ISSN 1062-8738, Bulletin of the Russian Academy of Sciences. Physics, 2012, Vol. 76, No. 12, pp. 1280–1282.
Original Russian Text © A.V. Pak, N.N. Yanyushkina, M.B. Belonenko, 2012, published in Izvestiya Rossiiskoi Akademii Nauk. Seriya Fizicheskaya, 2012, Vol. 76, No. 12, pp. 1434–1436.

Propagation of Extremely Short Optical Pulses in Impurity Carbon Nanotubes in Dispersive and Nonlinear Media

A. V. Pak[a], N. N. Yanyushkina[a], and M. B. Belonenko[b, c]

[a] *Volgograd State University, Volgograd, 400062 Russia*
[b] *Volgograd Institute of Business, Volgograd, 400048 Russia*
[c] *Entropique Inc., London, ON, N6J 3S2 Canada*
e-mail: pak.anastasia@gmail.com

Abstract—Maxwell equations describing an extremely short pulse propagating in impurity carbon nanotubes placed in a dispersive nonmagnetic medium are analyzed with allowance for the nonlinearity of the medium. The dependences of the magnetic field intensity on the initial pulse amplitude and the parameters of the medium are revealed.

DOI: 10.3103/S1062873812120258

INTRODUCTION

The propagation of extremely short 10^{-15} s pulses in optical media without damage to the material allows us to observe and study nonlinear phenomena that occur very rarely in the fields of pulses of long duration [1]. These phenomena include superbroadening of the time spectrum.

This work considers the dynamics of extremely short pulses that propagate in carbon nanotubes (CNTs) capable of displaying nonlinear properties in dispersive nonmagnetic media. Extremely short pulses are those that consist of several field oscillations [2–4]. The unique electrophysical characteristics of CNTs allow us to use them in different electronic devices (e.g., transistors and diodes) [5, 6]. The authors of [7] considered a case that is important from the practical point of view used to analyze propagation of pulses in waveguide structures. It considers both the nonlinearity and the dispersion of the medium. Impurity CNTs are considered because they are the best objects for experimental fabrication.

PROBLEM STATEMENT AND BASIC EQUATIONS

We consider a pulse of an alternating electric field propagating in a carbon nanotube system.

The Hamiltonian of the electron subsystem can be written as

$$H = \sum_{j,\Delta,\sigma} t_\Delta (c^+_{j\sigma} c_{j+\Delta\sigma} + c^+_{j+\Delta\sigma} c_{j\sigma}) + \sum_{l,\sigma} \varepsilon_{l\sigma} n^d_{l\sigma} + \sum_l U n^d_{l\uparrow} n^d_{l\downarrow} + \sum_{l,j,\sigma} \left(V_{lj} c^+_{j\sigma} d_{l\sigma} + h.c. \right), \quad (1)$$

where $a^+_{j\sigma}$ and $a_{j\sigma}$ are the operators of the generation and annihilation of electrons with spin σ at node j, and t_0 is the integral of the electron jumps determined by the overlapping of the functions of neighboring units.

The spectrum of electrons that describes the properties of the electron subsystem in the absence of Coulomb repulsion U (with allowance for the addition of impurities to the atomic surfaces of zig-zag CNTs) is [8]

$$E_l(k) = \frac{1}{2}\left[\varepsilon_k + \varepsilon_{l\sigma} \pm \sqrt{(\varepsilon_k - \varepsilon_{l\sigma})^2 + 4\frac{N_{imp}}{N}|V_{lj}|^2} \right], \quad (2)$$

where ε_k is the electron spectrum for an ideal nanotube, $\varepsilon_{l\sigma}$ is the energy of an electron with spin σ on impurity l, V_{lj} is the matrix element for hybridization of the electron states of impurity l and atom j of the crystal, N_{imp} is the number of the impurity atoms, and N is the number of unit cells. The expression for ε_k is [8]

$$\varepsilon(k) = \pm t_0 \sqrt{1 + 4\cos(ak)\cos(\pi q/n) + 4\cos^2(\pi q/n)},$$

where $q = 1, 2 \ldots n$, the nanotube is of the $(n, 0)$ type; $t_0 \approx 2.7$ eV; $a = 3b/2\hbar$, and $b = 0.142$ nm is the length of a C–C bond.

