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The Spectrum of Transverse Acoustic Phonons in Planar Multilayer Semiconductor Nanostructures

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Based on the elastic continuum model, the theory of displacement of acoustic phonons spectra, arising in flat semiconductor nanostructures, was developed. For the studied resonant tunneling structure, which can be an active element of a quantum cascade laser or detector, the spectrum of acoustic phonons modes has been calculated. The dependences of the acoustic phonon spectrum from geometric parameters of studied nanostructure were set. The results obtained in the paper can be used to further theoretical studies of the electrons interaction with the transverse acoustic phonons in multilayer semiconductor nanosystems.

Keywords: Quantum cascade laser, Quantum cascade detector, Resonant tunnel structure, Acoustic phonons, Transfer matrix.

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1. INTRODUCTION

Actually, the study of electron tunneling processes in planar semiconductor multilayer resonant tunneling structures (RTS) occupies an important place for an effective work of modern quantum cascade lasers (QCL) [1-3] and detectors (QCD). Much attention is paid to the theoretical study of interaction of electrons with optical phonons [4], constant electric [5, 6] and magnetic field [7] with the electron beam and its static and dynamic spatial charge [8, 9], but the acoustic phonons influence on the resonant tunneling is still practically unexplored. Also the value of contribution of electrons interaction with acoustic phonons in multilayer RTS is not been studied yet.

It was determined in papers [10, 11], the study of spectral parameters and active dynamic conductivity of the RTS as an active zones of QCL and efficiency, can largely describe the processes of generating or detecting electromagnetic waves, tunneling and relaxation of electron beam, and above all, solve the important task of optimizing efficiency and QCL by the selection of geometric design of their active zones.

Considering abovementioned, the important task is to study the spectrum of all types of acoustic phonons arising in nanostructures and effects of their interaction with electrons. However, these studies are efficient to do for the RTS, that are the active zones of QCL and efficiency.

Related researches of the acoustic phonons spectrum in the single quantum wells and wires are presented in the works [12-14]. From above it's obvious that the models of isolated nanosystems described in these works cannot be applied to multilayer RTS.

You can select two early papers [15, 16], where the acoustic phonon modes spread in an isotropic semiconductor layer, which is limited on both sides by another semiconductor environment were described.

In this paper, based on the elastic continuum model, the theory of displacement of an acoustic phonons spectra, arising in double-well semiconductor RTS with $In_{1-x}Ga_xAs$ – potential wells and $In_{1-x}Al_xAs$ potential barriers, was developed.

The results of this work can be used to develop a theory of electrons interaction with acoustic phonons in multilayer RTS.

2. THE ACOUSTIC PHONONS IN MULTILAYER RTS. ELASTIC CONTINUUM MODEL

The flat semiconductor RTS, consisting of two potential $In_{1-x}Ga_xAs$ – holes ((1), (3)) and potential – $In_{1-x}Al_xAs$ barrier ((2)), placed in an external semiconductor environment $In_{1-x}Al_xAs$ ((0) (4)) is examined In the Cartesian coordinate system. The axis Oz is perpendicular to planes of the nanosystem (Fig. 1).

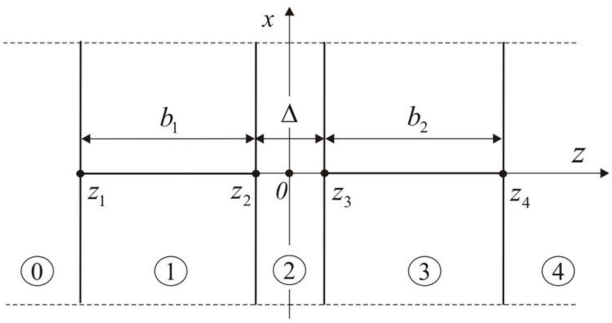

Fig. 1 – The geometric scheme of the multilayer RTS

In the model of elastic continuum the wave equation for the vector of an elastic displacement in the isotropic environment looks like:

$$\rho(z)\frac{\partial^2\bar{u}}{\partial t^2}=(C_{12}+2C_{44})\nabla\cdot(\nabla\cdot\bar{u})-C_{44}\nabla\times(\nabla\times\bar{u}) \quad (1)$$

where the density of the RTS material is defined as:

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$$\rho(z) = \sum_{p=1}^{4} \rho^{(p)} \left[\theta(z - z_{p-1}) - \theta(z - z_p) \right], \quad z_0 = -\infty; \quad z_5 = +\infty, \quad p = \overline{0,\,4} \tag{2}$$

$\rho^{(p)} = \begin{cases} \rho_0, \ p = 1, 3, \\ \rho_1, \ p = 0, 2, 4. \end{cases}$ – the density of the material, $C_{12}^{(p)} = \begin{cases} C_{12_0}, \\ C_{121}, \end{cases}$; $C_{44}^{(p)} = \begin{cases} C_{44_0}, & p = 1, 3, \\ C_{441}, & p = 0, 2, 4. \end{cases}$ – elastic constants of the p RTS layer , $\theta(z)$ - Heaviside unit function.

As the following equation is true to the transverse acoustic modes:

$$\nabla \cdot \bar{u} = 0; \ \nabla \times (\nabla \times \bar{u}) = -\nabla^2 \bar{u}\,, \tag{3}$$

so the equation (1) becomes:

$$\rho(z) \frac{\partial^2 \bar{u}}{\partial t^2} = C_{44} \nabla^2 \bar{u}\ . \tag{4}$$

Let consider that the transverse acoustic mode are spread in the direction of the axis Ox and have the wave vector q , so the elastic displacement $\bar{u}(z)$ can be found from the equation:

$$\bar{u}(x, y, z) = \bar{u}(z) e^{i(qx - \omega r)} \tag{5}$$

As the cross-phonon modes have only one nonzero component, so:

$$\bar{u}(z) = \left(0,\ u_y(z),\ 0\right), \tag{6}$$

Then, the solution of equation (4) can be represented as: $\bar{u}(z) = u_y(z) e^{i(qx - \omega t)}$, where the displacement is:

$$u_y(z) = \sum_{p=1}^{4} u_y^{(p)}(z) \left[\theta(z - z_{p-1}) - \theta(z - z_p) \right], \quad z_0 = -\infty; \quad z_5 = +\infty, \quad p = \overline{0,\,4} \tag{7}$$

And the components $u_y^{(p)}(z)$ can be obtained from the equation:

$$\frac{d^2 u_y^{(p)}(z)}{dz^2} - \left(q^2 - \frac{\omega^2}{\upsilon_t^{(p)2}} \right) u_y^{(p)}(z) = 0\ , \tag{8}$$

where

$$\upsilon_t^{(p)} = \sqrt{\frac{C_{44}^{(p)}}{\rho^{(p)}}} \tag{9}$$

- the transverse speed of sound in p layer of the RTS, moreover: $\upsilon_t^{(1)} = \upsilon_t^{(3)} = \upsilon_t^{(5)};\ \upsilon_t^{(2)} = \upsilon_t^{(4)}$.

As the acoustic waves should subside in the environment from the left and right side of the RTS, i.e. $z < z_1$ and $z > z_4$, then the solutions of equations (8) must satisfy the condition:

$$u(z)\big|_{z \to \pm\infty} = 0\ . \tag{10}$$

The solutions of equations (8), being presented in the expression (7) look like:

$$\begin{aligned} u_y(z) = {} & A_1 e^{\chi_t^{(1)} z} \left[\theta(z - z_0) - \theta(z - z_1) \right] + \left(A_2 \cos k_t^{(2)} z + B_2 \cos k_t^{(2)} z \right) \left[\theta(z - z_1) - \theta(z - z_2) \right] + \\ & + \left(A_3 e^{\chi_t^{(3)} z} + B_3 e^{-\chi_t^{(3)} z} \right) \left[\theta(z - z_2) - \theta(z - z_3) \right] + \left(A_4 \cos k_t^{(4)} z + B_4 \cos k_t^{(4)} z \right) \left[\theta(z - z_3) - \theta(z - z_4) \right] + \\ & + B_5 e^{-\chi_t^{(5)} z} \left[\theta(z - z_4) - \theta(z - z_5) \right], \end{aligned} \tag{11}$$

