Показано можливість створення сенсора на акустичних хвилях із застосуванням нанострижнів ZnO. Отримано частотне рівняння, що дозволить визначати швидкість поширення поверхневої хвилі при заданих геометричних параметрах стрижневих наноструктур, відомій густині їх розміщення на поверхні, а також керувати цією швидкістю, змінюючи указані параметри. Побудована модель спрощує процес розробки сенсорів та аналіз отриманих за допомогою сенсорів на акустичних хвилях результатів

Ключові слова: сенсор, акустична хвиля, нанострижні ZnO, гідротермальний метод, пружний півпростір

Показана возможность создания сенсора на акустических волнах с использованием наностержней ZnO. Получено частотное уравнение, которое позволит определять скорость распространения поверхностной волны при заданных геометрических параметрах стержневых наноструктур, известной плотности их размещения на поверхности, а также управлять этой скоростью, изменяя указанные параметры. Построенная модель упрощает процесс разработки сенсоров и анализ полученных с помощью сенсоров на акустических волнах результатов

Ключевые слова: сенсор, акустическая волна, наностержни ZnO, гидротермальный метод, упругое полупространство

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ZnO NANOSTRUCTURES AS SENSING ELEMENT OF ACOUSTIC WAVE SENSOR

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1. Introduction

Nowadays acoustic wave devices are widely applied in many industrial and scientific fields ranging from mobile devices and wireless communication, pressure and viscosity sensors to novel biosensors for DNA detection. Major advantages of acoustic wave sensors include: single sided planar structure, the ability to interact directly with the sensing medium, high sensitivity, low hysteresis, small size, direct frequency output signal and low power consumption. Acoustic wave sensors have great potential for further application in the systems of analysis and quality control of chemical and biological agents. The investigation of novel sensitive materials, their synthesis methods is an actual problem and continuously carried out. For further quality and accuracy enhancement, simplification of manufacturing and improvement of applying the simulation of novel acoustic wave sensors operation should be performed.

At the same time ZnO became a promising component in a wide range of nanoscale devices for future application. It is an attractive material for electronics, photonics and sensing due to having exotic and versatile properties such as mechanical, piezoelectric, optical and electrical properties, biocompatibility, nontoxicity, chemical and photochemical stability, high specific surface area, optical transparency, electrochemical activities and so on [1]. On other hand, ZnO is attracting considerable attention due to its unique ability to form a variety of nanostructures such as nanowires, nanoribbons/nanobels, nanocombs, nanorings, nanocages, nanocastle, nanofibers etc. ZnO nanorods/nanowires have been employed as bio- or gas sensitive element of acoustic wave sensors [2]. ZnO nanorods provide giant effective surface area and strong bonding sites and this way allow more precision managing of their properties and characteristics.

It is known [3] that a propagation velocity of ultrasonic waves in solids is determined by the shape of the surface along which the elastic disturbances propagate, by resiliency and inertia (density) of the continuum. Rayleigh surface waves or, generally speaking, surface acoustic waves obtain in a narrow not more than two wavelengths near-surface layer of a solid. It is suggested that the propagation velocity of Rayleigh (surface) waves can be controlled by changing of inertial properties of the material particles, which are located near the surface of an elastic half-space.

In this paper we suggest the simulation of the plane harmonic surface wave propagation process in an isotropic elastic half-space with rod nanostructures on surface for determining of the propagation velocity of surface waves at given geometric parameters of the rod nanostructures, at certain density of their placement on the surface of the half-space and attached masses. This model will simplify the development of ZnO nanorods SAW sensors and analysis of the results.

2. SAW sensors with ZnO nanorods and their simulation.

Problem definition

To obtain nanorods on surfaces of different materials such methods as vapor phase synthesis, laser ablation, electrochemical method, biotemplating method, chemical method are applied [4]. In particular, hydrothermal method allows synthesis of ordered rod structures which satisfy the requirements for acoustic wave sensors design at the same time being a rather simple and inexpensive.

Fig. 1 shows schematically the structure of the acoustic wave sensor using ZnO nanorods. Thus, two interdigitated transducers are formed on the piezoelectric substrate by photolithography, between them ZnO nanorods are grown by hydrothermal method.

