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Modeling of the Nano-acoustic-electronic Converter on the Basis of Graphene Nanotubes

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In the paper, the model of the nano-acoustic-electronic converter on the basis of a graphene nanotube is constructed and the amplitude-frequency characteristic is calculated. Within this model, the frequency dependences of the strain amplitude, surface concentration of electrons and electrostatic potential are determined. It is established that the nanoconverter sensitivity increases with increasing concentration of electrons and decreasing radius of the nanotube.

Keywords: Graphene nanotube, Acoustic wave, Acoustic-electronic interaction, Strain.

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1. INTRODUCTION

The unique electronic and mechanical properties of single-layer graphene, especially, high carrier mobility at room temperature (~ 10^5 cm²/V·s), electron-hole symmetry and high values of the Young modulus (~ 10^{12} Pa), make this material very promising for nanoelectronics [1], in particular, for the creation of high-speed single-electron transistors, photodetectors, infrared light-emitting diodes and low-barrier Schottky diodes based on graphene [2]. The nanotubes formed on the basis of graphene have a high resonance frequency (more than 3 GHz), since their Young modulus is equal to ~ 1 TPa [3-5] and, depending on the symmetry type, have metallic or semiconductor properties [5].

In order to create any device on the basis of graphene or experimentally determine the properties of graphene itself, it is necessary to have metal contacts. One of the methods for obtaining graphene consists in the thermal action on silicon carbide (SiC); as a result, silicon atoms leave the surface SiC layers and residual carbon atoms form a hexagonal structure generating an epitaxial graphene layer [6]. However, graphene monolayer acquires a negative charge, so that the Fermi level is shifted from its initial position at the Dirac point upward violating the electron-hole symmetry [1, 7]. To avoid this, the covalent bonds in the G-SiC system are broken by intercalation of hydrogen into the space between the sheet of graphene and the SiC substrate [8, 9].

The second method for obtaining epitaxial graphene is the catalytic growth of graphene on the surface of transition metals from gases containing carbon. A graphene nanotube can be represented as a result of gluing of a graphene sheet into a cylindrical surface. The electronic properties of a nanotube, such as the carrier concentration and mobility, band gap, conductivity, are determined by its geometry, whose main parameters are the diameter and chirality, i.e. the orientation angle of the graphite surface relative to the nanotube axis [10].

An important property of a nanotube is the presence in it of a strong interaction between its electronic characteristics and mechanical strain [11-14]. The band gap, carrier concentration, phonon spectrum, etc. vary due to strain. This, in turn, is manifested in the electrical conductivity of the nanotube. Thus, the nanotube is a very efficient converter of mechanical oscillations into an electrical signal and vice versa that makes it a unique element of nanoelectromechanical systems.

The frequency characteristic of the device is among the main specifications, which determine the possibility of practical application of the devices based on electromechanical properties of graphene nanotubes (GNT). The higher frequency of an electrical signal, on which this device responds adequately, the larger conversion rate of information and, finally, its efficiency increases [12].

The acoustic-electronic effects in a graphene nanotube are investigated and the amplitude-frequency characteristics of a nanoelectromechanical converter based on a graphene nanotube are calculated in this work.

2. MODEL

We consider a graphene nanotube of height H, radius R_0 and wall thickness d ($d << R_0$), which is subjected to an acoustic wave with frequency ω. We will assume that the wave propagates along the Oz axis, which coincides with the axial axis of the nanotube. The components of the displacement vector of the i-th carbon atom $\mathrm{u}_i(t,\mathrm{r})$ are found taking into account that the displacement of each carbon atom can be expanded in a series due to the atomic displacement $\mathrm{u}(\mathrm{r},t)$ in the continual approximation [10]:

$$\mathrm{u}_i - \mathrm{u}_0 \propto (\boldsymbol{\rho}_i \nabla)\mathrm{u}(\mathrm{r},t), \qquad (1)$$

where ρ_i is the radius-vector of the nearest neighbors; u_0 is the displacement vector of the central atom; $\mathrm{u}(\mathrm{r},t)$ is the field of atomic displacements determined in the cylindrical system of coordinates based on the following system of equations:

$$(\lambda + 2G)\frac{\partial \theta}{\partial r} = \rho \frac{\partial^2 u_r}{\partial t^2}, \qquad (2)$$

$$(\lambda + 2G)\frac{\partial \theta}{\partial z} = \rho \frac{\partial^2 u_z}{\partial t^2}, \qquad (3)$$

where λ, G are the Lame coefficients; ρ is the graphene density; $\theta = \frac{1}{r}\frac{\partial(ru_r)}{\partial r} + \frac{\partial u_z}{\partial z}$.

