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PROPAGATION OF THREE-DIMENSIONAL EXTREMELY SHORT OPTICAL PULSES IN STRAINED CARBON NANOTUBES

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Abstract. We investigate the extremely short optical pulses in strained carbon nanotubes in the three-dimensional case. The mechanical strain is taken into account in the framework of the gauge theory. We study the influence of the value of the mechanical stretching on the pulse shape.

Key words: extremely short pulses, carbon nanotubes, strain.

1. INTRODUCTION

The study of the phenomena arising from the interaction of electromagnetic radiation with matter plays a significant role in modern opto- and nano-electronics, due to a large number of practical applications [1]. The successes of modern laser technologies from the point of view of generating powerful electromagnetic radiation with certain characteristics, including extremely short laser pulses with durations corresponding to several half-periods of field oscillations [2], are an incentive for a comprehensive study of such pulses in various media [3–14], including carbon nanotubes (CNTs) [15–24]. Physical effects caused by the propagation of extremely short pulses in nonlinear media can be the basis for new energy transfer systems, optical information processing, and other compact devices for modern opto-electronics circuits [25], which are based on various micro- and nano-structures.

Previously, we considered the dynamics of extremely short optical pulses through an array of idealized carbon nanotubes or nanotubes with impurities. The influence of external strains in the one-dimensional case was also considered [26]. But, as is well-known, the dimension of the problem can significantly change the results. In this work, we study the dynamics of three-dimensional (3D) extremely short optical pulses in a medium with carbon nanotubes subjected to mechanical tension. The introduction of such deformations can significantly affect the propagation of optical pulses through the array of the carbon nanotubes.

2. BASIC EQUATIONS

The electron's spectrum for zig-zag carbon nanotubes of (n, 0) type has the following form:

$$\varepsilon(p,s) = \pm\gamma\sqrt{1+4\cos(ap)\cos(\pi s/n)+4\cos^2(\pi s/n)}, \quad (1)$$

where $\gamma \approx 2.7$ eV, $a = 3b/2\hbar$, $b = 0.142$ nm is the length of C-C bond, (p, s) is the quasimomentum, p is the component of the momentum along the CNT axis, $s = 0, .., n$. Different signs define the valence and conduction bands.

We are not taking into account the interaction between carbon nanotubes due to its weakness. The electric field vector $\boldsymbol{E}$ is directed along the axis of the nanotubes, and the electromagnetic pulse moves in the transverse direction.

The mechanical strain is taken into account in the framework of the gauge theory, which manifested itself in the appearance of a stress field. This field is determined by the corresponding vector potential $\boldsymbol{A}'$, which changes the momentum of electrons in a medium containing the array of carbon nanotubes. In deformed CNTs, all interatomic bonds turn out to be nonequivalent, and the three hopping integrals may not be equal to each other. The CNTs are a folded graphene sheet (ZOW plane) in the cylinder along the OW axis. Further, we write all the equations for graphene, and then we take into account the periodic boundary conditions. According to this fact, the calibration vector potential has the form: $\boldsymbol{A}' = (A_z, A_w)$ and its components can be written as [27]:

$$A'_z = \frac{\sqrt{3}}{2}(\gamma_3-\gamma_2), \qquad A'_w = \frac{1}{2}(\gamma_3+\gamma_2-2\gamma_1), \quad (2)$$

where $\gamma_{1,2,3}$ are the hopping integrals.

In the case of weak deformation of the crystal lattice, each hopping integral can be expanded in a series up to the second term [28]:

$$\gamma_i = \gamma + \frac{\beta\gamma}{a^2}\boldsymbol{r}_i(\boldsymbol{u}_i-\boldsymbol{u}_0), \quad (3)$$

where γ is the unperturbed hopping integral, $\boldsymbol{r}_i$ is the radius vector of nearest neighbors, $\boldsymbol{u}_\text{i}$ displacement vector of the i-th atom, $\boldsymbol{u}_0$ is the displacement vector of the central atom, and β is the electronic parameter of Gruneisen [29], which for carbon structures can be taken equal to 2.

In the continuum limit, one can expand the displacement of carbon atoms:

$$\boldsymbol{u}_i - \boldsymbol{u}_0 \propto \left(\boldsymbol{r}_i \nabla\right)\boldsymbol{u}, \tag{4}$$

where $\boldsymbol{u}$ is the displacement field.