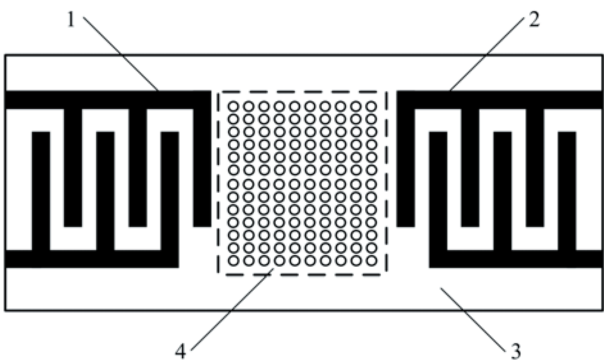

Fig. 1. The structure of the acoustic wave sensor: 1, 2 — interdigitated transducers, 3 - piezoelectric substrate, 4- array of ZnO nanostructures

Due to the fact that propagation velocity of ultrasonic waves in solids is determined by the shape of the surface along which the elastic disturbances propagate, by resiliency and inertia (density) of the continuum, propagation velocity of Rayleigh (surface) waves can be controlled by changing of inertial properties of the material particles, which are located near the surface of an elastic half-space. Thus, for the application of shown sensor design it is necessary to carry out preliminary consideration of harmonic surface waves propagation in an elastic half-space on which surface rod nanostructures are located. It is necessary to build a model by which the assessment of propagation velocity of surface waves at given geometric parameters of the rod-shaped nanostructures, at certain density values of their placement on the surface of half-space and attached masses will be feasible. Based on this model it will be possible to control propagation velocity of surface waves by changing these parameters.

The elastic half-space (Fig. 2) is considered. Rod nanostructures are located on its surface. Rod nanostructures are absolutely rigidly connected to the surface of the half-space at the base, i. e. in the plane $x_3 = 0$. The rods are arranged equidistantly along the axes Ox_1 and Ox_2 with the step Δ, so that the areal density on the surface of the half-space is $N = 1/\Delta^2$. The point masses M_0 are located at the free ends of the rod nanostructures. To fix the idea, we assume that all the nanostructures have the same geometric parameters, i. e. length L and unvarying along the length of the rod cross-section, which has the shape of a ring with the radii R_1 and R_2 $(R_2 > R_1)$, (Fig. 2) or a circle with the radius R_2. The rod nanostructures don't interact with each other, i. e. an energy transfer over the surface of the half- space is absent.

Suppose, a plane harmonic wave exists in the volume of the elastic half-space $(x_3 \le 0)$, its kinematic characteristics are determined by the displacement vector of material particles $\vec{u}(x_2,x_3)e^{i\omega t}$, here $\vec{u}(x_2,x_3)$ is the spatially developed amplitude of the displacement vector of material particles; $i = \sqrt{-1}$ – the imaginary unit; ω – is known angular frequency of the sign change of displacement; t – is time. We assume that the elastic wave propagates from left to right along axis Ox_2 (Fig. 2). In this case the components of the vector $\vec{u}(x_2,x_3)$ must be determined as follows:

$$u_1(x_2,x_3) = 0\,,\ u_2(x_2,x_3) = u_2(x_3)e^{-i\gamma x_2}\,,$$

$$u_3(x_2,x_3) = u_3(x_3)e^{-i\gamma x_2}\,, \qquad (1)$$

here γ is the wave number of the plane surface wave - the value to be determined in the course of the problem solving.

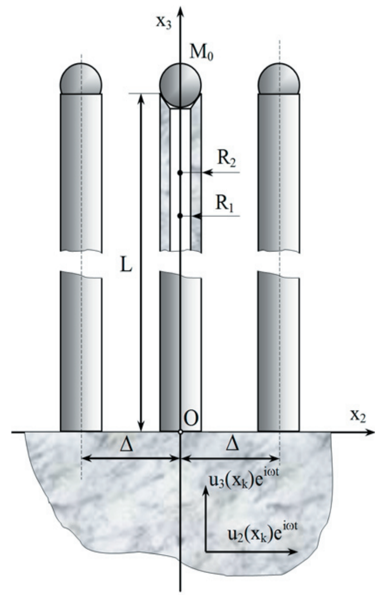

Fig. 2. The analytical model of the problem

Propagating surface wave imparts following motion to ends $x_3 = 0$ of rod nanostructures:

- vertical displacement $u_3(0)e^{-i\gamma x_2}$;
- horizontal displacement $u_2(0)e^{-i\gamma x_2}$;
- rotations in x_3Ox_2 plane by $\psi = \varepsilon_{23}(x_2,0)$,

where $\varepsilon_{23}(x_2,x_3) = (\partial u_2/\partial x_3 + \partial u_3/\partial x_2)/2$ is the elastic strain tensor components.

Obviously, that $\psi = \varepsilon_{23}(0)e^{-i\gamma x_2}$,

where $\varepsilon_{23}(0) = \left(-i\gamma u_3(0) + \partial u_2(x_3)/\partial x_3\big|_{x_3=0}\right)/2$.

It is clear that the above written expressions for the displacements of the ends of the rod nanostructures are accurate only in the case when the strong inequality $2R_2 << \lambda_R$ holds, i. e. when the maximum size of the cross-sectional diameter of the nanotube or nanorod substantially smaller than the Rayleigh wave λ_R. Otherwise, it's needed to use averaged over the cross sectional area of the rod nanostructures kinematic characteristics. In the following exposition we assume that the inequality $2R_2 << \lambda_R$ holds.

