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Dynamics of laser beams in a carbon nanotube array under mechanical loading

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In this paper, we study the effect of a stress field formed in a carbon nanotube array under mechanical loading on the properties of laser beams propagating in this medium. Using the method of slowly varying amplitudes and phases based on the wave equation, we obtain an equation characterizing the change in the intensity of the electric field of a Gaussian beam. We analyze the effect of the stress field on the parameters of laser radiation.

Keywords: carbon nanotubes, laser beams, mechanical load.

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1. Introduction

The study of the interaction of high-intensity laser radiation with matter is an important area of research in nonlinear optics. As modern theoretical [1–3] and experimental studies show, such studies contribute both to the discovery of new physical phenomena and to the search for promising materials for effective control of laser radiation characteristics. Carbon nanotubes (CNTs) are of particular interest in this context, since they demonstrate a unique ability to maintain stable propagation of electromagnetic fields [4].

The key factor in controlling the characteristics of laser radiation (such as localization, intensity [5], increase in output power [6]) is the nonlinearity of the medium. Media with nonlinear properties can include both traditional Kerr media [7] and plasma [8], which provide polarization control when interacting with a control beam, and modern materials with pronounced nonlinearity — in particular, carbon nanotubes.

In addition, the parameters of electromagnetic radiation can be influenced by external fields. Thus, the possibility of controlling extremely short optical pulses in anisotropic crystals using magnetic and acoustic fields is shown in Refs. [9,10]. All of these results were obtained by solving Maxwell's equations without using the approximation of slowly varying amplitudes and phases.

2. Theoretical part

In this study, this approximation is used to derive an analogue of the nonlinear Schrodinger equation describing the dynamics of a laser beam in a medium with CNTs under the action of a deformation field.

Let's us consider the propagation of an electromagnetic beam through a dielectric medium with carbon nanotubes. The wave vector is directed at a right angle to the CNT array. The work uses the assumption that all nanotubes are oriented along the x axis, and the inhomogeneities of the electromagnetic field along their axis are not taken into account, since it is shown that this does not significantly contribute to the femtosecond pulses under consideration [11].

The dependence of the energy Δ on the quasi-momentum for carbon nanotubes of the zig-zag type is described by the expression [12]:

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

p — the component of the quasi-pulse of an electron along the CNT axis, $s = \overline{1, m}$ — the number characterizing the quantization of the pulse along the perimeter of the nanotube ($m = 7$), which is determined by the diameter of the CNT ($\approx 0.55\,\text{nm}$), $a = 1.5b/\hbar$, b — the distance between carbon atoms in a graphene lattice, $\hbar$ — Planck's constant, $\gamma_0 \approx 2.7\,\text{eV}$ —integral overlaps. The sign „+“ corresponds to the conduction band, the sign „–“ corresponds to the valence band.

The electric field of the laser beam and the density of the electric current flowing through the CNT cross-section have the form $\mathbf{E} = \big(E(y, z, t), 0, 0\big)$ and $\mathbf{j} = \big(j(y, z, t), 0, 0\big)$. The equation for the component of the vector potential of laser radiation along the axis CNT —

$$\frac{\varepsilon}{c^2}\frac{\partial^2 A}{\partial t^2} = \frac{\partial^2 A}{\partial y^2} + \frac{\partial^2 A}{\partial z^2} + \frac{4\pi}{c}\,j(A), \tag{2}$$

here c is the speed of light in vacuum, ε is the dielectric constant of the medium in which the nanotubes are located.

Next, we take into account that CNTs are subjected to compression and stretching deformations, which leads to the appearance of a field of mechanical stresses [13]. This, in turn, corrects the pulse field:

$$A' = d \cdot u, \tag{3}$$

where d is the proportionality coefficient depending on the Gruneisen electronic parameter (2 for carbon nanotubes) [14], the Poisson coefficient and γ_0, u is field of elastic deformations.

We do not provide a detailed calculation [15] of the dependence of the vector potential on the deformation field (3) in this paper, but only show its general form.

Next, we write down the expression for the x-component of the electric current density:

$$j = 2e \sum_{s=1}^{m} \int_{\mathrm{BZ}}^{\infty} v(p, s) \cdot F \cdot dp, \tag{4}$$

where $v(p, s) = \partial\Delta(p, s)/\partial p$ is the electron velocity, F is the Fermi distribution function–Dirac, BZ is the Brillouin zone.

