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PROPAGATION OF LASER BEAMS IN AN ARRAY OF SEMICONDUCTOR CARBON NANOTUBES

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In this paper, we consider propagation of a monochromatic laser beam in an array of semiconductor carbon nanotubes. Initial distribution of the beam intensity is taken in the form of a Gaussian profile in the plane perpendicular to the wave vector. The electromagnetic field in an array of nanotubes is described by Maxwell equations, reduced to a multidimensional wave equation. With an approximation of the slowly varying amplitudes and phases, we derive the effective equation describing the time-averaged field intensity distribution of the laser beam in a medium. Numerical solution of the derived equations allows us to analyze the dependence of the diffractive spreading of the beam on its frequency and initial amplitude. Furthermore, the influence of the nanotube radius on the diffractive spreading of the laser beam is investigated.

Keywords: Carbon nanotubes; laser beam propagation; Gaussian profile.

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1. Introduction

Carbon nanotubes are promising objects for the use in creating a modern basis for nanoelectronics.[1] Nonlinearity of the electron dispersion of nanotubes leads to a wide range of properties, which can be observed in the fields of moderate intensity in the range between $\sim 10^3$ and 10^5 V/cm (see Refs. 2–7 and references therein). This fact, as well as the success of laser physics in the formation of powerful electromagnetic radiation with given parameters, became the impetus for comprehensive studies of electronic and optical properties of nanotubes with the presence of electromagnetic fields.$^{8–10}$ In particular, recent papers$^{11–15}$ have been devoted to the study of the propagation of extremely short electromagnetic pulses in arrays of nanotubes. In Ref. 11, the possibility of solitary electromagnetic waves propagation in the array of nanotubes has been demonstrated. The propagation of extremely short electromagnetic pulses in an array of nanotubes placed in a dispersive nonmagnetic dielectric medium was considered in Ref. 12, as well as the dependence of the pulse shape on the constants of the dispersion medium. References 13 and 14 were devoted to a study of the dynamics of two-dimensional electromagnetic waves and so-called ”light bullets” in arrays of nanotubes with metal inhomogeneities. The questions related to a stabilization of extremely short electromagnetic pulses in arrays of nanotubes are considered in Ref. 16. The areas of potential applicability of the results of these studies include, among others, optical information processing systems.

The above works were related to the propagation of electromagnetic pulses in nanotubes arrays, whose duration is comparable to a period of oscillation of the field within an optical range, that is several orders of magnitude smaller than the relaxation time in the system. However, there is still an open question about the propagation of quasi-stationary laser beams, the length of which substantially exceeds the period of field oscillation in the optical and infrared ranges, but still less than the relaxation time. The interest in studying this problem is evident, as this is one of the most promising tasks of modern optics, which consists in the creation of all-optical devices implementing the control of light by light. Such devices can be constructed based on media whose strongly nonlinear properties can effectively change the parameters of light beams, as well as their propagation with the least distortion and attenuation. Therefore, it seems timely to study the peculiarities of propagation of monochromatic laser beams and the influence of medium properties on time-averaged parameters of the beam field in an array of semiconducting carbon nanotubes. The latter is the actual scope of the present work. The rest of the article is organized as follows. In Sec. 2, we describe the basic formalism for the solution of the problem, Sec. 3 is devoted to the derivation of the effective equation describing the propagation of a monochromatic laser beams in an array of semiconducting carbon nanotubes. The results of our numerical simulations, as well as their analysis, are given in Sec. 4. Conclusions are given in Sec. 5.

2. Basic Relations and the Wave Equation

We consider the propagation of the laser beam in a bulk semiconductor array of single-walled carbon nanotubes of the zigzag-type $(m, 0)$, where the integer m (not a multiple of three) defines the nanotube radius through $R = \frac{bm}{2\pi}\sqrt{3}$. b is the distance between adjacent carbon atoms.^{2} We assume that the nanotubes are placed into a homogeneous dielectric medium, nanotube axes are parallel to a common axis Ox, and the distance between neighboring nanotubes is large compared to