In this case, the vertical movements $u_3(0)e^{-i\gamma x_2}$ initiate longitudinal oscillations in the nanorod, which, as a first approximation, can be considered as one-dimensional. In this case the vertical displacements $w_3(x_3)e^{i\omega t}$ of material particles of the rod satisfy Newton's second law in differential form, which is written in the form:

$$\frac{\partial^2 w_3(x_3)}{\partial x_3^2} + k^2 w_3(x_3) = 0 \forall x_3 \in [0,L], \quad (2)$$

where $k = \omega / v_{ст}$ is the wave number of longitudinal waves in a rod; $v_{ст} = \sqrt{E/\rho_0}$ is the rod velocity; E and ρ_0 are Young's modulus and the density of the rod material, respectively.

Horizontal displacements and rotations in the cross section $x_3 = 0$ cause harmonic oscillations of the lateral bending in the rod nanostructure. At the same time the longitudinal displacements $w_2(x_3)e^{i\omega t}$ of material particles of the rod satisfy the standard equation of the lateral bending, which is written in the form

$$\frac{\partial^4 w_2(x_3)}{\partial x_3^4} - \lambda^4 w_2(x_3) = 0 \forall x_3 \in [0,L], \quad (3)$$

where λ is the wave number of the harmonic oscillations of the lateral bending, and $\lambda^4 = \omega^2 \rho_0 S/(EJ_1)$; $S = \pi(R_2^2 - R_1^2)$ is the cross-sectional area of the rod; J_1 is the moment of inertia of the cross-section of the rod about Ox_1 axis. The geometric characteristic J_1 of the rod cross-section is calculated as follows [5]:

$$J_1 = \int_S x_2^2 dS = \int_0^{2\pi}\int_{R_1}^{R_2} \rho^3 \sin^2\phi \, d\phi d\rho = \pi(R_2^4 - R_1^4). \quad (4)$$

From (4) it follows that for the solid rod $(R_1 = 0)$ geometric characteristic is $J_1 = \pi R_2^4$.

Normal stresses $\sigma_{33}^*(0)$ or normal forces $N_3^*(0) = \sigma_{33}^*(0)S$ appear as a result of compression - tension oscillations of a nanorod in its cross section $x_3 = 0$. The surface density of the normal forces is $n_3^* = N_3^*(0)N = \sigma_{33}^*(0)SN$.

Oscillations of the lateral bending form the moment of flection M_8 and the lateral force $Q(0)$ in the cross-section $x_3 = 0$ of the fixed nanorod. The surface density of lateral forces is $n_2^* = Q(0)N$.

Thus, at the propagation of a plane surface wave in the half-space, on which surface $x_3 = 0$ nanostructured elements are located, the kinematic characteristics of elastic waves must satisfy the following boundary conditions:

$$c_{33kl} \left. \frac{\partial u(x_2, x_3)}{\partial x_k} \right|_{x_3 = 0} = n_3^*, \; k,l = 2,3, \quad (5)$$

$$2c_{32kl} \left. \frac{\partial u(x_2, x_3)}{\partial x_k} \right|_{x_3 = 0} = n_2^*, \; k,l = 2,3, \quad (6)$$

where c_{33kl} and c_{32kl} are the matrix elements of coefficients of elasticity of the half-space material; in (1.5) and (1.6) summation over repeated indices k and l is implied.

The last relations completely determine the sequence of steps for solving the problem of controlling the speed of propagation of surface acoustic waves. First, the density n_2^* and n_3^* of tangential and normal loads is evaluated, and then the components of the displacement vector $u_2(x_3)e^{-i\gamma x_2}$ and $u_3(x_3)e^{-i\gamma x_2}$ which satisfy the boundary conditions (5) and (6) are determined. Desired wave number γ and phase velocity $v_f = \omega/\gamma$ of surface waves are determined when these conditions are completed.

3. The response simulation of the nanostructured elements

We first define the response n_3^* of the array of nanostructures.

The solution of equation (2) is obvious:

$$w_3(x_3) = A\cos kx_3 + B\sin kx_3, \quad (7)$$

where A and B are constants to be determined.

