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Opto-acoustic effects in an array of carbon nanotubes

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In this paper, we investigate the propagation of electromagnetic waves in a piezoelectric composite comprising carbon nanotubes and piezoelectric fibers. This hybrid medium is initially subjected to the effects of an extremely short optical pulse consisting of just two oscillations of the electric field. On the basis of Maxwell's equations and the wave equation for the displacement vector of the medium, we obtain an effective governing equation for the vector potential of the electromagnetic field, as well as the displacement vector for the media. The dependence of the pulse shape on the parameters of the problem was analyzed, thereby revealing a non-trivial interplay between the characteristics of the pulse dynamics and the electrically induced mechanical vibrations of the medium. The uncovered properties could potentially offer promising prospects for the development of new materials for the optoelectronics industry. *Published by AIP Publishing.*
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I. INTRODUCTION

In recent years, due to the growing range of applications, researchers have increasingly paid more attention and interest to the problem of propagating extremely short electromagnetic pulses in various media.[1–7] This is essentially the consequence of two factors: (i) the related systems are associated with the well-known theory of solitons, and (ii) the fact that the study of these issues may lead to the development of significant practical applications.[8–12] On the other hand, the successes in the physics of nanostructures constantly offer new objects for the studies in this field. One of such fascinating nanostructures is carbon nanotubes (CNTs), the nonlinear properties of which have long been intensively and extensively studied.[13–16] In particular, many studies are devoted to the dynamics of intense and extremely short optical pulses—a.k.a. light bullets—in such media.[17–22] In particular, there were various aspects investigated, such as the effective equations, the dynamics of the pulse with the influence of impurities, the Coulomb interaction between electrons, the collisions between light bullets, and the influence of external fields to name a few.

Among the affected range of issues, however, there are a number of remaining challenges, which are not addressed in the papers cited above. First of all, it concerns the properties of the medium in which the carbon nanotubes were placed. In this regard, one can highlight Ref. 23, in which the impact of medium dispersion on the propagation of light bullets has been investigated. Meanwhile, as we know, the medium can have different properties (piezoelectric, magnetic, ferroelectric, and so forth), which may have a significant effect on the propagation of light bullets. In this paper, we set out to prove the last assertion and theoretically stimulate experiments in this area. Specifically, we consider CNTs placed in a particular environment, which can be subjected to electrically induced mechanical deformations—i.e., piezoelectric vibrations. Such hybrid media based on CNTs and piezoelectric fibers create unique conditions for the propagation of light bullets: the locally intense electric field, in turn, excites various nonlinear responses of the medium.

II. FORMULATION OF THE PROBLEM AND GENERAL EQUATIONS

Consider the propagation of extremely short electromagnetic pulses through an array of carbon nanotubes. The electric field of the pulse is assumed to be perpendicular to the nanotube axis (see Fig. 1). The dispersion law for a $(m,0)$ zigzag-type CNT reads

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

where $s = 1, 2, \ldots, m$ (m is not a multiple of three), $\gamma \approx 2.7$ eV is the overlap integral, $a = 3b/2\hbar$, $b = 0.142$ nm is the distance between carbon atoms.

In the presence of an external electric field $\mathbf{E}$, which is considered in the gauge $\mathbf{E} = -\frac{1}{c}\partial\mathbf{A}/\partial t$, it is necessary to replace the momentum with the generalized momentum, i.e., $p \to p - eA/c$ (e being the elementary charge and c the speed of light in vacuum). Maxwell's equations with the account of the gauge in a quasi-one-dimensional approximation can be written as follows:[24]

$$\frac{\partial^2\mathbf{A}}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2} + \frac{4\pi}{c}\mathbf{j} = \frac{4\pi}{c^2}\frac{\partial^2\mathbf{P}}{\partial t^2}, \tag{2}$$

where we neglect the diffraction spreading of the laser beam in the direction perpendicular to the axis of propagation. The vector potential is assumed to take the form $\mathbf{A} = \{0, 0, A(x,t)\}$, and the current is $\mathbf{j} = \{0, 0, j\}$. To account for the properties of the medium, we have added the term with the