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The solutions of the system of equations (2), (3) will be sought in the form

$$u_r(r,z,t) = U(r)e^{i\omega t}\cos kz \,,$$

$$u_z(r,z,t) = W(r)e^{i\omega t}\sin kz \,,$$

where $k = \omega/c_l$; c_l is the longitudinal velocity of acoustic vibrations.

The spatially inhomogeneous deformation caused by an acoustic wave modulates the surface energy σ that leads to the appearance of the lateral mechanical stress $\sigma_{rz} = \sigma_0 e^{i\omega t}\sin kz$, which is compensated by the shear stress in the medium. The boundary condition expressing the balance of the lateral stresses has the form

$$G\left(\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r}\right)_{r=R_0} = \sigma_0 \sin kz \,. \qquad (4)$$

Moreover, the quantization condition of acoustic phonon modes should be fulfilled [15]

$$\frac{1}{2Hd}\int_0^H \int_{R_0-d}^{R_0} \left(u_r^* u_r + u_z^* u_z\right) dz dr = \frac{\hbar}{2M\omega} \,, \qquad (5)$$

M is the mass of the carbon nanotube.

So, strain ξ on the graphene nanotube surface

$$\xi = \frac{\partial u_r}{\partial r} + \frac{u_r}{r} + \frac{\partial u_z}{\partial z} = \xi_0(R_0,\omega)\cos(\omega t - kz) \,, \quad (6)$$

where ξ_0 is the strain amplitude determined from the system of equations (2)-(5).

The periodic surface deformation leads to modulation of the conduction band bottom and, correspondingly, to re-distribution of the surface concentration of conduction electrons $n(x)$ and electrostatic potential $\varphi(x)$

$$n(z) = n_0 + n_1(z) = n_0 + n_1(k)e^{i\omega t + \alpha}\cos kz \,, \quad (7)$$

$$\varphi(z) = \varphi(k)e^{i\omega t + \alpha}\cos kz \,, \qquad (8)$$

where $n_1(k)$, $\varphi(k)$ are the amplitudes of the corresponding periodic perturbations.

Let us write the Poisson equation, which accounting (7)-(8) takes the form

$$-k^2\varphi(k) = \frac{e}{\varepsilon_0 \tilde{\varepsilon} d} n_1(k) \,, \qquad (9)$$

where ε_0, $\tilde{\varepsilon}$ are the dielectric constant and dielectric permittivity of the medium, respectively.

The electron current density is

$$j = n\mu_n \frac{d\chi}{dz} \,, \qquad (10)$$

where μ_n is the electron mobility and the electrochemical potential χ is determined by the relation [16, 17]

$$\chi(z) = k_B T \ln\frac{n(z)}{N_i} - e\varphi(z) + a_c\xi(z) \,, \qquad (11)$$

$N_i = 2\left(\frac{2\pi m k T}{h^2}\right)^{3/2}$ is the effective density of states; a_c is the constant of hydrostatic deformation potential of the conduction band. Taking into account (10), (11), the continuity equation can be written in the form

$$e\frac{\partial n}{\partial t} = k_B T\mu_n \frac{\partial}{\partial z}\left(n\frac{\partial}{\partial z}\ln\frac{n}{N_i}\right) - $$
$$- e\mu_n \frac{\partial}{\partial z}\left(n\frac{\partial \varphi}{\partial z}\right) + a_c\mu_n \frac{\partial}{\partial z}\left(n\frac{\partial \xi}{\partial z}\right). \qquad (12)$$

Substituting (6)-(8) into (12), we obtain

$$i\omega e n_1(k) = \mu_n k^2 n_0\left(e\varphi(k) - a_c\xi_0 - k_B T\frac{n_1(k)}{n_0}\right). \quad (13)$$

Having solved the system of equations (9) and (13), we derive

$$\varphi(k) = \frac{\xi_0 a_c / e}{\sqrt{\left(1 + \frac{k_B T k^2}{\Phi n_0}\right)^2 + \left(\frac{\omega e}{\Phi\mu_n n_0}\right)^2}} \,, \qquad (14)$$

$$\alpha = -arctg\frac{e\omega}{\Phi\mu_n n_0 + k_B T\mu_n k^2} \,,$$

where $\Phi = \dfrac{e^2}{\varepsilon_0\tilde{\varepsilon} d}$.

3. RESULTS AND DISCUSSION

In Fig. 1, Fig. 2 we illustrate the dependences of the mechanical strain and electrostatic potential amplitude on the acoustic wave frequency at different values of the radius and length of the carbon nanotube. The calculations were performed at the following parameter values: $\sigma_0 = 10^4$ Pa, $T = 300$ K, $\mu_n = 10^5$ cm^2/V·s, $a_c = 2.46$ eV, $d = 0.15$ nm. Size dependence of the elastic constants is taken into account in the calculations [18].