On the surface $x_3 = 0$ the displacement of the end $x_3 = 0$ of the rod $w_3(0) = A$ have to be equal to the displacement $u_3(0)e^{-i\gamma x_2}$ of element of the half-space. So $A = u_3(0)e^{-i\gamma x_2}$. According to Newton's third law $x_3 = L$:

$$ES \left. \frac{\partial w_3(x_3)}{\partial x_3} \right|_{x_3 = L} = -\omega^2 M_0 w_3(x_3)\Big|_{x_3 = L}. \quad (8)$$

Substituting in (8) the expression (7) after obvious transformations, we obtain the following result:

$$B = -A\frac{(kL\xi\cos kL - \sin kL)}{(kL\xi\sin kL + \cos kL)} = -u_3(0)e^{-i\gamma x_2}F_3(kL), \quad (9)$$

where $\xi = M_0/(\rho_0 LS)$ - is the relative mass of a point on the end of the rod $x_3 = L$ (Fig. 2); $F_3(kL)$ - is a frequency-dependent function.

A normal stress $\sigma_{33}^*(x_3)$ in a random cross-section of the rod is defined as follows:

$$\sigma_{33}^*(x_3) = E\frac{\partial w_3(x_3)}{\partial x_3} = $$
$$= kEu_3(0)e^{-i\gamma x_2}\left[-\sin kx_3 - F_3(kL)\cos kx_3\right]. \quad (10)$$

From (10) $\sigma_{33}^*(0) = -kEF_3(kL)u_3(0)e^{-i\gamma x_2}$.

$$n_3^* = -N\frac{ES}{L}F_3^*(kL)u_3(0)e^{-i\gamma x_2}, \quad (11)$$

where $F_3^*(kL) = kLF_3(kL)$.

Fig. 3 shows graphs of the frequency dependence of the functions $F_3^*(kL)$ that were calculated for different values of ξ and the fixed quality factor $Q_{ст} = 100$ of material of the nanorod.

Fig. 3, b shows shifts large-scaled resonance frequencies of longitudinal oscillations of rods at small values of the relative mass of a point on the end of the rod $x_3 = L$. The increase in the mass M_0 of a point is accompanied by an increase in the resonant frequency of the oscillating system.

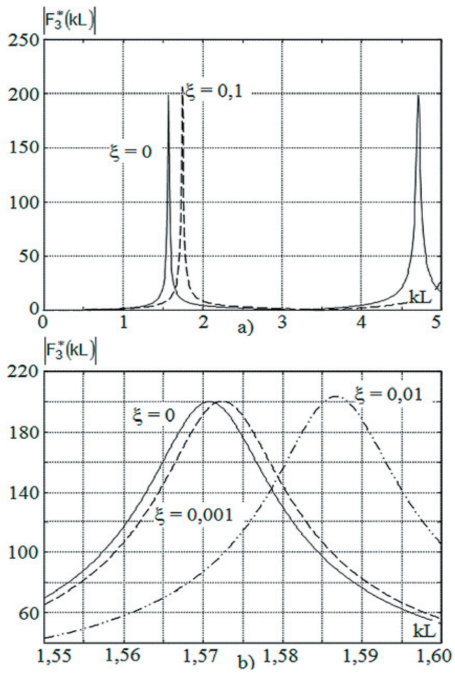

Fig. 3. Graphs of the frequency dependence of the functions $F_3^*(kL)$

The solution of the differential equation (3) has the form:

$$w_2(x_3) = C_1 \sin\lambda x_3 + D_1 \cos\lambda x_3 + C_2 \mathrm{sh}\lambda x_3 + D_2 \mathrm{ch}\lambda x_3, \quad (12)$$

where C_1, D_1, C_2 and D_2 - are constants to be determined.

The solution of (12) should implement the following conditions.

First of all, the conditions of the kinematic coupling of the rod cross-section $x_3 = 0$ with an element of the surface of the elastic half-space must be performed. The longitudinal displacement and rotation angles must be equal. The dynamic conditions at the end $x_3 = L$ must be performed too. There are vanishing of moment of flection and equation of the lateral force to the force of inertia of a point mass (Newton's third law). These speculations lead to the following system of equations for desired constants C_1, D_1, C_2 and D_2.

$$D_1 + D_2 = u_2(0)e^{-i\gamma x_2}, \quad (13)$$

$$C_1 + C_2 = \frac{1}{\lambda}\varepsilon_{23}(0)e^{-i\gamma x_2}, \quad (14)$$

$$-C_1 \sin\lambda L - D_1 \cos\lambda L + C_2 \mathrm{sh}\lambda L + D_2 \mathrm{ch}\lambda L = 0, \quad (15)$$

$$\begin{aligned} &C_1(-\cos\lambda L + \lambda L\xi \sin\lambda L) + D_1(\sin\lambda L + \lambda L\xi\cos\lambda L) + \\ &+ C_2(\mathrm{ch}\lambda L + \lambda L\xi \mathrm{sh}\lambda L) + D_2(\mathrm{sh}\lambda L + \lambda L\xi \mathrm{ch}\lambda L) = 0 \end{aligned}, \quad (16)$$

where $\xi = M_0/(\rho_0 LS)$ - is the relative mass of a point on the end of the rod $x_3 = L$.