Substituting (3) into (2) taking into account (4), we obtain:

$$\begin{aligned} A'_z &= \chi \frac{\beta\gamma}{a}\left(u_{zz} - u_{ww}\right), \\ A'_w &= -\chi \frac{2\beta\gamma}{a} u_{zw}, \end{aligned} \tag{5}$$

where χ is the a numerical parameter depending on the characteristics of the chemical bond in a substance, which can be set for CNT to be 1 [30].

Thus, the strain gauge field is proportional to the strain tensor $u_{\alpha\beta}$, which determines the local strain of the lattice. By setting the deformation field $\boldsymbol{u}$, we obtain that the strain tensor in the linear approximation has the form [31]:

$$u_{\alpha\beta} = \frac{\partial_\alpha u_\beta + \partial_\beta u_\alpha}{2}. \tag{6}$$

The calibration potential changes the band structure by calibrating the pulse by $-qA/c$ in the same way as the external electromagnetic field. The contributions of the electromagnetic field and lattice deformations are reduced to the sum of the corresponding vector potentials. The model does not take into account the rotations of interatomic bonds, *i.e.* $u_{zw} = 0$. Based on these assumptions, only one correction A_z is taken into account in the effective equation for the vector potential.

The longitudinal and transverse components of the strain tensor have the following relation [31]: $u_{zz} = -\mu u_{ww}$, where μ = 0.19 is the Poisson's ratio for CNTs [32].

In the 3D case, taking into account the transition to a cylindrical coordinate system, the equation describing the propagation of the electromagnetic field in the array of carbon nanotubes takes the form:

$$\begin{aligned} &\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial A}{\partial r}\right) + \frac{\partial^2 A}{\partial \varphi^2} + \frac{\partial^2 A}{\partial z^2} - \frac{\varepsilon}{c^2}\frac{\partial^2 A}{\partial t^2} + 4\pi j\left(A + A'\right) = 0, \\ &A' = \chi \frac{\beta\gamma u_{zz}}{a}\left(1+\mu\right), \end{aligned} \tag{7}$$

where ε is the dielectric constant of the medium, c is the light velocity; r, z, and φ are the coordinates in the cylindrical system, the current density j is determined by the formula [33]:

$$j = 2e\sum_{s=1}^{m}\int_{ZB} v(p,s)\cdot f(p,s)\,\mathrm{d}p, \tag{8}$$

where e is the electron charge, $v(p,s)=\partial\varepsilon(p,s)/\partial p$ is the electron velocity, $f(p,s)$ is the electron distribution function, $\varepsilon(p,s)$ is determined according to the formula (1), and the integration is carried out in the first Brillouin zone. We omit the calculation of current density in this paper, because it repeats the standard calculations for CNTs, see for example [33].

Further, we take into account that by virtue of cylindrical symmetry $\partial/\partial\varphi \to 0$.

3. MAIN RESULTS

The equation (7) is reduced to a dimensionless form and is solved numerically. The initial condition is chosen as an extremely short Gaussian pulse:

$$\begin{gathered} A(r,z,0) = Q\cdot\exp\left(-\frac{(z-z_0)^2}{l_z^2}\right)\exp\left(-\frac{r^2}{l_r^2}\right), \\ \frac{\mathrm{d}A(r,z,0)}{\mathrm{d}t} = \frac{2\cdot v\cdot Q\cdot(z-z_0)}{l_z^2}\exp\left(-\frac{(z-z_0)^2}{l_z^2}\right)\exp\left(-\frac{r^2}{l_r^2}\right), \end{gathered} \tag{9}$$

where Q is the amplitude of the electromagnetic pulse at the entrance to the medium with CNT, v is the initial pulse velocity upon entry into the medium, l_z, l_r determine the pulse width along the z and r directions, respectively, and z_0 is the initial coordinate of the center of momentum along the axis z.

The evolution of the electromagnetic pulse during its propagation in the medium with carbon nanotubes is shown in Fig. 1. We draw the field intensity I, which can be found as:

$$I = \frac{1}{c^2}\left(\frac{\partial A}{\partial t}\right)^2. \tag{10}$$

It can be seen that, in the absence of mechanical loading, the pulse spreads both in the longitudinal and transverse directions (Fig. 1d). In the case with $u \neq 0$, it propagates quite stably, experiencing only broadening in the transverse direction. Note that over time, a "tail" forms behind it (Fig. 1c).

