurity level j. We restrict ourselves to the consideration of four levels, since, as the level number increases, its contribution to the impurity parameters decreases. $\Delta(p,s)$ is the dispersion law for electrons of carbon nanotubes in the absence of impurity [14]:

$$\Delta\left(p,s\right)=\gamma\sqrt{1+4\cos\left(ap\right)\cos\left(\frac{\pi}{n}s\right)+4\cos^{2}\left(\frac{\pi}{n}s\right)}, \tag{2}$$

where $\gamma\approx 2$ eV, $a=3b/2\hbar$, $b=0.142$ nm is the distance between neighboring atoms in carbon nanotube with quasi-momentum (p,s), and p is the momentum component along the CNT axis, $s=0,..,n$.

Due to the distance between CNTs exceeds their diameter is about in 10 times, we can neglect the interaction between the tubes. We consider the geometry of our problem, in which the wave vector is perpendicular to the CNT array and the electric field strength vector $\mathbf{E}$ is co-directional the nanotube axis.

The acoustic field is due to the stress field, which appears due to the deformation field. It can be taken into account in the framework of the gauge theory. This field is determined by the vector potential $\mathbf{A}'$, which changes the momentum of electrons in a medium containing an array of carbon nanotubes. All interatomic bonds in CNTs under stress are nonequivalent; therefore, the neighboring hopping integrals may not coincide. We can consider CNTs as a rolled sheet of graphene and write down all the equations for it. Further, we should write the periodic boundary conditions. Then, the gauge vector potential has the form: $\mathbf{A}'=(A'_z,A'_x)$ [15]:

$$\begin{aligned}A'_x&=\frac{(\gamma_2+\gamma_3-2\gamma_1)}{2},\\ A'_z&=\frac{\sqrt{3}\,(\gamma_3-\gamma_2)}{2},\end{aligned} \tag{3}$$

where $\gamma_{1,2,3}$ is the modulation of hopping integrals due to displacements of carbon atoms.

The contributions of the electromagnetic field and lattice deformations are reduced to the sum of the corresponding vector potentials (the electromagnetic field of the pulse and the gauge) [16]:

$$\begin{gathered}\frac{\partial^2 A}{\partial x^2}+\frac{\partial^2 A}{\partial z^2}-\frac{\varepsilon}{c^2}\frac{\partial^2 A}{\partial t^2}+4\pi j\left(A+A'/e\right)=0,\\ A'=\chi\frac{\beta\gamma u_{zz}}{a}\cdot(1+\mu),\end{gathered} \tag{4}$$

where ε is the dielectric constant of the medium, β is the electronic Gruneisen parameter, which determines the change in the frequency of lattice vibrations with a change in the volume of the system [17] (for CNT we can take $\beta\approx 2$), $\mu=0.19$ is the Poisson's coefficient for carbon nanotubes [18], χ is the parameter depending on the characteristics of the chemical bond in the substance, which can be set for CNTs equal to 1, u_{zz} is the longitudinal component of the strain tensor, j is the current density, which is determined as:

$$j=2e\sum_{s=1}^{n}\int\limits_{BZ}v\left(p,s\right)\cdot f\left(p,s\right)dp, \tag{5}$$

where e is the electron charge, $v\left(p,s\right)=\partial\varepsilon_{imp}\left(p,s\right)/\partial p$, $f(p,s)$ is the Fermi distribution function, BZ means integration over the first Brillouin zone. Carrying out standard calculations of the current density for CNTs, we obtain the effective equation for the vector potential of the electric field:

$$\begin{aligned}&\frac{\partial^2 A}{\partial x^2}+\frac{\partial^2 A}{\partial z^2}-\frac{\varepsilon}{c^2}\frac{\partial^2 A}{\partial t^2}+\frac{4en_0\gamma_0 a}{c}\sum_{q=1}^{\infty}b_q\sin\left(\frac{aq\left(eA+A'\right)}{c}\right)=0,\\ &b_q=\frac{1}{N_F}\sum_s a_{sq}\int\limits_{BZ}dp\cdot\cos\left(pq\right)\frac{\exp\left(-\varepsilon_{imp}\left(p,s\right)/k_BT\right)}{1+\exp\left(-\varepsilon_{imp}\left(p,s\right)/k_BT\right)},\\ &a_{sq}=\int\limits_{BZ}dp\cdot\cos\left(pq\right)\cdot\varepsilon_{imp}\left(p,s\right),\end{aligned} \tag{6}$$

where n_0 is the electron concentration, k_B is the Boltzmann constant, T is the temperature, a_{sq} are the coefficients in the expansion of the electron dispersion law (1) in a Fourier series, N_F is the normalization constant for the Fermi distribution.

The initial condition with a Gaussian (7a) and a Bessel (7b) transverse profile is chosen in the following form:

$$\begin{aligned}A\left(x,z,0\right)&=Q_0\cdot\exp\left(-\frac{x^2}{l_x^2}-\frac{z^2}{l_z^2}\right),\\ \frac{dA\left(x,z,0\right)}{dt}&=\frac{2\cdot z\cdot v\cdot Q_0}{l_z^2}\cdot\exp\left(-\frac{x^2}{l_x^2}-\frac{z^2}{l_z^2}\right),\end{aligned} \tag{7a}$$

$$A(x,z,0) = Q_0 \cdot \exp\left(-\frac{z^2}{l_z^2}\right)\exp\left(-\frac{x}{l}\right),$$
$$\frac{dA(x,z,0)}{dt} = \frac{2\cdot z\cdot \upsilon\cdot Q_0}{l_z^2}\cdot J_0\left(\left|\frac{x}{l_x}\right|\right)\exp\left(-\frac{z^2}{l_z^2}\right)\exp\left(-\frac{x}{l}\right), \quad (7b)$$

where Q_0 is the initial amplitude of the electromagnetic pulse, l_x, l_z is the width of the pulse along the x and z-axis, υ is the pulse velocity along OZ, l is the cutoff parameter for Bessel function. All values are given here already in dimensionless form.

3. Main results and discussion

Equation (6) is solved numerically [19] with the following system parameters: CNT of the "zigzag" type $(7,0)$, $\varepsilon = 4$, $T = 293$ K, $\upsilon = 0.9$ (in units of the light speed).

The evolution of the electromagnetic field during its propagation in a medium with impurity carbon nanotubes under the action of an acoustic field is shown in Figs. 1 and 2 for the Gaussian and Bessel profiles, respectively.

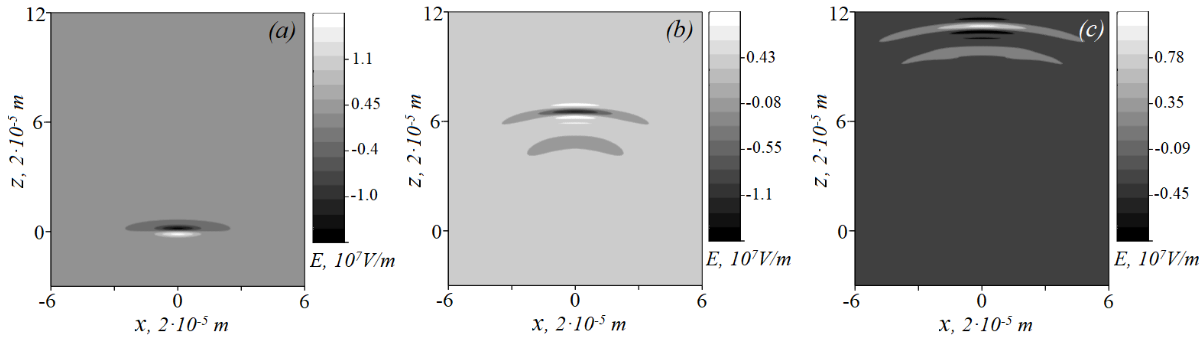

FIG. 1. Pulse evolution with a Gaussian profile ($u_{zz} = 0.1$): a) $t = 0$; b) $t = 7$; c) $t = 12$. The time unit corresponds to $2\cdot 10^{-14}$ s