Maxwell's equation for nonmagnetic dielectric media is reduced to the form [9]

$$\frac{\partial^2 \vec{E}}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2} + \frac{4\pi}{c}\frac{\partial \vec{j}}{\partial t} = \frac{4\pi}{c^2}\frac{\partial^2 \vec{P}_L}{\partial t^2} + \frac{4\pi}{c^2}\frac{\partial^2 \vec{P}_{NL}}{\partial t^2}, \quad (3)$$

where $\vec{E}$ is the electric field of the light wave; $\vec{P}_L = \alpha\vec{E}$ is the polarization response of the medium, linear over the field; $\vec{P}_{NL} = \eta|\vec{E}|^2\vec{E}$ is the nonlinear part of the polarization response; t is time, and c is the speed of light in a vacuum. In this problem, we used an elementary model describing the medium's nonlinearity. It considered that the polarization vector is parallel to the vector $\vec{E}$.

Equation (3) was modified to describe the propagation of pulses with a broad spectrum in a linear medium (for when $\eta = 0$) [10]. The dependence of the linear refraction index of isotropic optical media n in light frequency ω in the range of their transparency can be described with almost any level of accuracy by a correlation of the type [11, 12]

$$n^2(\omega) = N_0^2 + 2cN_0 a\omega^2 + 2cN_0 a_1\omega^4 + \ldots - 2cN_0 b\omega^{-2} - 2cN_0 b_1\omega^{-4}, \tag{4}$$

where $N_0, a, a_1, \ldots, b, b_1\ldots$ are empirical constants of the mediums' dispersion. Dispersion correlation (4) yields a wave equation of the type

$$\frac{\partial^2\vec{E}}{\partial x^2} - \frac{N_0^2}{c^2}\frac{\partial^2\vec{E}}{\partial t^2} = -\frac{2N_0}{c}a\frac{\partial^4\vec{E}}{\partial t^4} + \frac{2N_0}{c}a_1\frac{\partial^6\vec{E}}{\partial t^6} - \ldots + \frac{2N_0}{c}b\vec{E} - \frac{2N_0}{c}b_1\int_{-\infty}^{t}dt'\int_{-\infty}^{t'}\vec{E}dt'' + \ldots. \tag{5}$$

Equation (5) describes the propagation of pulses along the x axis in the forward and backward directions.

Comparing Eqs. (3) and (5), allowing for the Coulomb calibration

$$\vec{E} = -\frac{1}{c}\frac{\partial\vec{A}}{\partial t},$$

and restricting ourselves to the fourth derivative, we can demonstrate that the following type of equation is a generalization of Eq. (5) with the nonlinearity of the medium taken into account:

$$\frac{\partial^2\vec{A}}{\partial x^2} + \frac{2N_0}{c}a\frac{\partial^4\vec{A}}{\partial t^4} - \frac{2N_0}{c}b\vec{A} + \frac{4\pi}{c}\vec{j} - \frac{1}{c^2}(1+4\pi\alpha)\frac{\partial^2\vec{A}}{\partial t^2} - \frac{12\pi\eta}{c^4}\frac{\partial^2\vec{A}}{\partial t^2}\left(\frac{\partial\vec{A}}{\partial t}\right)^2 = 0. \tag{6}$$

Vector potential $\vec{A}$ has the form $\vec{A} = (0, 0, A(x,t))$.

The expression for current density is

$$\vec{j}_0 = e\sum_{ps}\vec{\upsilon}_s\left(p - \frac{e}{c}A(t)\right)\left\langle a_{ps}^{+}a_{ps}\right\rangle, \tag{7}$$

where $\upsilon_s(p) = \partial\varepsilon_s(p)/\partial p$, and the bent brackets denote averaging over the nonequilibrium density matrix $\rho(t)$: $\langle B\rangle = Sp(B(0)\rho(t))$.

Expanding $\upsilon_s(p)$ into a Fourier series yields the form

$$\upsilon_s(p) = \sum_k A_{ks}\sin(kp),$$

$$A_{ks} = \frac{1}{2\pi}\sum_p \upsilon_s(p)\sin(kp).$$

Substituting the result into Eq. (7), we perform summation over p and s:

$$j_0 = -en_0\sum_k D_k\sin\left(\frac{ke}{c}A(t)\right),$$

$$D_k = \sum_{s=1}^{m}\int_{-\pi/a}^{\pi/a} dpA_{ks}\cos(kp)\frac{\exp(-\beta\varepsilon_s(p))}{1+\exp(-\beta\varepsilon_s(p))}, \tag{8}$$

where n_0 is the density of equilibrium electrons in a CNT, and $\beta = 1/kT$.

