Shear Acoustic Phonons in Multilayer Arseneide Semiconductor Nanostructures

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Using the elastic continuum model, exact analytical solutions for the equations of motion for the elastic medium of a multilayer resonant tunneling nanosystem describing the shear modes of acoustic phonons are obtained. The expressions describing the components of the stress tensor arising in the studied nanostructure and boundary conditions for the components of the elastic displacement vector and the components of the stress tensor are obtained. Using the obtained equations of motion for the elastic medium and boundary conditions, the theory of the spectrum and phonon modes for shear acoustic phonons is developed in the proposed work for a plane arsenide semiconductor nanostructure. It is shown that the spectrum of the displaced acoustic phonons of the studied nanosystem is obtained from the dispersion equation following from the boundary conditions using transfer-matrix method. Using the orthonormality condition, the normalized modes of shear acoustic phonons are obtained. For the parameters of the three-barrier nanostructure – the active zone of a quantum cascade detector – the calculation of the spectrum of acoustic phonons and its dependences on the wave vector and the geometric parameters of the nanostructure has been performed. It is shown that the calculated dependences of the spectrum of acoustic phonons on the wave vector form three groups with boundary values equal to the corresponding energies of acoustic phonons in massive crystals. Also it is obtained that an increase in the thickness of the internal barrier at constant other geometrical parameters of the nanosystem leads to a steady decrease in the values of the phonon energy levels energies. The proposed theory can be used to study the scattering of electron fluxes on acoustic phonons in multilayer resonant-tunneling structures.

Keywords: Acoustic phonons, Phonon modes, Resonant-tunneling structure, Quantum cascade laser, Quantum cascade detector.

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1. INTRODUCTION

The rapid development of nanoscience as a part of solid state physics determines the current relevance and wide range of nanotechnology applications [1-3]. In particular, in the physics of semiconductor nanosystems, the creation of quantum cascade lasers (QCL) [4, 5] and detectors (QCD) [6, 7] operating in the terahertz range of electromagnetic waves is significant. To expand the capabilities of the above-mentioned nanodevices, it is important to take into account the effects of various kinds arising in multilayer semiconductor resonant tunneling structures (RTS), which are their functional elements.

Despite the fact that the effects of the interaction of electrons tunneled through a RTS with optical phonons, constant electric and high-frequency electromagnetic fields, have been sufficiently clarified and analyzed [8-11], studies of acoustic phonons and their influence on tunnel electron transport are practically absent. Attention should be paid only to a few papers, calculations of the acoustic phonons spectrum in which were performed for single quantum wells [12] and nanosystems of cylindrical and spherical symmetry [13, 14]. It should also be noted that the classification of acoustic phonons arising in a quantum well placed in a massive semiconductor medium and calculations of their spectra was investigated in [15]. However, for RTS, used in QCL and QCD due to the mutual consistency of their cascades, this theory is not applicable, primarily as it is necessary to use other boundary conditions for the displacement vector and the components of the stress tensor.

Based on the model of an elastic continuum, the theory of the spectrum and acoustic modes of shear phonons arising in two-well-RTS with GaAs – quantum wells and AlAs – quantum barriers was developed in the proposed work. Direct calculations of the spectrum of acoustic phonons were performed for the three-barrier RTS as the active band of QCD. It is shown that the developed theory can be the basis for studying the interaction of electrons with a shear acoustic phonon in multilayer RTS.

2. EQUATIONS FOR SHEAR ACOUSTIC PHONON MODES IN NANOSTRUCTURE. DISPERSION EQUATIONS FOR THE DETERMINATION OF THE ACOUSTIC PHONON SPECTRUM

We will explore the shear acoustic phonons arising in the RTS, consisting of two InxGa1-xAs potential quantum wells and internal In0.5Al0.5As potential barrier. The geometrical scheme of the nanosystem is presented in Fig. 1.