where

$$\chi_t^{(1)} = \chi_t^{(3)} = \chi_t^{(5)} = \sqrt{q^2 - \frac{\omega^2}{\upsilon_t^{(1)2}}}; \quad k_t^{(2)} = k_t^{(4)} = \sqrt{\frac{\omega^2}{\upsilon_t^{(2)2}} - q^2}\ . \tag{12}$$

The conditions of continuity of displacement vector components and stress tensor $\sigma_{yz}^{(p)}(z)$ are satisfied on the heteroboundaries of nanostructure:

$$\begin{cases} u_y^{(p)}(z)\big|_{z = z_p - 0} = u_y^{(p+1)}(z)\big|_{z = z_p + 0}, \\ \sigma_{yz}^{(p)}(z)\big|_{z = z_p - 0} = \sigma_{yz}^{(p+1)}(z)\big|_{z = z_p + 0}, \end{cases} \tag{13}$$

where the displacement vector components are defined as:

$$\sigma_{yz}(z) = C_{44} \left(\frac{\partial \bar{u}(z)}{\partial y} + \frac{\partial \bar{u}(z)}{\partial z} \right) = C_{44} \frac{\partial}{\partial z} \left(u_y(z) e^{iqx} \right) = C_{44} \frac{\partial u_y(z)}{\partial z} e^{iqx}\ . \tag{14}$$

From the equation (14) considering (11) we can find following:

$$\sigma_{yz}(z) = \begin{cases} \sigma_y^{(0)}(z), \ z < z_1, \\ \sigma_y^{(1)}(z), \ z_1 \le z < z_2, \\ \sigma_y^{(2)}(z), \ z_2 \le z < z_3, \\ \sigma_y^{(3)}(z), \ z_3 \le z < z_4, \\ \sigma_y^{(4)}(z), \ z > z_4, \end{cases} = \begin{cases} C_{44}^{(0)} \chi_t^{(0)} A_0 e^{\chi_t^{(0)} z}, \ z < z_1, \\ C_{44}^{(1)} k_t^{(1)} \left(-A_1 \sin k_t^{(1)} z + A_1 \cos k_t^{(1)} z \right), \ z_1 \le z < z_2, \\ C_{44}^{(2)} \chi_t^{(2)} \left(A_2 e^{\chi_t^{(0)} z} - B_2 e^{-\chi_t^{(0)} z} \right), \ z_2 \le z < z_3, \\ C_{44}^{(3)} k_t^{(3)} \left(-A_1 \sin k_t^{(3)} z + A_1 \cos k_t^{(3)} z \right), \ z_3 \le z < z_4, \\ -C_{44}^{(4)} \chi_t^{(0)} B_4 e^{-\chi_t^{(0)} z}, \ z > z_4. \end{cases} \tag{15}$$

With the use of the transfer matrix method, all the unknown coefficients $A_1, A_2, B_2, A_3, B_3, A_4, B_4, B_5$ are uniquely determined from the condition (10) and equation (13). The spectrum of phonons is determined by the dispersion equation:

$$\left|T(q,\, \omega)\right| = 0\,, \qquad (16)$$

where:

$$T(q,\, \omega) = T^{(0,1)}T^{(1,2)}T^{(2,3)}T^{(3,4)} \qquad (17)$$

is the transfer matrix of studied RTS.