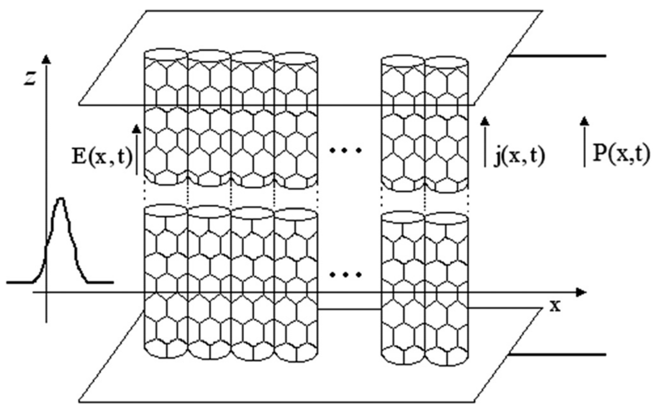

FIG. 1. Schematic drawing representing the geometry of the problem.

polarization vector **P**, directed along the CNT's axis (see Fig. 1).

Let us now express, in a standard fashion, the current density

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

where $v_s(p) = \partial\varepsilon_s(p)/\partial p$ and the brackets $\langle\ldots\rangle$ denote averaging with the nonequilibrium density matrix $\rho(t)$: $\langle B\rangle = \mathrm{Sp}(B(0)\rho(t))$. $C^{\dagger}_{ps}$ and C_{ps} are the creation and annihilation operators for excitations with quasi-momenta (p, s). Taking into account the relation $[C^{\dagger}_{ps\sigma}C_{ps\sigma}, H] = 0$, equations of motion for the density matrix give us the conservation equality $\langle C^{\dagger}_{ps\sigma}C_{ps\sigma}\rangle = \langle C^{\dagger}_{ps\sigma}C_{ps\sigma}\rangle_0$. Here $\langle B\rangle_0 = \mathrm{Sp}(B(0)\rho(0))$, $\rho_0 = \exp(-H/k_BT)/\mathrm{Sp}[\exp(-H/k_BT)]$ (k_B is the Boltzmann constant and T the temperature). The dispersion law $\varepsilon_s(p)$ can be expanded as a Fourier series

$$\varepsilon_s(p) = \frac{1}{2\pi}\sum_{sq} a_{sq}\cos(apq), \qquad a_{sq} = \int \cos(apq)\varepsilon_s(p)dp, \tag{4}$$

where the integration is performed over the first Brillouin zone, and q is any natural number.

To proceed, we use the following considerations. In a non-piezoelectric medium, electron dynamics is determined by Newton's second law, i.e., $d\mathbf{p}/dt = e\mathbf{E}$. With the gauge $\mathbf{E} = -\partial\mathbf{A}/c\partial t$, this yields a standard solution for the so-called "long" momentum, $\mathbf{p} = \mathbf{p}_0 - e\mathbf{A}/c$. If we account for the piezoelectric effects, electron dynamics is described by the equation $d\mathbf{p}/dt = e\mathbf{E} + ed\partial\mathbf{u}/\partial z$, where d is the piezoelectric coefficient, and $\mathbf{u}$ is the displacement vector of the medium. This latter equation with the account for Eqs. (3) and (4) leads us to a single effective equation for the vector potential in the form (subscripts z are omitted for clarity)

$$\frac{\partial^2 A}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} + \frac{4en_0}{c}\sum_{q=1}^{\infty} qb_q \sin\left(\frac{aqe(A+\eta)}{c}\right) - \frac{4\pi}{c^2}\frac{\partial^2 P}{\partial t^2} = 0, \tag{5}$$

$$b_q = \sum_s a_{sq}\int dp\cos(apq)\frac{\exp(-\varepsilon_s(p)/k_BT)}{1+\exp(-\varepsilon_s(p)/k_BT)}.$$