Taking into account the decomposition of the dispersion relation into a Fourier series and within the framework of the collisionless approximation, the equation (4) is converted to the following form:

$$j = -en_0\gamma_0 a \sum_{q=1}^{\infty} \sum_{s=1}^{m} b_{s,q} \sin\left(\frac{qa(eA + A')}{c}\right), \tag{5}$$

here n_0 determines the concentration of electrons,

$$b_{s,q} = -q\,\frac{\alpha_{s,q}}{\gamma_0}\,\frac{\int_{-\pi}^{\pi} \cos(qr) \exp\left(-\sum_{q=1}^{\infty} \frac{\alpha_{s,q}\cos(qr)}{k_\mathrm{B}T}\right) dr}{\int_{-\pi}^{\pi} \exp\left(-\sum_{q=1}^{\infty} \frac{\alpha_{s,q}\cos(qr)}{k_\mathrm{B}T}\right) dr}, \tag{6}$$

$k_\mathrm{B} \approx 1.38\,\mathrm{J/K}$, T is the temperature,

$$\alpha_{s,q} = \frac{a}{\pi} \int_{\mathrm{BZ}}^{\infty} \cos(p \cdot a \cdot q)\Delta(p, s)\,dp. \tag{7}$$

Taking into account the above formulas (5)–(7), the wave equation (2) describing the dynamics of laser radiation in a medium with carbon nanotubes in the presence of a deformation field can be written as:

$$\frac{ea}{c}\left(\frac{\partial^2 A}{\partial y^2} + \frac{\partial^2 A}{\partial z^2}\right) - \frac{ea\varepsilon}{c^3}\frac{\partial^2 A}{\partial t^2} - \omega_0^2 \sum_{q=1}^{\infty} \sum_{s=1}^{m} b_{s,q} \sin\left(\frac{qa}{c}(eA + A')\right) = 0,$$

$$\omega_0 = 2ea\sqrt{\pi n_0 \gamma_0} \tag{8}$$

or, given the sine of the sum,

$$\frac{ea}{c}\left(\frac{\partial^2 A}{\partial y^2} + \frac{\partial^2 A}{\partial z^2}\right) - \frac{ea\varepsilon}{c^3}\frac{\partial^2 A}{\partial t^2} - \omega_0^2 \sum_{q=1}^{\infty} \sum_{s=1}^{m} \left[b_{s,q}^1 \sin\left(\frac{qae}{c}A\right) + b_{s,q}^2 \cos\left(\frac{qae}{c}A\right)\right] = 0,$$

$$b_{s,q}^1 = b_{s,q} \cos\left(\frac{qa}{c}A'\right), \quad b_{s,q}^2 = b_{s,q} \sin\left(\frac{qae}{c}A'\right). \tag{9}$$

Let's represent the dimensionless component of the vector potential as

$$\tilde{\mathbf{A}} = \frac{ea}{c}A = \tilde{\mathbf{A}}_0(y, z)\cos(\omega t - kz - \varphi), \tag{10}$$

$\tilde{\mathbf{A}}_0(y, z)$ is the envelope of the x-components of the vector potential, $k = \omega\sqrt{\varepsilon}/c$ is the modulus of the wave vector, φ is the initial phase.

Based on the method of slowly varying amplitudes and phases [16], it is possible to obtain an equation for the intensity of an electromagnetic beam $|\Phi|^2 = |\tilde{\mathbf{A}}_0(y, z)|^2$, taking into account the representation of $\sin(\mu\cos\eta)$ and $\cos(\mu\cos\eta)$ using Bessel functions of the first kind and averaging over period $2\pi/\omega$:

$$\frac{\partial^2\Phi}{\partial\xi^2} + 2i\kappa\frac{\partial\Phi}{\partial\tau} - \Phi\sum_{q=1}^{\infty}\sum_{s=1}^{m}\left(qb_{s,q}^1 \sum_{r=0}^{\infty} \frac{(-1)^{\prime} q^{2r+1}|\Phi|^{2r}}{2^{2r} r!(r+1)!}\right) - \Phi\sum_{q=1}^{\infty}\sum_{s=1}^{m}\left(b_{s,q}^2 \sum_{r=0}^{\infty} \frac{(-1)^{\prime} q^{2r}|\Phi|^{2r}}{2^{2r} r!r!} \times \left(1 - \frac{q^2|\Phi|^2}{2(r+1)(r+2)}\right)\right) = 0 \tag{11}$$

(ξ, τ) represent dimensionless coordinates, κ is a dimensionless wave vector, $b_{s,q}$ are determined during the calculation of the velocity of conduction electrons in carbon nanotubes. Since these coefficients decrease quite rapidly with q, we will limit the sum of q to only ten terms.