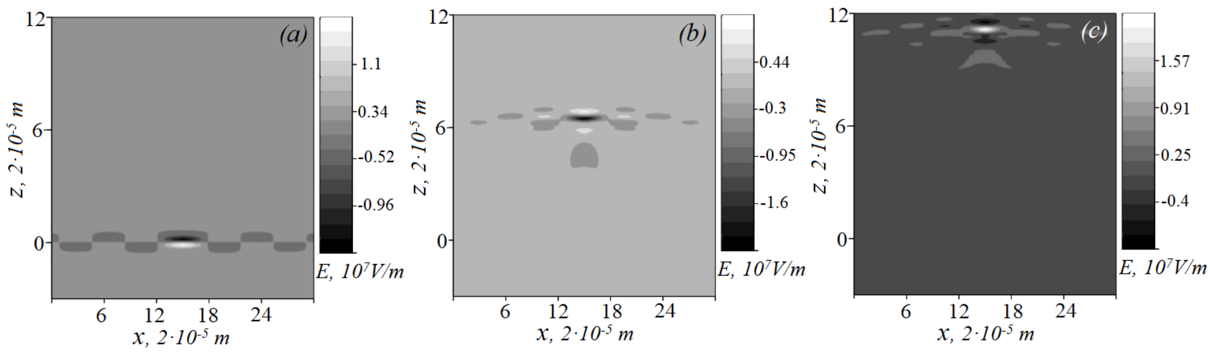

FIG. 2. Pulse evolution with a Bessel profile ($u_{zz} = 0.1$): a) $t = 0$; b) $t = 7$; c) $t = 12$. The time unit corresponds to $2\cdot 10^{-14}$ s

From the above dependencies, we can say that the pulse propagates about 10 of its wavelengths regardless of the cross-sectional shape. Therefore, it moves stably even under the action of deformation. Although the fields are assumed to be strong, there is no significant change in the character of the pulse propagation with a Bessel profile. It should be noted, that for the same values of the initial pulse amplitude with a Gaussian profile, a noticeable decrease in the diffraction effect is observed, which is associated with the nonlinear properties of the medium. Note that in both cases (Figs. 1, 2) a "tail" appears behind the main pulse, which is clearly visible on the following Figs. 3 and 4. Figs. 1 and 2 show only a part of the computational domain for clarity of the behavior of the main pulse.

The dependence of the shape of the electromagnetic pulse on the magnitude of the acoustic field is shown in Fig. 3.

It can be seen, that the mechanical load on the CNT has a greater effect on the pulse with a transverse Gaussian profile as compared to the Bessel pulse, even in the case of small values of the u_{zz}. This can be associated with the pulse with a transverse Bessel cross section and has the property of immunity from diffraction. Note that the mechanical tension on the CNT changes the dispersion law of electrons in the CNT, and, therefore, changes the form of the nonlinearity of the medium. As before, nonlinearity has a stronger effect on the Gaussian pulse dynamics.

Next, we investigate the effect of impurities in strained CNTs on the pulse propagation process (Fig. 4).