The quantity η in Eq. (5) is related to the non-zero component of the displacement vector u of the medium as follows:

$$\eta = -cd\int_{-\infty}^{t}\frac{\partial u(z,t')}{\partial z}dt'. \tag{6}$$

Here, we consider one of the simplest models possible, such that the induced polarization in the medium admits linear variations with the applied electric field and is directed parallel to the electric field due to the piezoelectric effect

$$P = d\frac{\partial u}{\partial z}. \tag{7}$$

It is worth noting that Eq. (5) must be supplemented with the equation for the displacement vector u[25–27]

$$\frac{\partial^2 u}{\partial x^2} - \frac{1}{v_a^2}\frac{\partial^2 u}{\partial t^2} + \frac{d}{\rho}\frac{\partial u}{\partial z} = 0, \tag{8}$$

where ρ is the medium density, and v_a is the speed of sound in the medium.

Within the framework of the model described above, it is necessary to make a couple of remarks. First, we take into consideration only one component of the displacement vector **P**, which can obviously be easily generalized. Also, we do not take into account the fact that the environment can have some nonlinear acoustic properties, thereby resulting in the possibility of having the polarization vector not being colinear with the electric field.

III. RESULTS OF THE NUMERICAL MODELING

Equation (5) was solved numerically using the direct cross-type difference scheme.[28] The initial condition is chosen in the form of extremely short pulses consisting of two electric field fluctuations and can be written in the form

$$A(x,0) = Qx\exp\left(-\frac{x^2}{\gamma}\right), \quad \frac{dA(x,0)}{dt} = \frac{2x^2v}{\gamma}Q\exp\left(-\frac{x^2}{\gamma}\right), \quad \gamma = (1-v^2)^{1/2}, \quad u(x,0) = 0, \quad \frac{du(x,0)}{dt} = 0, \tag{9}$$

where Q and v are the initial pulse amplitude and velocity, respectively. The evolution of the electromagnetic field during its propagation through the sample is shown in Fig. 2. Due to the fact that Eq. (5) is sufficiently close to the integrable sine-Gordon equation, the pulse propagates preserving its shape in the initial stage. Then the non-integrable terms in Eq. (5) begin to play a non-negligible role resulting in the appearance of a tail behind the pulse, which has approximately zero area. Note that, as shown by the results of numerical calculations, the type of carbon nanotubes only