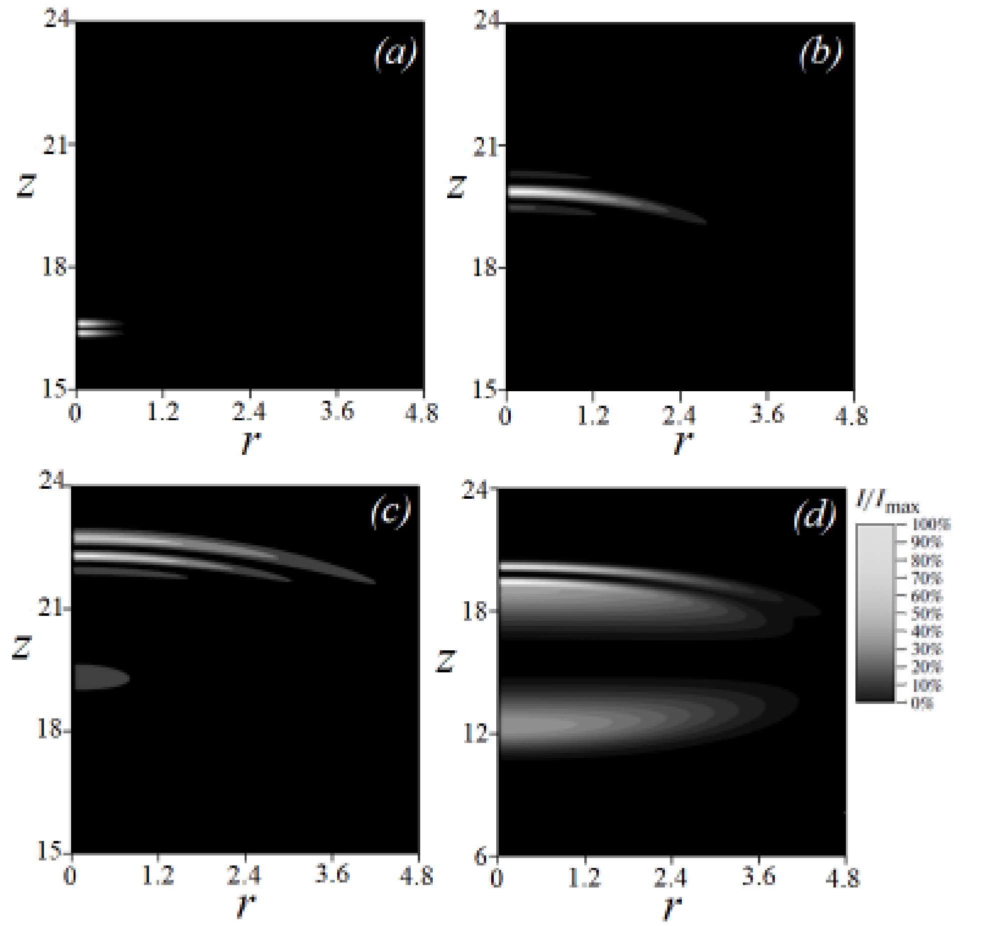

Fig. 1 – The intensity of the electric field of the 3D electromagnetic pulse, taking into account the strain field: a) $t = 0$; b) $t = 5.0$; c) $t = 7.5$; d) $t = 7.5$. For figures (a–c) $u = 0.1$, for figure (d) $u = 0$. Here I_{max} is the maximum intensity for each time point. All values in dimensionless units.

The dependence of the intensity of the electric field on the longitudinal coordinate is shown in Fig. 2.

From the dependences shown in Fig. 2 we can conclude that an increase in the strain tensor reduces the "tail" following the main pulse and contributes to the concentration of the main energy of the pulse in the central region.

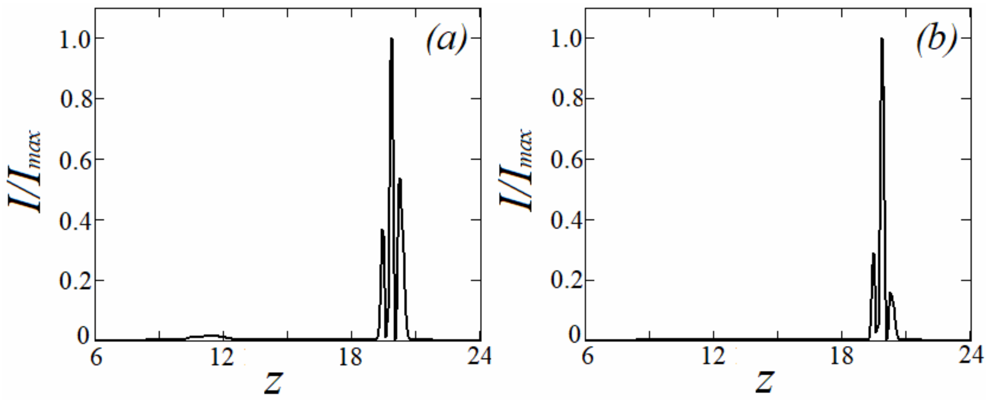

Fig. 2 – The intensity of the electric field of the 3D electromagnetic pulse (longitudinal section): a) $u = 0.01$; b) $u = 0.1$ ($t = 5.0$). All values in dimensionless units.