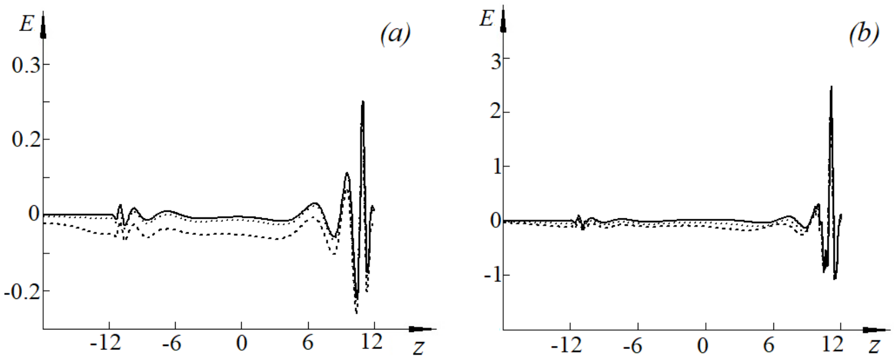

FIG. 3. The dependence of the electric field strength E (longitudinal section at the pulse center: $t = 12$, $D = 0.1\gamma$) on the coordinate z for different longitudinal components of the strain tensor: a) Gaussian profile: the solid curve corresponds to $u_{zz} = 0$, the dotted curve – $u_{zz} = 0.01$, the dashed curve – $u_{zz} = 0.05$; b) Bessel profile: the solid curve corresponds to $u_{zz} = 0$, the dotted curve – $u_{zz} = 0.05$, the dashed curve – $u_{zz} = 0.1$. The z-unit corresponds to $2 \cdot 10^{-5}$ m, along the E-axis – 10^7 V/m, in time – $2 \cdot 10^{-14}$ s

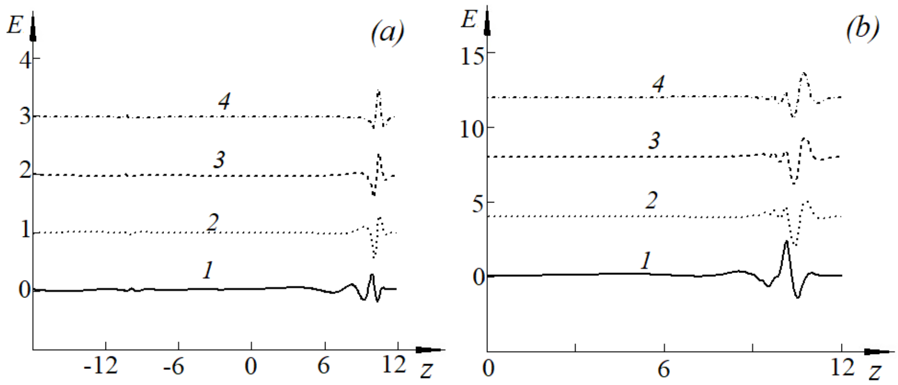

FIG. 4. The dependence of the electric field strength E (longitudinal section at the pulse center: $t = 12$, $u_{zz} = 0.01$) on the coordinate z for the different impurity parameters ($D = -R = -Q$): (a) Gaussian profile – for clarity, each i-th curve is shifted up by $(i-1)$ units; (b) Bessel profile – for clarity, each i-th curve is shifted up by $4(i-1)$ units: curve 1 corresponds to $D = 0$ (no impurity), curve 2 – $D = 0.3\gamma$, curve 3 – $D = 0.5\gamma$, curve 4 – $D = 1.0\gamma$. The unit along the z-axis corresponds to $2 \cdot 10^{-5}$ m, along the E-axis E – 10^7 V/m, in time – $2 \cdot 10^{-14}$ s

It can be seen from the given dependencies that the impurity parameters allows us to not only change the shape, but also the pulse amplitude. We also note that for pulses of both cross sections (Gaussian and Bessel), pulse inversion is observed when impurity carbon nanotubes are introduced into the medium (curves 2–4).

4. Conclusion

Let us formulate the main results from the work:

1. There is a localized pulse propagation in dielectric medium with impurity carbon nanotubes under mechanical strain. Dispersive broadening of pulses during propagation can be compensated for by selecting the appropriate parameters of the acoustic field and impurity.
2. For a pulse with a transverse Gaussian profile, the effect of the acoustic field is more pronounced than for a pulse with a Bessel profile.
3. It is observed, that due to the impurity introduction, it is possible to control the amplitude and shape of few-cycle optical pulse with different profiles.

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