The finite-difference Besse scheme [17] of the second order of accuracy is used to solve equation (11), with initial conditions in the form of a Gaussian beam:

$$\Phi(\xi, 0) = \Phi_0 \cdot \exp\left(\frac{\xi^2}{L^2}\right). \tag{12}$$

Here Φ_0 is the initial intensity, depending on the frequency and amplitude of the electric field of the beam, L is the beam width.

3. Results

Figure 1 shows the field intensity distribution in the CNT array (7.0) with the following parameters:

$$T = 77\,\mathrm{K}, \quad \varepsilon = 4, \quad n_0 = 2 \cdot 10^{18}\,\mathrm{cm}^{-3},$$

$$\gamma_0 = 2.7\,\mathrm{eV}, \quad \omega_0 \approx 10^{14}\,\mathrm{s}^{-1}.$$

There is a significant spreading of the beam over time, which leads to a decrease in amplitude by about 35% of the initial value. Our studies have shown that the degree of broadening depends on the frequency and initial amplitude of the electric field of the laser beam. Namely, higher-amplitude laser beams are less susceptible to diffraction,

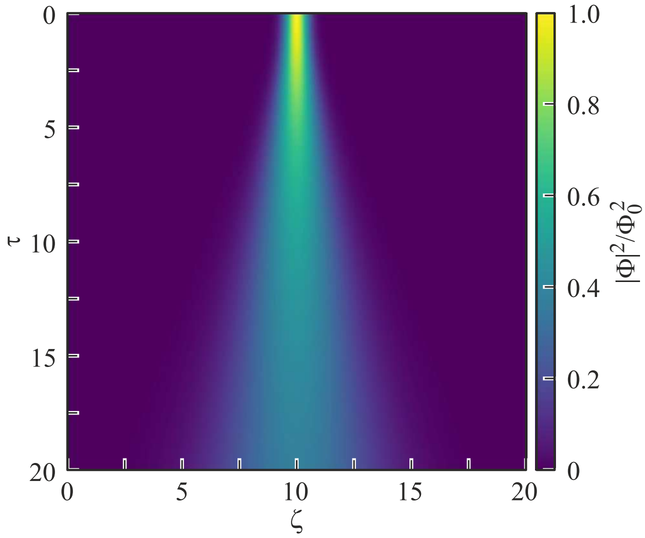

Figure 1. Dependence of the laser beam intensity on coordinates ξ and τ.

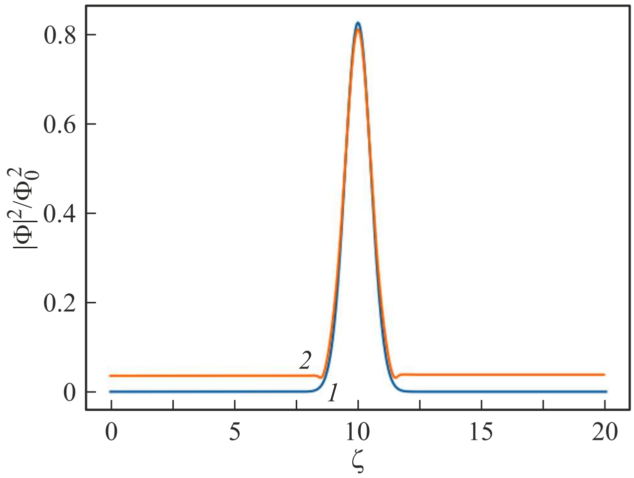

Figure 2. Dependence of the laser beam intensity on the coordinate ξ at $\tau = 15$: curve *1* — without taking into account the deformation, *2* — taking into account the deformation.

and a similar behavior is observed with an increase in frequency ω. So, for $\omega = 2 \cdot 10^{14}\,\mathrm{s}^{-1}$, the absolute change in beam width relative to the original ($\sim 6 \cdot 10^{-4}$ cm) is $6.6 \cdot 10^{-4}$ cm and $2 \cdot 10^{-5}$ cm for $\omega = 10^{15}\,\mathrm{s}^{-1}$.

Figure 2 shows the dependence of the beam intensity on the spatial coordinate in the presence/absence of a deformation field.

4. Conclusion

From the above dependencies, it can be concluded that the presence of deformation of carbon nanotubes (values up to 10 % were considered) has a weak effect on the parameters of the laser beam and manifests itself in a decrease in intensity of no more than 1.5 %.

Thus, based on the constructed model describing the dynamics of a laser beam in a medium with CNTs exposed to a deformation field, it was found that compression/stretching of carbon nanotubes does not lead to significant changes in the beam. This allows CNTs to be used in optical applications where mechanical stress is possible, for example, in waveguide systems.

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Conflict of interest

The authors declare no conflict of interest.

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