The equation determinant $D_0(\lambda L,\xi)$ of system (13) – (16) is written as follows:

$$\begin{aligned} &D_0(\lambda L,\xi) = \\ &= 2\left[1 + \cos\lambda L \mathrm{ch}\lambda L + \lambda L\xi(\mathrm{sh}\lambda L \cos\lambda L - \mathrm{ch}\lambda L \sin\lambda L)\right]. \end{aligned} \quad (17)$$

It is obvious that the equation

$$D_0(\lambda L,\xi) = 0, \quad (18)$$

has infinite set of roots $\lambda_n L$ ($n = 1,2,...$ - number of the root), which correspond to an infinite set of resonant frequencies $\omega_p^{(n)}$ of oscillating system.

Because $\lambda L = g\sqrt{kL}$ is the dimensionless wavenumber, where g - dimensionless geometric parameter $g = \sqrt[4]{SL^2/J_1}$ (for a given cross-sectional shape of the nanotube $g = \sqrt[4]{L^2/(R_2^2 + R_1^2)}$), obviously $\lambda_n L = g\sqrt{k_n L}$.

For nanotubes with dimensions $L = 10^{-6}$ m, $R_2 = 50$ nm, $R_1 = 25$ nm ($g = 4{,}2295$) dimensionless frequency $k_1 L$ depend on parameter ξ like that:

$\xi = 0$, $k_1L = 1{,}231766$; $\xi = 0{,}0001$, $k_1L = 1{,}231519$; $\xi = 0{,}001$, $k_1L = 1{,}229317$; $\xi = 0{,}01$, $k_1L = 1{,}208592$; $\xi = 0{,}1$, $k_1L = 1{,}082022$.

It is clearly seen that the increase in mass M_0 of a point is accompanied by a decrease of the first resonance frequency of lateral oscillations of a nanorod. It can be noted that the value of the first resonance frequency of lateral oscillations are more sensitive to changes in parameter ξ than the value of the first resonance frequency of longitudinal oscillations of a rod.

The lateral force $Q(x_3) = EJ_1 \partial^3 w_2(x_3)/\partial x_3^3$ at $x_3 = 0$, i.e., in the plane of the fixing of the nanotube on the surface of the elastic half-space defined by the following equation:

$$Q(x_3)\big|_{x_3=0} = EJ_1\lambda^3(-C_1 + C_2), \quad (19)$$

Where constants C_1 and C_2, defined from (13) – (16) are:

$$\begin{aligned} C_1 = &\frac{e^{-i\gamma x_2}}{D_0(\lambda L,\xi)}\Big[u_2(0)(\cos\lambda L \mathrm{sh}\lambda L + 2\lambda L\xi\cos\lambda L \mathrm{ch}\lambda L + \\ &+ \sin\lambda L \mathrm{ch}\lambda L) + \frac{\varepsilon_{23}(0)}{\lambda}(1 + \cos\lambda L \mathrm{ch}\lambda L + 2\lambda L\xi \sin\lambda L \mathrm{sh}\lambda L)\Big], \end{aligned}$$

$$\begin{aligned} C_2 = &\frac{e^{-i\gamma x_2}}{D_0(\lambda L,\xi)} \times \\ &\times\left[-u_2(0)(\cos\lambda L \mathrm{sh}\lambda L + 2\lambda L\xi\cos\lambda L \mathrm{ch}\lambda L + \sin\lambda L \mathrm{ch}\lambda L) + \right. \\ &+ \frac{\varepsilon_{23}(0)}{\lambda} \times \\ &\left.\times(1 - \sin\lambda L \mathrm{sh}\lambda L - 2\lambda L\xi \sin\lambda L \mathrm{sh}\lambda L + \cos\lambda L \mathrm{ch}\lambda L)\right]. \end{aligned} \quad (20)$$

Substituting (20) in the definition (16) of the lateral force we define:

$$Q(x_3)\big|_{x_3=0} = -2\omega^2 m_{\text{ст}} e^{-i\gamma x_2}\left[u_2(0)f_1(\lambda L) + L\varepsilon_{23}(0)f_2(\lambda L)\right], \quad (21)$$

where $m_{\text{ст}} = \rho_0 LS$ - is a mass of a nanorod;

$$\begin{aligned} f_1(\lambda L) = &\frac{1}{\lambda L D_0(\lambda L,\xi)}(\cos\lambda L \mathrm{sh}\lambda L + 2\lambda L\xi\cos\lambda L \mathrm{ch}\lambda L + \\ &+ \sin\lambda L \mathrm{ch}\lambda L), \end{aligned}$$

$$f_2(\lambda L) = \frac{1}{(\lambda L)^2 D_0(\lambda L,\xi)}(\sin\lambda L \mathrm{sh}\lambda L + 2\lambda L\xi \sin\lambda L \mathrm{ch}\lambda L). \quad (22)$$