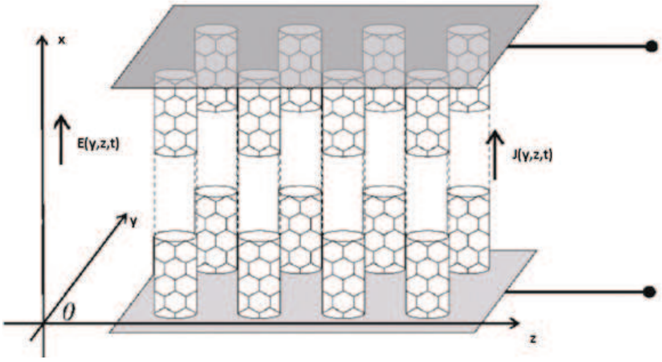

Fig. 1. Geometry of the problem.

their diameter. While applications exist where this may not be the case,[17–21] the latter assumption allows us to neglect the interaction between nanotubes. Given the geometry, the dispersion law of conduction electrons in the nanotube has the form

$$\Delta(p_x, s) = \gamma_0 \left\{ 1 + 4\cos\left(p_x \frac{d_x}{\hbar}\right)\cos\left(\pi\frac{s}{m}\right) + 4\cos^2\left(\pi\frac{s}{m}\right)\right\}^{1/2}, \tag{1}$$

where the quasi-momentum is represented as $\mathbf{p} = \{p_x, s\}$, $s = 1, 2, \ldots, m$ is the number characterizing the quantization of momentum along the perimeter of the nanotube, γ_0 is the overlap integral, and $d_x = 3b/2$.[2]

Propagation of monochromatic laser beam in an array of carbon nanotubes will be considered here in a direction perpendicular to the axes of nanotubes, i.e. along the axis Oz. We assume that the electric field of the laser beam, $\mathbf{E} = \{E(y,z,t), 0, 0\}$, is oriented along the axis Ox, and the frequency of the beam field satisfies the inequality $2\pi/\tau \ll \omega < 2\gamma_0 d/3\hbar R$, where τ is the electron relaxation time (roughly, the time in which electrons fall to the bottom of the conduction band). The left part of the above inequality allows us to use the collisionless approximation, while the right part means that we neglect the interband transitions in semiconductor nanotubes.[2,22] The geometry of the problem is transparently illustrated on Fig. 1.

The electromagnetic field in an array of nanotubes can be described by Maxwell's equations,[23] which (in a chosen geometry) can be reduced to the equation

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

where $A(y,z,t)$ and $j(y,z,t)$ are the projections of the vector potential $\mathbf{A} = (A(y,z,t), 0, 0)$ and the current density $\mathbf{j} = (j(y,z,t), 0, 0)$ along the direction of axis Ox; ε is the permittivity of medium, and c is the speed of light in vacuum. The electric field of the laser beam is determined by the known relation $c\mathbf{E} = -\partial\mathbf{A}/\partial t$.

The electric field of the laser beam along the axis Ox is assumed to be uniform. Note that the field inhomogeneity along the axis Ox can lead to accumulation of electric charges, and accordingly, we would need to consider the field generated by this charge, which is a separate problem. This is considered to be out of the scope of this paper.

We find the conduction current density in an array, following the approach developed in Ref. 24. Representing the electron energy spectrum (1) as a Fourier series, we write the expression for the projection of the current density on the axis following the collisionless approximation:

$$j = -en_0 \frac{d_x}{\hbar}\gamma_0 \sum_{s=1}^{m}\sum_{\alpha=1}^{\infty} G_{\alpha,s} \sin\left(\alpha \frac{ed_x}{c\hbar} A\right), \tag{3}$$

where e is the electron charge, n_0 is the concentration of conduction electrons in an array of nanotubes,

$$G_{\alpha,s} = -\alpha \frac{\delta_{\alpha,s}}{\gamma_0} \frac{\int_{-\pi}^{\pi} \cos(\alpha\zeta)\exp\{-\sum_{\alpha=1}^{\infty} \theta_{\alpha,s}\cos(\alpha\zeta) d\zeta\}}{\int_{-\pi}^{\pi} \exp\{-\sum_{\alpha=1}^{\infty} \theta_{\alpha,s}\cos(\alpha\zeta) d\zeta\}}, \tag{4}$$