In the (17):

$$T^{(p,p+1)} = \begin{pmatrix} t_{11}^{p,p+1} & t_{12}^{p,p+1} \\ t_{21}^{p,p+1} & t_{22}^{p,p+1} \end{pmatrix} \qquad (18)$$

is the transfer matrix between p and $p+1$ layers of the RTS, moreover transfer matrix elements are defined as:

$$t_{11}^{p,p+1} = \begin{cases} \dfrac{1}{2}\left(1 - \dfrac{C_{44}^{(p)}\chi_t^{(p)}}{C_{44}^{(p+1)}k_t^{(p+1)}}\right)e^{-\chi_t^{(0)}z_p}\cos k_t^{(p+1)}z_p; \\ \dfrac{1}{2}\left(1 - \dfrac{C_{44}^{(p+1)}k_t^{(p+1)}}{C_{44}^{(p)}\chi_t^{(p)}}\right)e^{\chi_t^{(0)}z_p}\sec k_t^{(p)}z_p \end{cases} \quad t_{12}^{p,p+1} = \begin{cases} \dfrac{1}{2}\left(1 + \dfrac{C_{44}^{(p)}\chi_t^{(p)}}{C_{44}^{(p+1)}k_t^{(p+1)}}\right)e^{-\chi_t^{(0)}z_p}\sin k_t^{(p+1)}z_p; & p = 0;\, 2 \\ \dfrac{1}{2}\left(1 + \dfrac{C_{44}^{(p+1)}k_t^{(p+1)}}{C_{44}^{(p)}\chi_t^{(p)}}\right)e^{\chi_t^{(0)}z_p}\sec k_t^{(p)}z_p; & p = 1;\, 3 \end{cases}$$

$$t_{21}^{p,p+1} = \begin{cases} \dfrac{1}{2}\left(1 + \dfrac{C_{44}^{(p)}\chi_t^{(p)}}{C_{44}^{(p+1)}k_t^{(p+1)}}\right)e^{\chi_t^{(0)}z_p}\cos k_t^{(p+1)}z_p; \\ \dfrac{1}{2}\left(1 + \dfrac{C_{44}^{(p+1)}k_t^{(p+1)}}{C_{44}^{(p)}\chi_t^{(p)}}\right)e^{\chi_t^{(0)}z_p}\csc k_t^{(p)}z_p \end{cases} \quad t_{22}^{p,p+1} = \begin{cases} \dfrac{1}{2}\left(1 - \dfrac{C_{44}^{(p+1)}k_t^{(p+1)}}{C_{44}^{(p)}\chi_t^{(p)}}\right)e^{\chi_t^{(0)}z_p}\sin k_t^{(p+1)}z_p; & p = 0;\, 2 \\ \dfrac{1}{2}\left(1 - \dfrac{C_{44}^{(p)}\chi_t^{(p)}}{C_{44}^{(p+1)}k_t^{(p+1)}}\right)e^{-\chi_t^{(0)}z_p}\sec k_t^{(p)}z_p; & p = 1;\, 3 \end{cases} \qquad (19)$$

$$t_{12}^{0,1} = t_{21}^{0,1} = t_{11}^{3,4} = t_{22}^{3,4} = 0.$$

The acoustic phonons spectrum are completely determined by the equations (18-19) and $\Omega_{n\bar{q}} = \hbar\omega_{n\bar{q}}$.

3. DISCUSSION OF THE RESULTS

Based on the developed theory, the calculation of the acoustic phonons spectrum of the nanostructure, consisting of two potential $In_{0.53}Ga_{0.47}As$ wells and potential $In_{0.52}Al_{0.48}As$ barrier, placed in the environment, $In_{0.52}Al_{0.48}As$ has been done. Geometric parameters of the RTS are the following: potential wells: $b_1 = b_2 = 10$ nm, barrier -. $\Delta = 5$ nm. Physical parameters of the RTS are: the density of the potential wells and barriers material $\rho_0 = 5{,}50 \cdot 10^3\ kg/\mathrm{m}^3$; $\rho_1 = 4{,}76 \cdot 10^3\ kg/\mathrm{m}^3$, and the elastic constants $C_{44_0} = 5{,}96 \cdot 10^{10}\mathrm{N/m^2}$; $C_{44_1} = 4{,}76 \cdot 10^{10}\ \mathrm{N/m^2}$.