As seen from Fig. 1, a sharp increase in the mechanical strain amplitude is observed in the carbon nanotube for the acoustic wave frequency of $\omega \sim c_l/L$ (Fig. 1b) and $\omega \sim c_l/R_0$ (Fig. 1a). An increase in the carbon nanotube radius leads to a decrease in the resonance frequencies and an increase in the strain amplitude. This is explained by the fact that a monotonic increase in the elastic constants is observed with decreasing nanotube radius [18].

In Fig. 2 we show the dependence of the electrostatic potential amplitude on the acoustic wave frequency for different values of the carbon nanotube radius (Fig. 2a) and its length (Fig. 2b). As seen from Fig. 2, the amplitude of the electric potential induced by an acoustic wave substantially depends on the acoustic wave frequency and the nanotube geometry. A monotonic decrease in the electrostatic potential amplitude occurs with decreasing carbon nanotube radius and length. This is explained by the fact that graphene nanotubes of smaller sizes are less sensitive to strain. As seen from Fig. 2, in the frequency range of $10^9\ \text{s}^{-1} < \omega < 10^{11}\ \text{s}^{-1}$, the amplitude of the electric potential induced by an acoustic wave almost does not depend on the nanotube radius.

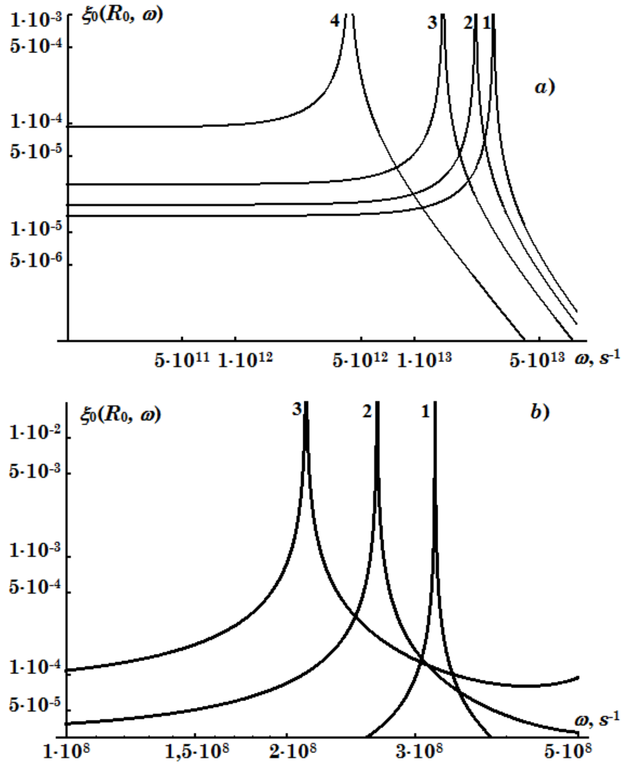

Fig. 1 – Dependence of the strain amplitude on the acoustic wave frequency at different values of the graphene nanotube radius: 1 – R_0 = 0.5 nm; 2 – R_0 = 0.8 nm; 3 – R_0 = 1.5 nm; 4 – R_0 = 5 nm (a) and length: 1 – L = 100 μm; 2 – L = 120 μm; 3 – L = 150 μm (b)