In light of the above, Eq. (5) (after it is madet dimensionless) can be written as

$$\frac{\partial^2 B}{\partial x'^2} - (1+4\pi\alpha)\frac{\partial^2 B}{\partial t'^2} - 12\pi\eta\frac{\partial^2 B}{\partial t'^2}\left(\frac{\partial B}{\partial t'}\right)^2 + \frac{2N_0 a}{c}\frac{\partial^4 B}{\partial t'^4} - \frac{2N_0 bB}{c} + \sin(B) + \sum_{k=2}^{\infty}B_k\sin(kB) = 0, \tag{9}$$

$$B = \frac{eaA}{c};\quad x' = \frac{ea}{c}\sqrt{8\pi\gamma};\quad t' = t\frac{ea}{c}\sqrt{8\pi n_0\gamma|B_1|}.$$

NUMERICAL SIMULATION

The analyzed Eq. (9) was numerically solved using a cross-type direct difference scheme. The time and coordinate steps were determined from the standard stability conditions. The steps of the difference scheme were sequentially reduced by half until the solution changed at the 8th significant sign. The initial condition was chosen as

$$B(x,t) = Q\exp\left(-\frac{(x-\upsilon t)^2}{\gamma}\right),$$

$$\gamma = (1-\upsilon^2)^{1/2},$$

where Q is the pulse amplitude. υ determines the pulse propagation rate, and γ specifies the width of the initial pulse.

The evolution of the electric field over time is shown in Fig. 1.

Comparing Figs. 1a and 1b, we can state that taking linear (α parameter) and nonlinear (η parameter) polarization of the medium into account yields a reduction in pulse amplitude and the leveling of the two pulse maxima. This can be attributed to a pulse expending energy on medium polarization, and to the formed nonlinearity that levels the pulse amplitudes. The pulse amplitude does not rise further due to dispersion effects.

The evolution of an ultrashort optical pulse depends most strongly on the initial pulse amplitude. Figure 2 exemplifies such a dependence. We believe this effect is related to the periodic character of nonlinearity in Eq. (10).

Our calculations showed that the nature of an impurity does not affect the propagation of a pulse in the nanotube medium, since the presence of an impurity yields an additional localized absorption level in the energy band structure of the CNT. This level is, however, too deep to affect the analyzed effects. This statement is in agreement with the results from other studies on impurity structures [8, 13].

Based on the results from numerical calculations, we may conclude that medium dispersion and nonlinearity influence the propagation of ultrashort pulses in CNTs, nonlinear processes turn out to be more important than those of dispersion.

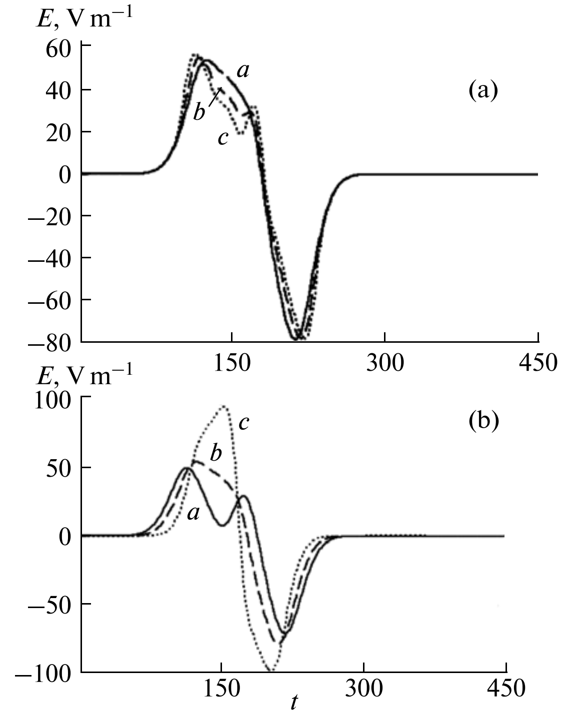

Fig. 1. Time dependence of an electric field determined by the potential in Eq. (9). Dimensionless time is plotted on the x axis (unity corresponds to 3×10^{-16} s), while the y axis represents the dimensionless value of the electric field (unity corresponds to 10^8 V/m). All quantities are in dimensionless units. (a) (*a*) $\alpha = 0.5$, (*b*) $\eta = 0.1$, (*c*) $\eta = 0.3$, (*d*) $\eta = 0.5$; (b) (*a*) $\eta = 0.1$, (*b*) $\alpha = 0.9$, (*c*) $\alpha = 0.5$, (*d*) $\alpha = 0.1$.