The 0x3 axis is directed perpendicular to the interfaces of the nanosystem media. In view of this and the designations in Fig. 1, the density of the nanostucture material medium can be represented as

\[ \rho(x_3) = \sum_{p=0}^{6} \rho(p) \left[ \theta(x_3 - x_3^{(p)}) - \theta(x_3 - x_3^{(p+1)}) \right], \]

(1)

where \( x_3^{(0)} = -\infty; \ x_3^{(7)} = +\infty, \ p = 0, 6, \) and \( \rho(p) = \begin{cases} \rho_0, & p = 1, 3, 5 \\ \rho_1, & p = 0, 2, 4. \end{cases} \) is the density of the correspond-
ing nanosystem layer material, $\theta(x_i)$ is the Heaviside unit function.

$$\text{Fig. 1 – Geometric scheme of the three-barrier RTS}$$

Using the elastic continuum model, the equation of motion for the elastic displacement vector in the isotropic case looks like:

$$\rho(x_i) \frac{\partial^2 \mathbf{u}(x_i, x_2, x_3)}{\partial t^2} = \frac{\partial \sigma_j(x_i, x_2, x_3)}{\partial x_j}, \quad j = 1, 2, 3,$$  \hspace{1cm} (2)

where $\sigma_j(x_1, x_2, x_3)$ is the stress tensor. Equation (2) can be reduced to the form:

$$\rho(x_3) \frac{\partial^2 \mathbf{u}(x_3)}{\partial t^2} = (C_{12} + 2C_{34}) \nabla \cdot (\nabla \cdot \mathbf{u}) - C_{34} \nabla \times (\nabla \times \mathbf{u}),$$  \hspace{1cm} (3)

$$\mathbf{u} = \mathbf{u}(x_1, x_2, x_3),$$

where $u_{ij}^{(p)} = \sqrt{(C_{12} + 2C_{34})/\rho^{(p)}}$ is the propagation velocity of longitudinal and transverse waves, respectively.

Solutions of equations (8) are as follows:

$$u_{l}^{(p)}(x_3) = A_{l}^{(p)} e^{-\omega_{l}^{(p)} x_3} + B_{l}^{(p)} e^{\omega_{l}^{(p)} x_3};$$

$$\pm c_{l}^{(p)} = \sqrt{\frac{\omega^2}{\nu_l^{(p)}}} = \sqrt{\frac{\omega^2}{\nu_l^{(p)}}}.$$  \hspace{1cm} (9)

To find $u_{l}^{(p)}(x_3)$ and $u_{l}^{(p)}(x_3)$, the conditions (6) are used. Since

$$\nabla \times \left( \mathbf{u}_l(x_3) + \mathbf{u}_l(x_3) \right) = 0$$  \hspace{1cm} (10)

where

$$C_{12}^{(p)} = \sum_{p=0}^{6} C_{12}^{(p)} \left[ \theta(x_3 - x_3^{(p)}) - \theta(x_3 - x_3^{(p+1)}) \right] =$$

$$\begin{cases} C_{12}^{(p)} & p = 0, 2, 4, \\ C_{12}^{(p)} & p = 1, 3, 5 \end{cases}$$

are the elastic constants for the corresponding $p$-th RTS layer.

In the case of shear acoustic phonons $\pi(x_1, x_2, x_3) = \pi(x_1) \pi(x_3)$ where the vector $\mathbf{u} = \mathbf{u}(x_3)$ has two non-zero components:

$$\mathbf{u}_l(x_3) = \mathbf{u}_l(x_3) + \mathbf{u}_l(x_3) = \left( u_{l}^{(p)}(x_3); 0; u_{l}^{(p)}(x_3) \right).$$  \hspace{1cm} (5)

Vectors $\mathbf{u}_l(x_3)$, $\mathbf{u}_l(x_3)$ can be represented in the form:

$$\mathbf{u}_l(x_3) = \mathbf{u}_l(x_3) + \mathbf{u}_l(x_3);$$

$$\mathbf{u}_l(x_3) = \mathbf{u}_l(x_3) + \mathbf{u}_l(x_3),$$

where for the components $u_{l}^{(p)}(x_3)$ and $u_{l}^{(p)}(x_3)$ of shear acoustic phonons, the following conditions are satisfied:

$$\nabla \times \mathbf{u}_l^{(p)}(x_3) = 0; \nabla \cdot (\nabla \times \mathbf{u}_l^{(p)}(x_3)) = \nabla^2 \mathbf{u}_l^{(p)}(x_3);$$

$$\nabla \times \mathbf{u}_l^{(p)}(x_3) = 0; \nabla \times \mathbf{u}_l^{(p)}(x_3) = -\nabla^2 \mathbf{u}_l^{(p)}(x_3).$$  \hspace{1cm} (6)