$\theta_{\alpha,s} = \delta_{\alpha,s}/k_B T$, and $\delta_{\alpha,s}$ are the coefficients in the expansion of the spectrum (1) into a Fourier series.[25] The latter are explicitly given by

$$\delta_{\alpha,s} = \frac{d_x}{\pi\hbar}\int_{-\pi\hbar/d_x}^{\pi\hbar/d_x} \Delta(p_x, s)\cos\left(\alpha\frac{d_x}{\hbar}p_x\right) dp_x\,. \tag{5}$$

Note that in Eq. (3) the current density is explicitly dependent on the vector potential $\mathbf{A}$. Therefore, it might be assumed that the change of the vector potential by a constant (which does not yield any physical consequences) causes changes in the current density. However, in reality, this does not happen, because while deriving Eq. (3) it was assumed that the vector potential initially (at $t = 0$) is zero, which therefore fixes the gauge choice. Substituting the expression for the conduction current Eq. (3) into Eq. (2) gives us the wave equation describing the evolution of the field in an array of nanotubes:

$$\varepsilon\frac{\partial^2\Phi}{\partial t^2} - c^2\left(\frac{\partial^2\Phi}{\partial y^2} + \frac{\partial^2\Phi}{\partial z^2}\right) + \omega_0^2 \sum_{s=1}^{m}\sum_{\alpha=1}^{\infty} G_{\alpha,s}\sin(\alpha\Phi) = 0\,, \tag{6}$$

where $\Phi(y,z,t) = ed_x A(y,z,t)/c\hbar$ is the dimensionless projection of the vector potential onto the axis Ox, ω_0 is the characteristic frequency, defined by the formula

$$\omega_0 = 2\frac{ed_x}{\hbar}\sqrt{\pi\gamma_0 n_0}\,. \tag{7}$$

3. Effective Equation

We now turn to the description of the field of a monochromatic laser beam using the dimensionless projection of the vector potential on the axis Ox in the following way:

$$\Phi(y,z,t) = \Phi_0(y,z)\cos(\omega t - kz - \psi) \tag{8}$$

where $\Phi_0(y,z) = A_0(y,z)ed_x/c\hbar$, $A_0(y,z)$ is the envelope of the projection of the vector potential on the axis Ox, $k = \omega/v$ is the absolute value of a wave vector, $v = c/\sqrt{\varepsilon}$ is the speed of light in the medium, and ψ is the initial phase. At this point we substitute Eq. (8) into Eq. (6) and use an approximation of slowly-varying amplitudes and phases,[26] then simplify the obtained equation assuming that the conditions $|\partial\Phi_0/\partial z| \ll k|\Phi_0|$ and $|\Phi_0\partial\psi/\partial z| \ll |\partial\Phi_0/\partial z|$ apply. Next, we take into account the relation $\sin(\mu\cos(\zeta)) = 2\sum_{l=1}^{\infty}(-1)^{l+1}J_{2l-1}(\mu)\cos[(2l-1)\zeta]$ (Ref. 25) and take an average over the period of oscillations of the beam field, $2\pi/\omega$. As a result, using the expansion[25]

$$J_1(\zeta) = \frac{\zeta}{2}\sum_{l=1}^{\infty}\frac{(-1)^l}{l!\Gamma(l+2)}\left(\frac{\zeta}{2}\right)^{2l},$$

we obtain an effective equation for the complex function $\phi = \phi(y,z) = \Phi_0(y,z)\exp(i\psi)$, which determines the amplitude of the vector potential

$$\frac{\partial^2\phi}{\partial y^2} + 2ik\frac{\partial\phi}{\partial z} - \frac{\omega_0^2}{c^2}\phi\sum_{\alpha=1}^{\infty}\left\{\left[\alpha\sum_{l=0}^{\infty}\frac{(-1)^l\alpha^{2l}|\phi|^{2l}}{l!2^{2l}\Gamma(l+2)}\right]\sum_{s=1}^{m}G_{\alpha,s}\right\} = 0\,, \tag{9}$$

where $\Gamma(\zeta)$ is the Euler gamma function.[25] As is known, the practically measured physical quantities are the intensity, energy, or power of electromagnetic radiation, which are proportional to the square of the absolute value of electric field vector.[27] Taking into account the expression (8) and the chosen gauge for a vector potential, the value $I = \langle|\mathbf{E}|^2\rangle$ (the average being taken over the period $2\pi/\omega$) takes the form