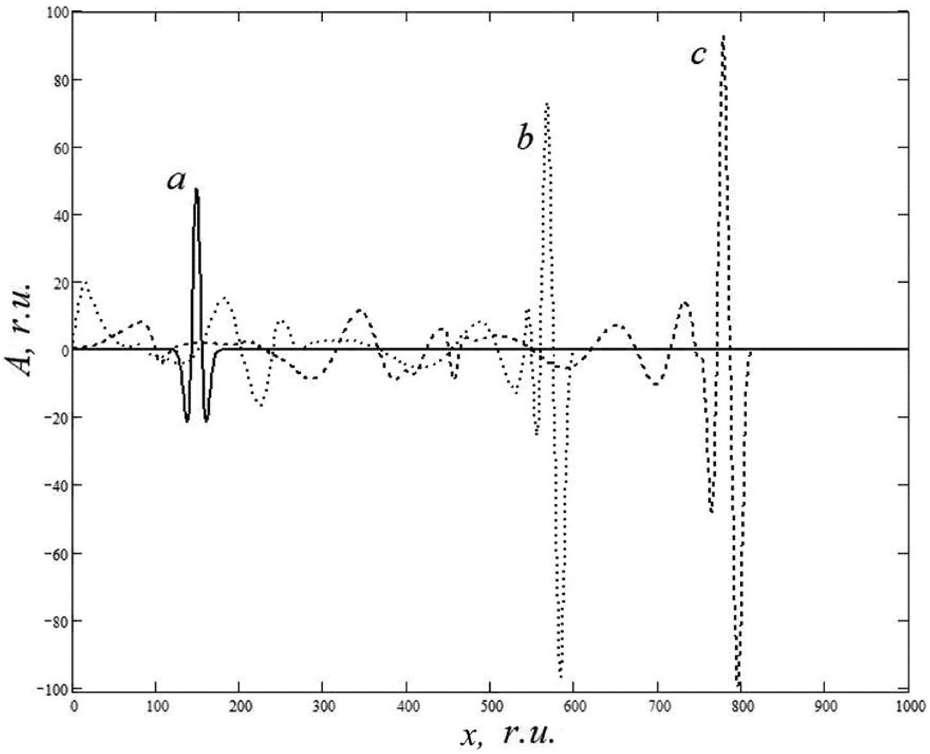

FIG. 2. Dependence of the vector potential on coordinate ($v/c = 0.95$): (a) initial pulse; (b) $t = 5.0 \times 10^{-12}$ s; and (c) $t = 7.5 \times 10^{-12}$ s. All quantities are given in relative units.

weakly affects the dynamics of the pulse. This behavior occurs for all types of semiconductor nanotubes. Also note the appearance of a "tail," which is also not related to the type of CNTs. Lastly, it is worth noting the increase in the pulse amplitude as it propagates through the sample.

The dependence of the pulse shape on the initial pulse velocity is shown in Fig. 3. Such a behavior can be explained by the transition to a moving coordinate system which leads to narrowing of the pulse. Also note that the evolution of the extremely short pulse depends, in general, on the initial pulse amplitude. Moreover, low-amplitude pulses propagate with almost unchanged shape. Larger amplitude pulses undergo major changes due to the effects of nonlinearity and wavefront interference with its decay.

We also investigated the influence of the piezoelectric coefficient d on the pulse propagation through the sample,

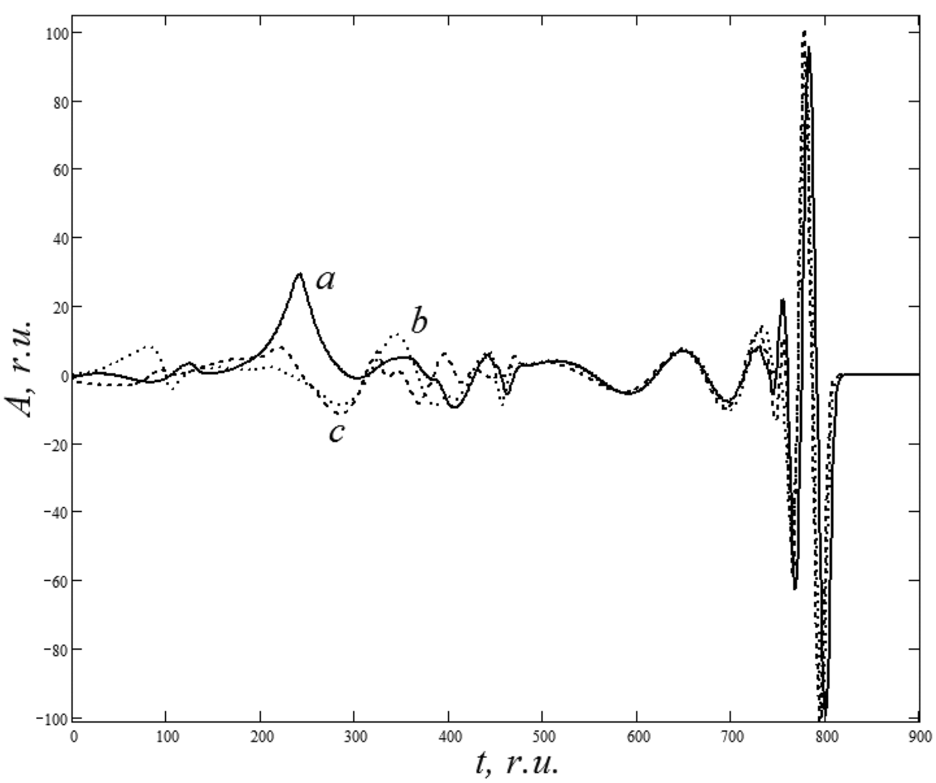

FIG. 3. Dependence of the vector potential on time for different values of the initial speed of pulse: (a) $v/c = 0.93$; (b) $v/c = 0.95$; and (c) $v/c = 0.93$. All quantities are given in relative units.