The dependence of the intensity of the electric field on the transverse coordinate is presented in the Fig. 3.

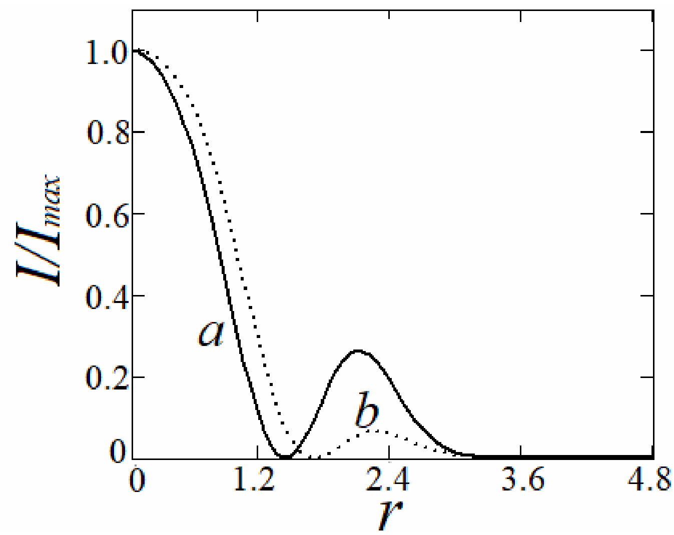

Fig. 3 – The intensity of the electric field of the 3D electromagnetic pulse (transverse section): a) $u = 0.01$; b) $u = 0.1$ ($t = 5.0$). All values in dimensionless units.

It can be seen, that with an increase in the strain tensor, the "side" peak of the pulse decreases, which indicates the effect of stabilization of the electromagnetic wave due to an increase in the degree of deformation of carbon nanotubes.

The dependence of the intensity of the electric field on the initial pulse velocity is shown in Fig. 4.

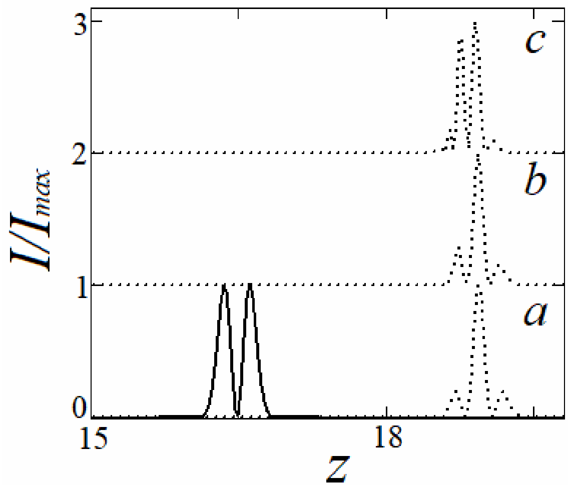

Fig. 4 – The electric field intensity of the 3D electromagnetic pulse for different values of the initial pulse velocity: a) $v = 0.93\ c$; b) $v = 0.95\ c$; c) $u = 0.98\ c$ (dotted curves for time $t = 5.0$). The solid line shows the pulse intensity at time $t = 0$ for clarity. All values in dimensionless units.

According to Fig. 4, the closer the pulse velocity at the entrance to the medium with deformed carbon nanotubes to the speed of light in vacuum, the better the initial shape of the extremely short optical pulse is preserved.

Next, we study the stability of the obtained solutions with respect to perturbations of the momentum field E that depend on the angle φ. The stability analysis can be carried out on the basis of the linearized equation (7), which for small perturbations δA has the form:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\delta A}{\partial r}\right)+\frac{\partial^2\delta A}{\partial z^2}-\frac{\varepsilon}{c^2}\frac{\partial^2\delta A}{\partial t^2}+\frac{4ae^2qn_0}{c^2}\times$$
$$\times\sum_{q=1}^{\infty}b_q\cos\left(\frac{aeq\left(A+\eta\right)}{c}\right)\delta A\exp\left(-\frac{t}{t_{rel}}\right)=0. \qquad (11)$$

Due to the linearity of (11), δA can be found as:

$$\delta A\propto\delta A\left(r,z,t\right)\exp\left(i\cdot n\cdot\varphi\right), \qquad (12)$$

where n is the azimuthal number.