$$I = \frac{1}{2}\left(\frac{\hbar\omega}{ed_x}\right)^2|\phi|^2\,. \tag{10}$$

4. The Results of Numerical Simulation

Propagation of a laser beam in a system of semiconductor carbon nanotubes is considered here with the typical values of system parameters: $\gamma_0 = 2.7$ eV, $b = 0.142$ nm, $d_x \approx 0.213$ nm, $n_0 = 2\cdot 10^{18}$ cm^{-3}, $T = 77$ K, $\varepsilon = 4$, and $\omega_0 \approx 10^{14}$ s^{-1} [see Eq. (7)]. Note that the collisionless approximation used in the current study is justified when considering the processes on a time scale not exceeding the relaxation time $\tau \approx 3\cdot 10^{-13}$ s,[2] which allows the laser beam to pass a distance $z = ct/\sqrt{\varepsilon} \approx 5\cdot 10^{-3}$ cm.

We further assume that the initial field intensity distribution $I(y,0)$ of the incident laser beam (in the plane $z = 0$) has a Gaussian profile. In view of the relation (10), the latter is determined by the distribution of $\phi(y,0)$:

$$\begin{aligned}\mathrm{Re}[\phi(y,0)] &= a\exp\left[-\frac{(y-y_0)^2}{L^2}\right],\\ \mathrm{Im}[\phi(y,0)] &= 0\,,\end{aligned} \tag{11}$$

where L is the beam half-width, y_0 is the coordinate of the maximum field intensity of the beam along the axis Oy, and a is the dimensionless parameter determined by the frequency and initial amplitude of the electric field of the incident beam (in the plane $z = 0$):

$$a = \frac{E_0 e d_x}{\hbar\omega}\sqrt{2}\,, \tag{12}$$

as it follows from Eq. (10) with account of Eq. (11).

The choice of initial conditions in the form of (11) is due to the fact that the Gaussian intensity distribution is known to be of great interest from a practical point of view in a wide range of applications. This is due to the fact that the minimal diffraction spreading is observed for Gaussian beams and such beams are closest to the reality, being an approximation, most simply and completely describing the properties of laser radiation.[27–31]

To our knowledge, Eq. (9) has no exact analytical solutions in a general case. In the present study it is solved numerically together with the initial condition (11). For the numerical solution of this equation we apply the implicit difference scheme. Difference scheme steps in both time and coordinates where iteratively decreased twice until the solution became unchanged in the eighth decimal place.

Figure 2 represent the typical results of modeling of a monochromatic laser beam in an array of semiconductor carbon nanotubes.

Figure 2 shows the field intensity distribution in an array of nanotubes during the propagation of a Gaussian beam with half-width $L = 6 \cdot 10^{-4}$ cm in a nanotube array of the $(7, 0)$ type for the above-mentioned values of other parameters of the system. The field intensity is represented by the ratio $I/E_0^2 = |\phi|^2/a^2$ [see Eqs. (10)–(12)], different values of which are set in correspondence to the linear dependence of the shades of gray scale. Most bright areas correspond to high intensity zones, and the darkest to the low ones. Horizontal and vertical axes on Fig. 2 correspond to the dimensionless coordinates $\nu = y\omega_0/c$ and $\zeta = z\omega_0/c$, respectively. For the values of the parameters chosen above, units on the axes $O\nu$ and $O\xi$ correspond to distances $\Delta y = \Delta z \approx 3 \cdot 10^{-4}$ cm. Figure 2 highlights

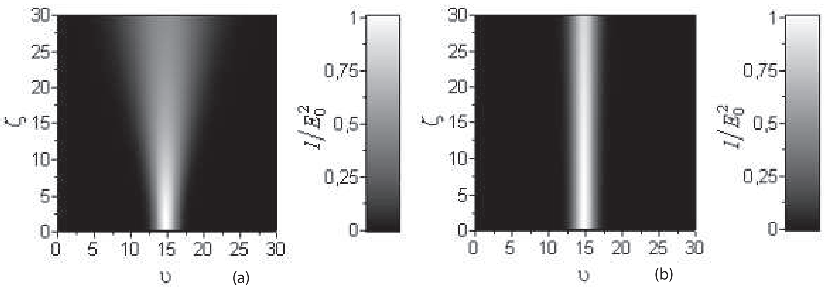

Fig. 2. Propagation of a Gaussian laser beam for different values of E_0 and ω. (a) $E_0 = 10^3$ V/cm, $\omega = 2 \cdot 10^{14}$ s^{-1}; (b) $E_0 = 10^6$ V/cm, $\omega = 10^{15}$ s^{-1}. The axes are scaled using dimensionless coordinates $\nu = y\omega_0/c$ and $\zeta = z\omega_0/c$.