The tangential load or density n_2^* of lateral forces on the density of the surface of an elastic half-space $x_3 = 0$ is proportional to the surface density N of sources of lateral forces, i.e.:

$$n_2^* = NQ(x_3)\big|_{x_3=0} = \\ = -2\omega^2 N m_{ст} e^{-i\gamma x_2}\left[u_2(0) f_1(\lambda L) + L\varepsilon_{23}(0) f_2(\lambda L)\right]. \quad (23)$$

Thus, the reactions n_2^* and n_3^* of nanostructured elements on the surface of an elastic half-space are defined. Now we need to determine the wave number γ of surface waves, which create and balance these reactions.

4. The evaluation of kinematic characteristics of Relay waves in the half-space with nanostructures elements on its surface

Amplitude values $u_k(x_k)$ $(k = 1,2,3)$ of the components of the displacement vector $\vec{u}(x_k)e^{i\omega t}$ are determined by Newton's second law in differential form, which for an isotropic to elastic properties of solid in the absence of bulk forces is written as follows:

$$(\mu + 2G)\,\mathrm{grad\,div}\,\vec{u}(x_k) - G\,\mathrm{rot\,rot}\,\vec{u}(x_k) + \\ + \rho_0\omega^2\vec{u}(x_k) = 0 \;\forall\, x_k \in V, \quad (24)$$

where μ and G - are Lame elastic constants of an isotropic solid; ρ_0 - is a density of a material; V - is a half-space volume.

The displacement vector $\vec{u}(x_k)$ of material particles, as, indeed, the vector of any physical nature, can be written in the form of Helmholtz representation [3], i.e.:

$$\vec{u}(x_k) = \mathrm{grad}\,\Phi(x_k) + \mathrm{rot}\,\vec{\Psi}(x_k), \quad (25)$$

where $\Phi(x_k)$ and $\vec{\Psi}(x_k)$ - are scalar and vector potentials of the wave field of elastic displacements of material particles of solid.

If $\mathrm{div}\,\vec{\Psi}(x_k) = 0$ in any point of solid, then, substituting the Helmholtz representation (25) into the steady harmonic oscillations equation (24), we can get two of the Laplace equation of the form:

$$\nabla^2\Xi_1(k_\ell) = 0, \quad (26)$$

$$\nabla^2\Xi_1(k_s) = 0, \quad (27)$$

Where $\Xi_1(k_\ell) = \nabla^2\Phi(x_k) + k_\ell^2\Phi(x_k)$,

$\Xi_2(k_\ell) = -\mathrm{rot\,rot}\,\vec{\Psi}(x_k) + k_s^2\vec{\Psi}(x_k)$

are functions; k_ℓ and k_s - are wave numbers of longitudinal (index ℓ) and shift (index s) of noninteracting harmonic waves, and $k_\ell = \omega/v_\ell$ and $k_s = \omega/v_s$, where v_ℓ and v_s - are velocities of longitudinal and shift waves, respectively, with values $v_\ell = \sqrt{(\mu + 2G)/\rho_0}$ and $v_s = \sqrt{G/\rho_0}$.

Since the solutions of the Laplace equation (3.3) and (3.4) are harmonic functions [7] certainly bounded above, the harmonic functions $\Xi_1(k_\ell)$ and $\Xi_2(k_s)$ are constants, and are not equal. If the domain of existence of solutions of the Laplace equation is unbounded (space, half-space, infinite layer, and infinite rod), these constants are zero (otherwise it violates the principle of physical feasibility of the process) and the potentials $\Phi(x_k)$ and $\vec{\Psi}(x_k)$ satisfy the Helmholtz equation, i. e.:

$$\nabla^2\Phi(x_k) + k_\ell^2\Phi(x_k) = 0, \quad (28)$$

$$-\mathrm{rot\,rot}\,\vec{\Psi}(x_k) + k_s^2\vec{\Psi}(x_k) = 0. \quad (29)$$

It is easy to show that the displacement field of the material particles of an elastic half-space, where components of the displacement vector are given by (1), is completely determined by the following potentials:

$$\Phi(x_2, x_3) = \Phi(x_3)e^{-i\gamma x_2}, \quad \Psi_1(x_2, x_3) = \Psi_1(x_3)e^{-i\gamma x_2}, \quad (30)$$

where the components of the vector potential $\Psi_2(x_2, x_3)$ and $\Psi_3(x_2, x_3)$ are equal to zero. Substituting the assumed solutions (3.7) in the Helmholtz equation (28) and (29), we obtain:

$$\frac{\partial^2\Phi(x_3)}{\partial x_3^2} - \alpha^2\Phi(x_3) = 0, \quad \frac{\partial^2\Psi_1(x_3)}{\partial x_3^2} - \beta^2\Psi_1(x_3) = 0, \quad (31)$$

where $\alpha = \sqrt{\gamma^2 - k_\ell^2}$ and $\beta = \sqrt{\gamma^2 - k_s^2}$ - are lagging in phase by the angle $\pi/2$ components Ox_3 of the wave vector $\vec{k}_\ell$ and $\vec{k}_s$.