Solutions of equation (3) taking into account (5), (6) will be found in the form:

$$\mathbf{u}(x_1, x_2, x_3) = \mathbf{u}_l(x_3) e^{i(qx_1 + \omega t)}.$$  \hspace{1cm} (7)

Then equation (3) within the $p$-th RTS layer splits into two equations:

$$\frac{d^2 u_{l}^{(p)}(x_3)}{dx_3^2} - \left( q^2 - \frac{\omega^2}{\nu_l^{(p)}} \right) u_{l}^{(p)}(x_3) = 0;$$

$$\frac{d^2 u_{l}^{(p)}(x_3)}{dx_3^2} - \left( q^2 - \frac{\omega^2}{\nu_l^{(p)}} \right) u_{l}^{(p)}(x_3) = 0,$$  \hspace{1cm} (8)

and

$$\nabla \times \left( \mathbf{u}_l(x_3) + \mathbf{u}_l(x_3) \right) = 0,$$  \hspace{1cm} (11)

then from (11) and (12), respectively, we get:

$$\frac{\partial \mathbf{u}_l(x_3)}{\partial x_3} = \frac{\partial \mathbf{u}_l(x_3)}{\partial x_3} = 0;$$

$$\frac{\partial \mathbf{u}_l(x_3)}{\partial x_3} + \frac{\partial \mathbf{u}_l(x_3)}{\partial x_3} = 0.$$  \hspace{1cm} (12)

Accounting of (7) gives:

$$u_{l}^{(p)}(x_3) = \frac{i}{q} \frac{\partial u_{l}(x_3)}{\partial x_3} = e^{i\pm \omega_{l}^{(p)} x_3};$$

$$u_{l}^{(p)}(x_3) = \frac{i}{q} \frac{\partial u_{l}(x_3)}{\partial x_3} \left( A_{l}^{(p)} e^{-\pm \omega_{l}^{(p)} x_3} - B_{l}^{(p)} e^{\pm \omega_{l}^{(p)} x_3} \right);$$

$$u_{l}^{(p)}(x_3) = \frac{i}{q} \frac{\partial u_{l}(x_3)}{\partial x_3} \left( A_{l}^{(p)} e^{-\pm \omega_{l}^{(p)} x_3} - B_{l}^{(p)} e^{\pm \omega_{l}^{(p)} x_3} \right).$$  \hspace{1cm} (13)
Now the solutions of equations (8) within the RTS can be represented as:

\[ u_s(x_3) = u_{s_1}^{(p)}(x_3) + u_{s_2}^{(p)}(x_3) = \left( B_i^{(0)} e^{-\xi_i^{(0)} x_3} + B_i^{(0)} e^{-\xi_i^{(0)} x_3} \right) \theta(-z) + \left( A_i^{(6)} e^{-\xi_i^{(6)} x_3} + A_i^{(6)} e^{-\xi_i^{(6)} x_3} \right) \theta(x_3 - x_3^{(5)}) + \]

\[ + \sum_{p=1}^{5} \left( A_i^{(p)} e^{-\xi_i^{(p)} x_3} + B_i^{(p)} e^{\xi_i^{(p)} x_3} + A_i^{(p)} e^{-\xi_i^{(p)} x_3} + B_i^{(p)} e^{\xi_i^{(p)} x_3} \right) \theta(x_3 - x_3^{(p-1)}) - \theta(x_3 - x_3^{(p)}) \]}

(15)

In expressions (15) it is taken into account that from a physical point of view deformation cannot grow infinitely when \( x_3 \to \pm \infty \), which requires enforcement of condition:

\[ u_{s_3}(x_3) \mid_{x_3 \to \pm\infty} \to 0. \]}

(16)

Condition (16) is ensured by equating to zero the coefficients in expressions (15) at \( x_3 < 0 \) and \( x_3 > x_3^{(5)} \), that is \( A_0^{(0)} = A_0^{(5)} = 0, B_i^{(5)} = B_i^{(5)} = 0 \).