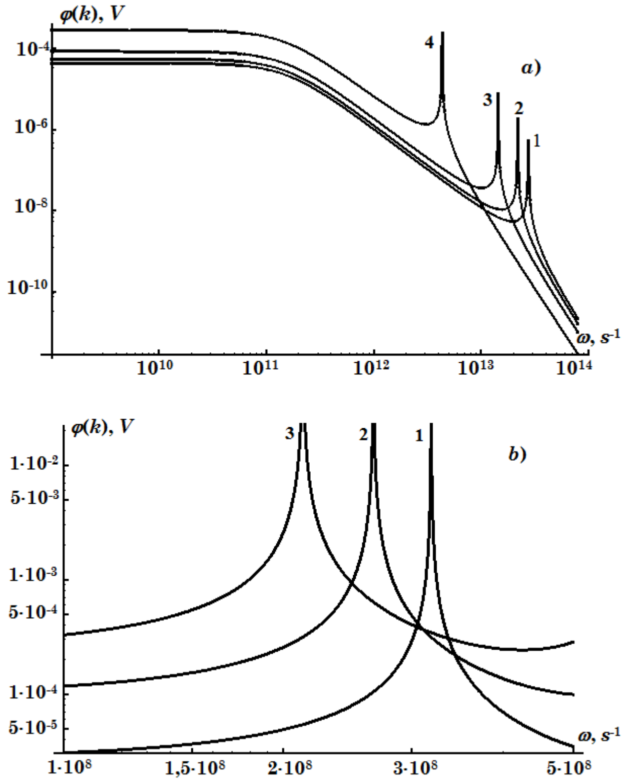

Fig. 2 – Dependence of the electrostatic potential amplitude on the acoustic wave frequency at different values of the graphene nanotube radius: 1 – R_0 = 0.5 nm; 2 – R_0 = 0.8 nm; 3 – R_0 = 1.5 nm; 4 – R_0 = 5 nm (a) and its length: 1 – L = 100 μm; 2 – L = 120 μm; 3 – L = 150 μm (b)

In Fig. 3 we present the dependence of the electrostatic potential amplitude on the acoustic wave frequency at different values of the surface electron concentration. A monotonic increase in the electrostatic potential amplitude is observed with increasing electron concentration. Moreover, an increase in the electron concentration leads to the expansion of the frequency range, in which the electrostatic potential is constant. When the acoustic wave frequency exceeds a certain value, which depends on the electron concentration, then the electrostatic potential amplitude decreases sharply. This is due to the fact that the local displacement of the conduction band bottom on account of strain is compensated by the electrostatic displacement. As seen from Fig. 3, a slight decrease in the resonance frequencies of the electrostatic potential is observed with increasing surface electron concentration.

We should also note that the electrostatic potential amplitude is proportional to the electron mobility in the graphene nanotube.

The sensitivity of the acoustic-electronic converter is determined by the relation

$$\gamma_\varphi = \left.\frac{d\varphi}{d\sigma}\right|_{T=const}. \qquad (15)$$

Substituting (14) into (15), we obtain the expression for the acoustic-electronic converter sensitivity, which depends on the electron concentration and mobility and also graphene nanotube geometry.

$$\gamma_\varphi = \frac{a_c / e}{\lambda\sqrt{\left(1+\frac{k_B T k^2}{\Phi n_0}\right)^2+\left(\frac{\omega e}{\Phi \mu_n n_0}\right)^2}}. \qquad (16)$$

As seen from formula (16), the sensitivity of the acoustic-electronic converter increases with increasing electron concentration and mobility. In addition, a decrease in the graphene nanotube thickness leads to an increase in the converter sensitivity. The sensitivity of the acoustic-electronic converter based on the graphene nanotube of the radius of 0.5 nm and the surface electron concentration of $n_0 = 10^6$ cm^{-2} is equal to ~ 10^{-4} μV/Pa. Thus, varying technologically the geometric sizes and electron concentration, it is possible to predictably increase the converter sensitivity in the specified frequency range.

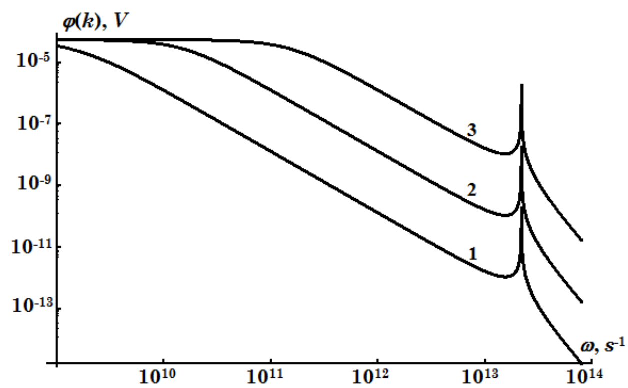

Fig. 3 – Dependence of the electrostatic potential amplitude on the acoustic wave frequency at different values of the surface electron concentration: 1 – $n_0 = 10^4$ cm^{-2}; 2 – $n_0 = 10^6$ cm^{-2} and 3 – $n_0 = 10^8$ cm^{-2}

4. CONCLUSIONS

The model of the nano-acoustic-electronic converter based on the graphene nanotube has been developed in the work. The proposed model takes into consideration the size dependences of the elastic constants and sound velocities in graphene.

The frequency dependences of the strain amplitude, surface electron concentration and electrostatic potential amplitude have been established in the framework of the given model.

It is ascertained that the converter sensitivity increases with increasing electron concentration and mobility and decreasing nanotube radius.

It is shown that a monotonic decrease in the electrostatic potential amplitude occurs with decreasing radius of the graphene nanotube. This is explained due to the fact that graphene nanotubes of smaller sizes are less sensitive to strain.

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