The solutions of equation (3.8), which do not contradict the physical sense of the problem, are as follows:

$$\Phi(x_3) = Ae^{\alpha x_3}, \quad \Psi_1(x_3) = Be^{\beta x_3}, \quad (32)$$

where A and B - are constants, which are determined from the conditions of implementation of Newton's third law to the $x_3 = 0$ surface of an elastic half-space, i.e., from the boundary conditions (1.5) and (1.6). In respect to an isotropic solid, moduli of elasticity are determined by the Lame constants μ and G moreover $c_{ijkl} = \mu\delta_{ij}\delta_{kl} + G(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$, where $\delta_{ij},...,\delta_{jk}$ are Kronecker symbols, the left part of these conditions are written as follows:

$$\sigma_{33}(x_2, x_3) = 2G\varepsilon_{33}(x_2, x_3) + \mu\,\mathrm{div}\,\vec{u}(x_2, x_3) = \\ = 2G\varepsilon_{33}(x_2, x_3) - k_\ell^2\Phi(x_2, x_3), \quad (33)$$

$$\sigma_{32}(x_2, x_3) = 2G\varepsilon_{32}(x_2, x_3), \quad (34)$$

where $\varepsilon_{33}(x_2, x_3) = \partial u_3(x_2, x_3)/\partial x_3$ - is compression-stretching deformation along the axis Ox_3;

$\varepsilon_{32}(x_2, x_3) = \left[\partial u_2(x_2, x_3)/\partial x_3 + \partial u_3(x_2, x_3)/\partial x_2\right]/2$ - is shearing strain in the plane x_3Ox_2.

Substituting the Helmholtz representation (25) solutions (32), we obtain $u_1(x_2, x_3) = 0$ the other two components of the amplitude values of the displacement vector of the material particles are defined by the following expressions:

$$u_2(x_2, x_3) = \left(-i\gamma Ae^{\alpha x_3} + \beta Be^{\beta x_3}\right)e^{-i\gamma x_2}, \quad (35)$$

$$u_3(x_2,x_3) = (\alpha A e^{\alpha x_3} + i\gamma B e^{\beta x_3}) e^{-i\gamma x_2} . \quad (36)$$

Defined by (3.12) and (3.13) displacement vector components correspond to the following values of the amplitudes of spatially developed the strain tensor components:

$$\varepsilon_{33}(x_2,x_3) = (\alpha^2 A e^{\alpha x_3} + i\gamma\beta B e^{\beta x_3}) e^{-i\gamma x_2} , \quad (37)$$

$$\varepsilon_{32}(x_2,x_3) = \frac{1}{2}\left[-2i\gamma\alpha A e^{\alpha x_3} + (\gamma^2+\beta^2) B e^{\beta x_3}\right] e^{-i\gamma x_2} . \quad (38)$$

Substituting (3.14) and (3.15) in the determination of mechanical stresses (3.10) and (3.11), we obtain:

$$\sigma_{33}(x_2,x_3) = G\left[(\gamma^2+\beta^2) A e^{\alpha x_3} + 2i\gamma\beta B e^{\beta x_3}\right] e^{-i\gamma x_2} , \quad (39)$$

$$\sigma_{32}(x_2,x_3) = G\left[-2i\gamma\alpha A e^{\alpha x_3} + (\gamma^2+\beta^2) B e^{\beta x_3}\right] e^{-i\gamma x_2} . \quad (40)$$

From (3.13) и (3.15) $u_2(x_2,0) = (-i\gamma A + \beta B) e^{-i\gamma x_2}$,

$u_3(x_2,0) = (\alpha A + i\beta B) e^{-i\gamma x_2}$

and $\varepsilon_{32}(0) = \left[-2i\gamma A + (\gamma^2+\beta^2) B\right]/2$.