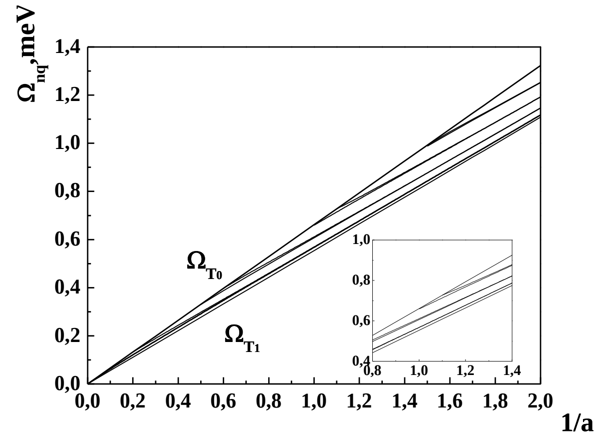

Fig. 2 – The dependences of the transverse phonons spectrum ($\Omega_{n\bar{q}}$) from the internal barrier position (Δ)

Fig. 2 shows the dependence of the energy spectrum of acoustic phonons from the wave vector $q = \dfrac{1}{a}$, where $a = b_1 + \Delta + b_2$. From the Fig. 2 it's obvious, that, mentioned above spectrum dependences $\Omega_{n\bar{q}}$ from q, are located in the energy interval: $\Omega_{T_1} \le \Omega_{n\bar{q}} \le \Omega_{T_0}$, where Ω_{T_0} and Ω_{T_1} - are the energies of the transverse phonons in massive crystal $In_{0.53}Ga_{0.47}As$ and $In_{0.52}Al_{0.48}As$ (where $\Omega_{T_0}(q), \Omega_{T_1}(q) \sim q$). The spectrum of acoustic phonons of the RTS consists of the phonon mode groups, each of which contains two modes of positive and negative dispersion. With the increasing of q, the phonon energies values within each of these groups grow and converge with each other and at the same time $\Omega_{n\bar{q}} \to \Omega_{T_0}$.

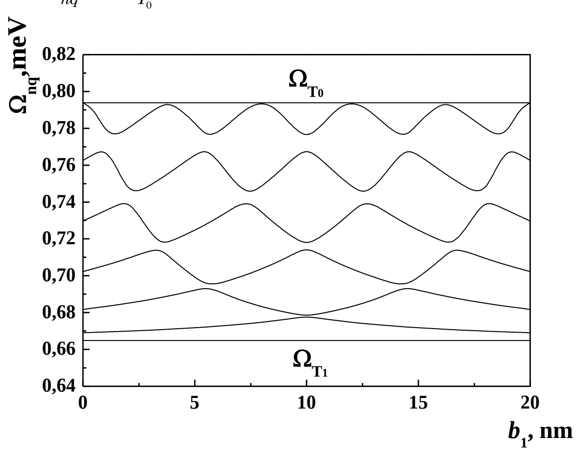

Fig. 3 – The dependences of the transverse phonons spectrum ($\Omega_{n\bar{q}}$) from the internal well position (b_1) in the general potential well at $q = 1.2$

Fig. 3 shows the dependence of the acoustic phonons spectrum $\Omega_{n\bar{q}}$ from the position of the inner barrier (b) for $q = 1.2$. The figure shows that the dependences $\Omega_{n\bar{q}}$ from b are within the limits: $\Omega_{T_1} = 0{,}66\ \text{meV} \le \Omega_{n\bar{q}} \le 0{,}79\ \text{meV} = \Omega_{T_0}$, and $\Omega_{n\bar{q}} < \Omega_{n+1\bar{q}}$, $n = 1, 2, .., 6$. For each of phonons mode $\Omega_{n\bar{q}}$, $n = 1, 2, .., 6$ on the dependence schedule of b, n maximums are formed and from $n = 2$, $n - 1$ minimums.