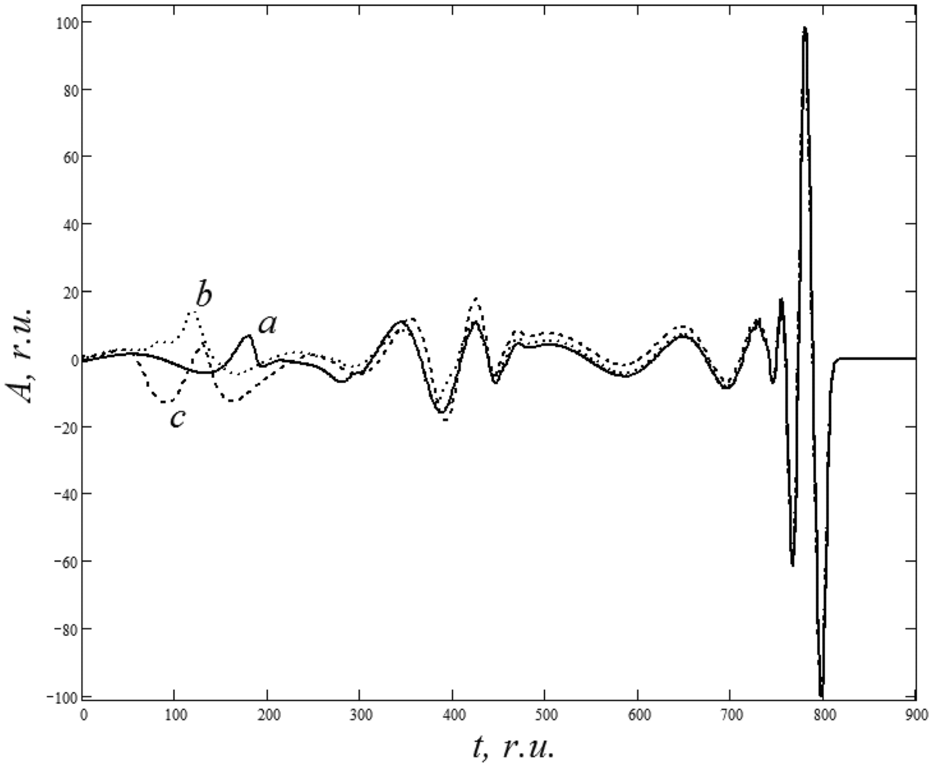

FIG. 4. Dependence of the vector potential on time for different values of the piezoelectric coefficient: (a) $d = 0.01$; (b) $d = 0.05$; and (c) $d = 0.1$. All quantities are given in relative units.

which is illustrated in Fig. 4. The figure shows that, as expected, this parameter only determines the shape of the "tail," but has no effect on the main pulse. Moreover, the larger the value of d, the greater the fluctuations in the pulse "tail" due to the piezoelectric effect. That is, one can control the generation of the terahertz pulse by changing the piezoelectric coefficient d.

IV. CONCLUSIONS

As a result of our study, the following conclusions can be made:

(i) Over time, there is an increase in the amplitude of the extremely short optical pulse in a piezoelectric medium with CNTs, which allows the use of this medium in devices for amplification of pulses.
(ii) The emergence of the "tail" behind the extremely short pulse may be useful for generating terahertz pulses.
(iii) The pulse behavior strongly depends on the value of the piezoelectric coefficient d, which determines the character of the oscillations in the "tail" following the main pulse.

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