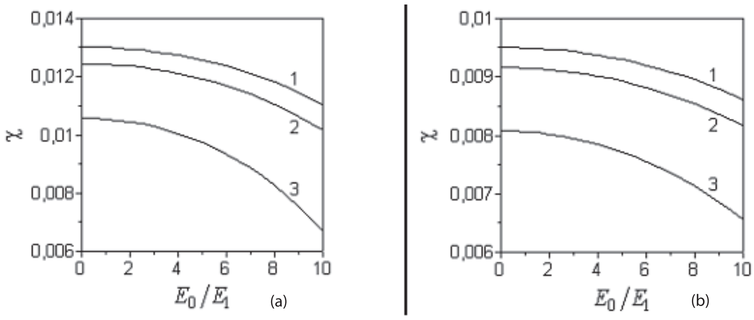

Fig. 3. Behavior of $\chi(E_0)$ at fixed ω for different values of m: $1 - m = 7$; $2 - m = 8$; $3 - m = 10$. The values of ω used are: (a) $\omega = 5 \cdot 10^{14}$ s^{-1}; (b) $\omega = 7 \cdot 10^{14}$ s^{-1}. Unit on the horizontal axis corresponds to a field $E_1 = 10^5$ V/cm .

that during the propagation of the Gaussian laser beam in an array of nanotubes diffraction spreading occurs. After the distance $\Delta z \approx 9{\cdot}10^{-3}$ cm $\gg \lambda$ ($\lambda = 2\pi c/\omega\sqrt{\epsilon}$ is the wavelength of the beam in the medium), the beam remains visible and has a peak intensity $I_{\text{peak}} \approx 0.5 \cdot E_0^2$ at $E_0 = 10^3$ V/cm and $\omega = 3 \cdot 10^{14}$ s^{-1} [$\lambda \approx 4.7{\cdot}10^{-4}$ cm, Fig. 2(a)]; or $I_{\text{peak}} \approx 0.8{\cdot}E_0^2$ at $E_0 = 10^6$ V/cm and $\omega = 10^{15}$s^{-1} [$\lambda \approx 9.4 \cdot 10^{-5}$ cm, Fig. 2(b)]. Thus, changing the frequency and initial amplitude of the laser beam can effectively influence the spreading of the beam in an array of nanotubes.

The process of diffraction spreading of the laser beam clearly exhibited in Fig. 2 is quantified here by the dimensionless measure

$$\chi = \frac{\Delta I_{\text{peak}}}{E_0^2 \Delta\xi} = \frac{\Delta|\phi_{\text{peak}}|^2}{a_0^2 \Delta\zeta}\,, \tag{13}$$

which is a ratio of the relative change of the peak intensity of the beam field and the dimensionless distance $\Delta\zeta = \omega_0 \Delta z/c$, corresponding to that change.

Figure 3 shows the dependence of the diffraction spreading χ on the initial amplitude E_0 of the field intensity of the beam, incident on an array of nanotubes of the type $(m, 0)$ at a fixed frequency ω of the field for different values of the index m. It is clear from the figure that the values of the parameter χ that characterizes the diffraction spreading of the laser beam decrease in a nonlinear way with increasing the amplitude of its electric field. We also note the strong dependence of the absolute value of χ on the frequency ω, which in turn suggests that we can substantially reduce the diffraction spreading by relatively small variation in the laser frequency.