To determine the coefficients \( B_i^{(0)}, B_i^{(1)}, A_i^{(0)}, A_i^{(1)}, B_i^{(1)}, A_i^{(1)}, B_i^{(1)}, \) the continuity conditions of the displacement vector components \( u_s(x_3), u_s(x_3) \) and the components of the stress ten-

\[ \sigma_{s_3}(x_3) = C_{44}^{(p)} \left( \frac{\partial u_{s_3}^{(p)}(x_3)}{\partial x_3} + \frac{\partial u_{s_3}^{(p)}(x_3)}{\partial x_3} \right) = C_{44}^{(p)} \left( iqu_{s_3}^{(p)}(x_3) + \frac{\partial u_{s_3}^{(p)}(x_3)}{\partial x_3} \right) e^{q_3} = \]

\[ = C_{44}^{(p)} \left( -2 \frac{\partial}{\partial x_3} A_i^{(0)} e^{-\xi_i^{(0)} x_3} + 2 \frac{\partial}{\partial x_3} B_i^{(0)} e^{\xi_i^{(0)} x_3} - \left( \frac{q^2}{\xi_i^{(0)} x_3} + \xi_i^{(0)} x_3 \right) A_i^{(0)} e^{-\xi_i^{(0)} x_3} + \left( \frac{q^2}{\xi_i^{(0)} x_3} + \xi_i^{(0)} x_3 \right) B_i^{(0)} e^{\xi_i^{(0)} x_3} \right) e^{q_3} ; \]

\[ \sigma_{s_3}(x_3) = C_{12}^{(p)} \nabla u_{s_3}(x_3) + 2 C_{44}^{(p)} \frac{\partial u_{s_3}^{(p)}(x_3)}{\partial x_3} = \left( iC_{12}^{(p)} u_{s_3}^{(p)}(x_3) + \frac{\partial u_{s_3}^{(p)}(x_3)}{\partial x_3} \right) e^{q_3} = \]

\[ = \left( iC_{12}^{(p)} u_{s_3}^{(p)}(x_3) + C_{11}^{(p)} \frac{\partial u_{s_3}^{(p)}(x_3)}{\partial x_3} \right) e^{q_3} = i \left( qC_{12}^{(p)} - \frac{q^2}{C_{11}^{(p)}} \right) A_i^{(0)} e^{-\xi_i^{(0)} x_3} + \]

\[ + q C_{12}^{(p)} \frac{\partial}{\partial x_3} \left( B_i^{(0)} e^{\xi_i^{(0)} x_3} + q \left( C_{12}^{(p)} - C_{11}^{(p)} \right) A_i^{(0)} e^{-\xi_i^{(0)} x_3} + q \left( C_{12}^{(p)} - C_{11}^{(p)} \right) B_i^{(0)} e^{\xi_i^{(0)} x_3} \right) ; \]

\[ C_{12}^{(p)} = C_{11}^{(p)} - 2 C_{44}^{(p)} . \]

The ratio between the coefficients is established using the transfer matrix method:

\[ A_i^{(p)}, B_i^{(p)}, A_i^{(p)}, B_i^{(p)} \] of the \( p \)-th and \( p+1 \)-th RTS layers.
where, taking into account (15), (17), the matrix $M_p$ is defined as:

$$\begin{pmatrix}
e^{-\kappa^2 q i^q} & e^{\kappa^2 q i^q} & e^{-\kappa^2 q i^q} & e^{\kappa^2 q i^q} \\
\frac{q}{i} & \frac{q}{i} & -\frac{q}{i} & \frac{q}{i} \\
2C_{44} \chi_1(q) e^{-\kappa^2 q i^q} & -2C_{44} \chi_1(q) e^{\kappa^2 q i^q} & 2C_{44} \chi_1(q) e^{-\kappa^2 q i^q} & -2C_{44} \chi_1(q) e^{\kappa^2 q i^q} \\
iq \chi_1(q) & iq \chi_1(q) & iq \chi_1(q) & iq \chi_1(q)
\end{pmatrix}$$