Substituting these values into the definition of reactions n_2^* and n_3^*, and substituting results into the boundary conditions (1.5) and (1.6), in the left sides of which values of $\sigma_{32}(x_2,0)$ and $\sigma_{33}(x_2,0)$ are written, after obvious transformations we obtain:

$$\alpha_{11}(\omega) A + i\alpha_{12}(\omega) B = 0 , \quad (41)$$

$$-i\alpha_{21}(\omega) A + \alpha_{22}(\omega) B = 0 , \quad (42)$$

where:

$$\alpha_{11}(\omega) = \gamma^2 + \beta^2 + NS\frac{E}{GL}\alpha F_3^*(kL) ;$$

$$\alpha_{12}(\omega) = 2\gamma\beta + NS\frac{E}{GL}\gamma F_3^*(kL) ;$$

$$\alpha_{21}(\omega) = 2\gamma\alpha + 2NS\left[\gamma k_s^2 L f_1(\lambda L) + \gamma\alpha (k_s L)^2 f_2(\lambda L)\right] ,$$

$$\alpha_{22}(\omega) = \gamma^2 + \beta^2 +$$

$$+ NS\left[2\beta k_s^2 L f_1(\lambda L) + (\gamma^2+\beta^2)(k_s L)^2 f_2(\lambda L)\right].$$

In writing the expressions for calculating the coefficients $\alpha_{21}(\omega)$

and $\alpha_{22}(\omega)$

it was taken into account that $m_{ст}/G = \rho_0 LS/G = LS/v_s^2$,

where $v_s = \sqrt{G/\rho_0}$ - is shear wave velocity.

The homogeneous system of algebraic equations (41) and (42) has nontrivial (non-zero) solutions for the coefficients A and B only if the determinant Δ_R of this system is equal to zero, i. e.:

$$\Delta_R = \alpha_{11}(\omega)\alpha_{22}(\omega) - \alpha_{12}(\omega)\alpha_{21}(\omega) = 0 . \quad (43)$$

The relation (43) has a sense of the condition of existence of Rayleigh surface wave at a given frequency ω and can be read as follows: constants A and B are not equal to zero, i. e. in the elastic half-space with a nanostructured surface Rayleigh wave propagates, only in the case when the wave numbers α and γ satisfy the equation (43).

It is easy to see that at zero surface density ($N = 0$) of nanostructures, condition (43) becomes to the standard [3] condition for the existence of classical Rayleigh wave, i. e.

$$\Delta_R\big|_{N=0} = (\gamma^2+\beta^2)^2 - 4\gamma^2\alpha\beta = 0 .$$

If $N \neq 0$, as it follows from (43), the wave number γ becomes non-linear dependence on frequency, i. e., there is frequency dispersion of the velocity propagation and, consequently, there are differences between the phase and group velocities of propagation of individual spectral components in the case of existence of pulse ultrasonic signals in a half-space. The frequency dispersion particularly appears at the resonant frequencies of nanostructural elements. Because on the resonance frequency the oscillating system (nanostructure element) consumes from the source of oscillations, i. e., from the surface wave, the maximum amount of energy, it can be argued that the velocity of propagation of surface waves at these frequencies will decrease sharply.

The most significant difference from the classical Rayleigh wave is in the fact that due to the energy transfers between the material particles of the elastic half-space and nanostructured elements, in which energy is dissipated, the wave number γ in equation (43) should be considered as a complex number where imaginary part is dramatically increased at resonance frequencies of nanostructural elements.

5. Conclusion

In this paper the feasibility of the development of surface acoustic wave sensors with ZnO nanostructures as sensing element is shown.

The process of propagation of a plane harmonic surface wave in an isotropic elastic half-space with the rod nanostructures on surface is observed. The frequency equation from which we can determine the velocity of propagation of a surface wave for a given geometrical parameters of the rod nanostructures, the values of the density of their distribution on the surface of the half-space and added masses is obtained. It is clear that variation of these parameters can change (control) the speed of propagation of a surface wave.

Performed simulation extends the range of tools for further development of nanorods-based SAW sensors due to comprehensive math-based explanation of their operating principles.

Further continuation of the simulation and adjustment of hydrothermal method of ZnO nanorods growing will simplify the creation of reliable and sensitive sensors on surface acoustic waves.

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Abstract

In spite of the wide application of SAW devices the investigation of novel sensitive materials, their synthesis methods is continuously carried out. For further quality and accuracy enhancement, simplification of manufacturing and improvement of applying the simulation of novel acoustic wave sensors operation should be performed. In ZnO nanorods-based sensors propagating surface wave imparts following motion to the ends of hydrothermally grown between two interdigitated transducers rod nanostructures: vertical displacement, horizontal displacement and rotations in plane. Thus, response of nanostructured elements to that displacements and kinematic characteristics of Relay waves are evaluated. During the simulation the frequency equation from which we can determine the velocity of propagation of a surface wave for a given geometrical parameters of the rod nanostructures, the values of the density of their distribution on the surface of the half-space and added masses is obtained. This model simplifies the development and analysis of the results from ZnO nanorods-based SAW sensors for biological and chemical agents, including molecules, cells and tissues. Performed simulation extends the range of tools for further development of nanorods-based SAW sensors due to comprehensive math-based explanation of their operating principles

Keywords: *sensor, acoustic wave, ZnO nanorods, hydrothermal method, elastic half-space*