Figure 4 demonstrates the dependence of χ on the frequency ω of the beam field at a fixed initial amplitude of the electric field E_0 for the cases of beam propagation in a homogeneous dielectric without nanotubes (curve 1), as well as in an array of nanotubes with different values of m (curves 2–4). The main conclusion from Fig. 4 is that the rate of diffraction spreading decreases with increasing frequency. Dependencies $\chi(E_0)$ and $\chi(\omega)$, as shown in Figs. 3 and 4, can be attributed, in our opinion, to the dependence of the dispersion and nonlinearity (which, in turn, are

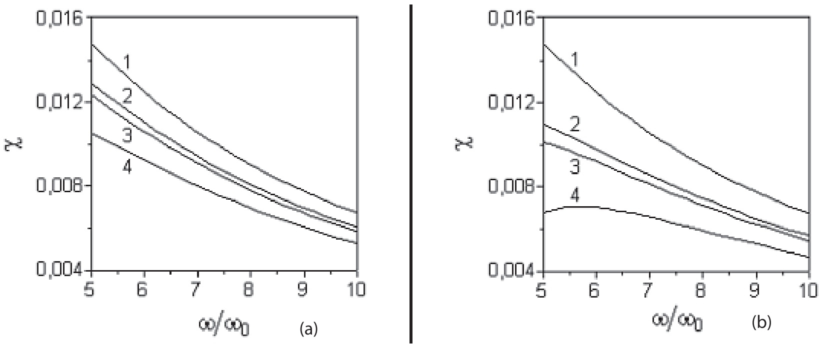

Fig. 4. Behavior of $\chi(\omega)$ at fixed E_0. Curve 1 corresponds to a homogeneous dielectric without nanotubes ($\varepsilon = 4$); curves 2–4 demonstrate the results for an array of nanotubes in various cases: 2 – $m = 7$; 3 – $m = 8$; 4 – $m = 10$. The values of E_0 used are: (a) $E_0 = 10^3$ V/cm; (b) $E_0 = 10^6$ V/cm.

determined by the quantity $2ik\partial\phi/\partial z$ and the term containing the sum over α in Eq. (9), respectively) on the frequency ω and amplitude E_0 of the initial field of the laser beam.

This kind of dependence in Figs. 3 and 4 is connected to the fact that the nonlinearity results in a focusing effect on the laser beam. Speaking the language of classical optics, the laser beam changes the effective refractive index of the medium in which it propagates. The latter leads to the formation of the region, similar to the optical waveguide; with a high refraction index at the edges. As a result, the laser beams of greater amplitude are less susceptible to diffraction, which in turn leads to the dependence on the frequency shown in Fig. 4. This is due to the fact that the frequency appears in the non-linear (the last one) term in Eq. (9). This, in turn, allows for a simple test of the predicted effects either by the measurement of the radius of the laser beam at the output of a medium containing carbon nanotubes, or by the threshold effect (see Fig. 2), which leads to the fact that the laser beam of a small-amplitude just decreases its amplitude due to a diffraction spreading.

Note that the spreading of a laser beam propagating in a nonlinear medium of the array of nanotubes placed in a dielectric is much less intense than in a homogeneous dielectric in the absence of nanotubes (see Fig. 4), as nonlinearity significantly compensates the dispersion spreading. Figures 3 and 4 also show that the value of the parameter m affects the process of spreading of the laser beam, that is reflected in change of the shape of the curves $\chi(E_0)$ and $\chi(\omega)$ with changing m (see the curves 2–4 of Figs. 3 and 4). With the growth of the index m, the spreading rate χ decreases. This relationship can be attributed to the reconstruction of the electron energy spectrum of nanotubes due to changes in the parameter m. As shown in Ref. 34, an increase in m leads to an increase in the effective nonlinearity, which prevents spreading of the electromagnetic wave. Thus, changing the parameters of the incident radiation, can effectively reduce the intensity of its spreading during the propagation through an array of nanotubes. This fact, in our opinion, may be crucial in the choice of semiconductor arrays of carbon nanotubes as the basis for the development of optoelectronic devices to control the laser field.

5. Conclusion

The main results of our work can be summarized as follows:

(i) We derived the effective equation describing the propagation of a monochromatic Gaussian laser beam in an array of semiconducting carbon nanotubes.
(ii) The numerical simulation revealed that the laser beam in an array of nanotubes, experiencing diffraction spreading, propagates a significant distance, conserving the peak intensity at a level acceptable for practical applications.
(iii) Increasing the frequency and amplitude of the initial field of the laser beam leads to a weakening of its diffraction spreading in an array of nanotubes.
(iv) Increasing the nanotube structural parameter m leads to a weakening of the diffraction spreading of the laser beam.

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