(19)

Now the coefficients $B_1^{(0)}, B_1^{(1)}$ in the medium to the left of the RTS can be expressed through the coefficients $A_1^{(0)}, A_1^{(1)}$ in the medium to the right of the RTS:

$$\begin{pmatrix}0 \\
B_1^{(0)} \\
0 \\
B_1^{(1)}
\end{pmatrix} = T^{(0,6)} \begin{pmatrix}A_1^{(0)} \\
0 \\
A_1^{(1)} \\
0
\end{pmatrix},$$

(20)

where

$$T^{(0,6)} = T(q, \omega) = T^{(1,2)} T^{(2,3)} T^{(3,4)} T^{(4,5)} T^{(5,6)}$$

(22)

is the transfer matrix of nanostructure.

The physical parameters of the studied RTS with GaAs – quantum wells and AlAs – quantum barriers. The geometric parameters of the three-barrier RTS were chosen as follows: quantum well widths $d_1 = d_2 = 2 \text{ nm}$, potential barrier widths $d_1 = d_2 = d_3 = 1 \text{ nm}$. The physical parameters of the nanostructure are as follows: material density of potential barriers and wells $\rho_0 = 3.76 \text{ g/cm}^3$; $\rho_1 = 5.32 \text{ g/cm}^3$, respectively, elastic constants $C_{11} = 12.02 \times 10^{11} \text{ dyn/cm}^2$; $C_{11} = 11.90 \times 10^{11} \text{ dyn/cm}^2$; $C_{44} = 5.99 \times 10^{11} \text{ dyn/cm}^2$; $C_{44} = 5.94 \times 10^{11} \text{ dyn/cm}^2$.

In Fig. 2 we show the spectrum of acoustic phonons $\Omega_{33}(q) = \hbar \omega_{\alpha,\beta}(q)$ depending on the wave vector $q = 1/(d_1 + d_2 + d_3 + d_4 + d_5)$.

As can be seen from Fig. 2, the dependencies $\Omega_{33}(q) = \hbar \omega_{\alpha,\beta}(q)$ form three different groups (I, II, III) whose energy values lie within the intervals $I(\Omega_1 \leq \Omega \leq \Omega_1)$, II$(\Omega_1 \leq \Omega \leq \Omega_2)$, III$(\Omega_1 \leq \Omega \leq \Omega_2)$, where
\[ \Omega_{\phi}(q) = \Omega_{\phi}^{GaAs}(q); \quad \Omega_{\psi}(q) = \Omega_{\psi}^{AlAs}(q); \]
are the corresponding values of the transverse and longitudinal acoustic phonon energies for massive AlAs and GaAs crystals, respectively.

\[ \Omega_{\phi}(q) = \Omega_{\phi}^{GaAs}(q); \quad \Omega_{\psi}(q) = \Omega_{\psi}^{AlAs}(q); \]

Fig. 2 – Dependence of the acoustic phonon spectrum groups with different dispersions on the wave vector \( q \).

At the same time, for the I and III groups of the spectrum, the variance of the dependences is as follows: the energy values begin at the values \( \Omega_{ny}(q) = \Omega_{ny}(q) \)
and \( \Omega_{ny}(q) = \Omega_{ny}(q) \), respectively, and with increasing \( q \) they also grow, reaching values \( \Omega_{ny}(q) = \Omega_{ny}(q) \)
and \( \Omega_{ny}(q) = \Omega_{ny}(q) \). For the II group, the values of the phonon energy begin at \( \Omega_{ny}(q) = \Omega_{ny}(q) \), and with increasing \( q \) they increase reaching values \( \Omega_{ny}(q) = \Omega_{ny}(q) \). It should be noted that the dependences for the I and III groups of the spectrum have a similar behavior, consisting in the approximation of the curves for the adjacent levels \( \Omega_{ny}(q) \) and \( \Omega_{ny+1}(q) \), however, for the III group, the adjacent level except for the approximation, can be seen from Fig. 2 tend to merge with increasing \( q \). By their physical nature, phonons of the I group belong to the transverse displacements of the medium and of the III group – to the longitudinal displacements.