Next, we can calculate the corresponding corrections to the electric field:

$$\delta E=-\frac{1}{c}\frac{\partial\delta A}{\partial t}. \qquad (13)$$

Equation (11) is solved numerically with initial conditions of the form similar to (9).

Figures 5 and 6 show the corresponding results for the electric field. These figures present the maximum modulus of the quantity δE (in the entire computational domain) depending on time and number *n*.

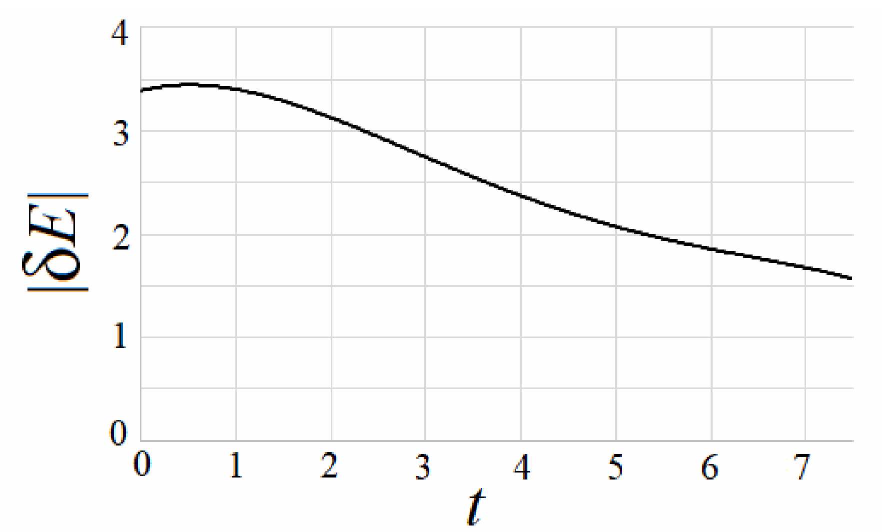

Fig. 5 – The dependence of maximum $|\delta E|$ on time ($n = 11$, $u = 0.1$). The unit on the vertical axis corresponds to 10^7V/m.

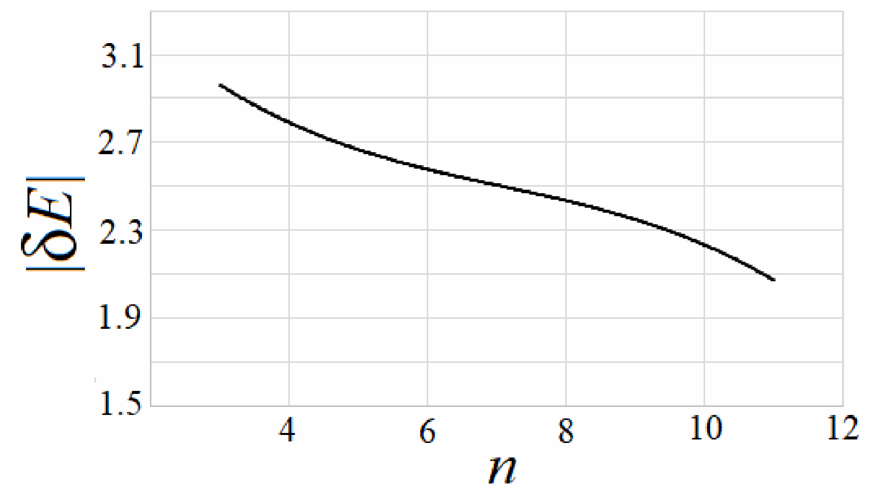

Fig. 6 – The dependence of maximum $|\delta E|$ on n ($t = 5.0$). The unit on the vertical axis corresponds to 10^7V/m.

Figure 5 shows that perturbations decrease over time, and this behavior is stable at large times. According to Fig. 6, the faster the perturbation decreases, the larger the number n is. The graphs in Figs. 5 and 6 allow us to conclude that the obtained solutions are stable with respect to perturbations in angle φ.

4. CONCLUSIONS

The key results of this work are summarized as follows:

1. It is shown that the mechanical stretching of carbon nanotubes significantly affects the dynamics of three-dimensional extremely short optical pulses.
2. The larger the strain, the more stable the pulse becomes. Thus, the mechanical stress is a controlling parameter for the electromagnetic field.
3. It is revealed that the initial pulse velocity into a medium with carbon nanotubes also exerts a stabilizing effect on the pulse shape.
4. It is shown that the pulses propagating in the CNT array taking into account the mechanical load are stable with respect to angular perturbations.

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