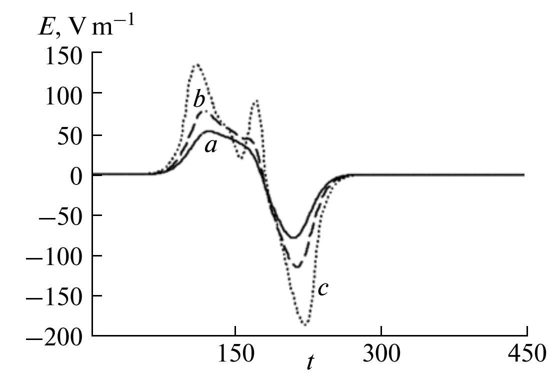

Fig. 2. Time dependence of the electric field determined by the potential in Eq. (9) for different initial pulse amplitudes. Dimensionless time is plotted on the x axis (unity corresponds to 1×10^{-16} s), while the y axis represents the dimensionless value of the electric field (unity corresponds to 10^7 V/m). (*a*) Q = 2; (*b*) $Q = 3$, (*c*) $Q = 5$.

CONCLUSIONS

The key conclusions from this work are below.

—An effective equation for the dynamics of extremely short optical pulses in impurity carbon nanotubes have been derived (with medium dispersion and nolinearity taken into account).

—The shape of extremely short optical pulses depends on the initial pulse amplitude, which is related to the character of carbon nanotube nonlinearity.

—It was shown that the propagation of extremely short optical pulses in a dispersive nonmagnetic medium (with the medium nonlinearity taken into account) depends mainly on nonlinear processes, while the effect of dispersion constants *a* and *b* is much weaker.

—The characteristics of impurity atoms (the hybridization energy and adatom levels) do not affect the propagation of an optical pulse in a nanotube medium, due to an additional level of adsorption very deep in the valence band.

ACKNOWLEDGMENTS

This work was supported by the federal target program Scientists and Science Teachers of an Innovative Russia, 2009–2013 (project no. 14.740.11.0374); and by the Russian Foundation for Basic Research (project no. 11-02-97054).

REFERENCES

1. Von der Linde, D. and Schuler, H., *J. Opt. Soc. Am. B*, 1999, vol. 13, no. 1, pp. 216–222.
2. Baltuska, A., Wei, Z., Pshenichnikov, M.S., and Wiersma, D.A., *Opt. Lett.*, 1997, vol. 22, no. 2, pp. 102–104.
3. Nisoli, M., De Silvestri, S., Svelto, O., et al., *Opt. Lett.*, 1997, vol. 22, no. 8, pp. 522–524.
4. Brabec, Th. and Krausz, F., *Rev. Mod. Phys.*, 2000, vol. 72, no. 2, pp. 545–591.
5. Novoselov, K.S., et al., *Science*, 2004, vol. 306, pp. 666–669.
6. Novoselov, K.S., et al., *Nature*, 2005, vol. 438, pp. 197–200.
7. Yanyushkina, N.N., Belonenko, M.B., and Lebedev, N.G., *Opt. Spektrosk.*, 2011, vol. 111, no. 1, pp. 92–97.
8. Belonenko, M.B., Popov, A.S., Lebedev, N.G., et al., *Phys. Lett. A*, 2011, vol. 375, p. 946.
9. Slepyan, G.Ya., Maksimenko, S.A., Kalosha, V.P., et al., *Phys. Rev. A*, 1999, vol. 60, no. 2, p. R777.
10. Vinogradova, M.B., Rudenko, O.V., and Sukhorukov, A.P., *Teoriya voln* (Waves Theory), Moscow: Nauka, 1990.
11. Kozlov, S.A., *Vestn. Molodykh Uchenykh. Ser. Fiz.*, 2000, vol. 1, p. 7.
12. Born, M. and Wolf, E., *Principles of Optics*, Oxford: Pergamon, 1969; Moscow: Nauka, 1973.
13. Nemilentsau, A.M., Slepyan, G.Ya., Khrutchinskii, A.A., and Maksimenko, S.A., *Carbon*, 2006, vol. 44, pp. 2246–2253.