Fig. 3 illustrates the dependences of the phonon energy on the position \( b = d_3 + d_4 \) of the internal potential barrier in the total potential well calculated with the value of the wave vector \( q = 1.7 \), while the other geometric parameters of the RTS are constant.

Fig. 4 shows the dependences of the phonon mode energies for the I and III groups on the thickness \( d_3 \) of the internal barrier calculated for \( q = 1.7 \).

In addition, as can be seen from Fig. 3, two curves \( \Omega_2 = \Omega_n(q) \) are formed in each dependency group. With a change of \( b \) for \( n = 1 \) and \( n = 2 \) in both curves, one and two maxima are formed, respectively. This suggests that the processes of branch formation for the transverse and longitudinal components of the phonon modes are weakly coupled.

As can be seen from Fig. 4, an increase in the thickness of the internal barrier at constant other geometrical parameters of the nanosystem leads to a steady decrease in the values of the phonon energy levels energies. In this case, there is a gradual convergence of the first and second phonon energy levels in each group.

4. CONCLUSIONS

Using the model of an elastic continuum, the theory of the energy spectrum and phonon modes of shear acoustic phonons arising in a two-dimensional plane nanostructure is developed. It is shown how the acoustic modes can be normalized for the studied type of acoustic phonons. Using the developed theory on the example of a double-well nanosystem with GaAs – quantum wells and AlAs – quantum barriers, we cal-
culated the spectrum of shear acoustic phonons. The properties of the shear acoustic phonons spectrum arising in the nanostructure on its geometrical parameters are established. The developed theory can be used as a basis for further investigation of the interaction processes of electrons with shear acoustic phonons in multilayer arsenide semiconductor nanosystems.

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Зміщувальні акустичні фонони в багатошарових арсенідних напівпровідникових наноструктурах

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З використанням моделі пружного континууму отримані точні аналітичні розв’язки для рівнянь руху пружного середовища багатошарової резонансної тунельної наносистеми, що описують зміщуваль- ні моди акустичних фононів. Отримано вирази, що задають компоненти тензора напружень, які виникають в досліджуваній наноструктурі, а також граничні умови для компонент вектора пружного зміщення та компонент тензора напружень. З використанням отриманих рівнянь руху для пружного середовища і граничних умов у пропонованій роботі для плоскої арсенідної напівпровідникової наноструктури розроблена теорія спектра і фононних мод для зміщувальних акустичних фононів. Показано, що спектр зміщувальних акустичних фононів досліджуваної наносистеми отримується з дисперсійного рівняння, що випливає з граничних умов застосуванням методу трансфер-матриці. Викорис- товуючи умову ортогональність, отримані нормалізовані моди звукових акустичних фононів. Для параметрів трійки тунельної наноструктури - активної зони квантового каскадного детектора - виконано розрахунок спектру акустичних фононів і його залежностей від хвильового вектора і геометричних параметрів наноструктури. Показано, що розраховані залежності спектра акустичних фононів від хвильового вектора утворюють три групи з граничними значеннями, рівними відповідним енергіям акустичних фононів в мазингових кристалах. Також встановлено, що збільшення товщини внутрішнього бар’єра при постійних інших геометричних параметрах наносистеми призводить до стійкого зменшення значень енергій рівнів фононів. Розглянута теорія може бути застосована для дослідження розсіяння електронних потоків на акустичних фононах в багатошарових резонансно-тунельних структурах.

Ключові слова: Акустичні фонони, Фононні моди, Резонансно-тунельна структура, Квантовий каскадний лазер, Квантовий каскадний детектор.