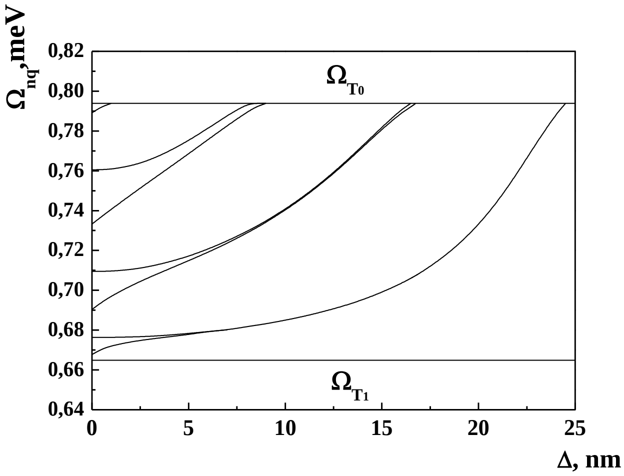

Fig. 4 – The dependences of the transverse phonons spectrum $\Omega_{n\bar{q}}$ from the internal barrier thickness (Δ) at constant size of the nanostructures, calculated at $q = 1.2$

The dependences of the energy spectrum of phonons from the thickness of the inner potential barrier at constant general size of nanostructure $a = b_1 + \Delta + b_2$, where $q = 1.2$ are presented at the Fig. 4. Fig. 4 shows that, similar to previously studied dependencies, acoustic phonon mode are located within the limits: $\Omega_{T_1} = 0{,}66\ \text{meV} \le \Omega_{n\bar{q}} \le 0{,}79\ \text{meV} = \Omega_{T_0}$. For each of the three groups of phonon modes , containing two modes with positive and negative dispersion, the dependences $\Omega_{n\bar{q}}$ of (Δ) increases, bounding together and reaching maximum values $\Omega_{T_0} = 0{,}79\ \text{meV}$.

4. CONCLUSION

In presented paper, with the use of elastic continuum model, the theory of the transverse acoustic phonons spectrum in planar multilayer semiconductor nanostructures has been developed, that can serve as an active element of a quantum cascade laser or detector.

On the example of the nanosystems with two potential wells and barriers, with the use of the advanced theory, the acoustic phonons spectrum was calculated.

The dependences of the phonon spectrum from geometric parameters of studied nanostructure were set in this paper.

The results obtained in the paper can be used to develop a theory of the electrons interaction with the transverse acoustic phonons in multilayer semiconductor nanosystems.

Спектр поперечних акустичних фононів у плоских багатошарових напівпровідникових наноструктурах

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У моделі пружного континууму розвинена теорія енергетичного спектру поперечних акустичних фононів, що виникають у плоских напівпровідникових наноструктурах. Для досліджуваної резонансно-тунельної структури, що може виконувати роль активного елемента квантового каскадного лазера чи детектора, розраховано спектр акустичних фононних мод. Встановлено залежності спектру акустичних фононів від геометричних параметрів досліджуваної наноструктури. Розвинена теорія може бути використана для подальшого теоретичного дослідження процесів взаємодії електронів з акустичними фононами у багатошарових наноструктурах.

Ключові слова: Квантовий каскадний лазер, Квантовий каскадний детектор, Резонансно-тунельна структура, Акустичні фонони, Трансфер-матриця.

Спектр поперечных акустических фононов в плоских многослойных полупроводниковых наноструктурах

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В модели упругого континуума развита теория энергетического спектра поперечных акустических фононов, возникающих в плоских полупроводниковых наноструктурах. Для исследуемой резонансно-туннельной структуры, которая может выполнять роль активного элемента квантового каскадного лазера или детектора, рассчитан спектр акустических фононных мод. Установлены зависимости спектра акустических фононов от геометрических параметров исследуемой наноструктуры. Развитая теория может быть использована для дальнейшего теоретического исследования процессов взаимодействия электронов с акустическими фононами в многослойных наноструктурах.

Ключевые слова: Квантовый каскадный лазер, Квантовый каскадный детектор, Резонансно-туннельная структура, Акустические фононы, Трансфер-матрица.

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