Acoustic phonons in multilayer nitride-based AlN/GaN resonant tunneling structures

I V Boyko 1,3, M R Petryk 1 and J Fraissard 2

1 Mathematical Modeling of Mass Transfer Laboratory, Ternopil Ivan Puluj National Technical University, 56 Ruska str., 46001 Ternopil, Ukraine
2 Sorbonne Universites, ESPCI-LPEM, 10 rue Vauquelin, F-75231 Paris, France
3 Author to whom any correspondence should be addressed.
E-mail: boyko.i.v.theory@gmail.com and jacques.fraissard@upmc.fr

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Abstract

The study of physical processes associated with acoustic phonons in nitride-based nanosystems is of great importance for the effective operation of modern nanoscale devices. In this paper, a consistent theory of acoustic phonons arising in multilayer nitride-based semiconductor resonant tunneling structures, that can function as a separate cascade of a quantum cascade laser or detector is proposed. Using the physical and geometric parameters of a typical nanostructure, the spectrum of various types of acoustic phonons and the corresponding normalized components of the elastic displacement vector are calculated. It has been established that the spectrum of acoustic phonons of a multilayer nanostructure consists of two groups of the shear phonons dependencies and three groups of dependencies for a mixed spectrum of flexural and dilatational phonons. The dependencies of the acoustic phonons spectrum of the nanostructure and the components of the elastic displacement vector on its geometric parameters are studied. It has been established that for the components of the displacement vector for shear phonons have a decrease in the absolute values of their maxima with increasing of energy level number. The components of flexural and dilatational phonons behave respectively as symmetric and antisymmetric functions relatively the center of an separate selected layer of the nanostructure. The proposed theory can be further applied to study the interaction of electrons with acoustic phonons in multilayer resonant tunneling structures.

1. Introduction

Modern quantum cascade lasers (QCL) [1–3] and detectors (QCD) [4–6] of the near and mid infrared ranges of electromagnetic waves use plane multilayer nanostructures based on double GaN, AlN and triple AlGaN compounds of nitride semiconductor materials as their active elements. The characteristic feature of the mentioned materials is the possibility of nanodevices operation based on them in a wide temperature range and the generation of a constant electric field caused by the piezoelectric effect in the nanostructure layers. For the nanostructures based on such semiconductors, phonon processes, especially processes associated with acoustic phonons and electron scattering on them, are rather poorly studied. Acoustic phonons propagating in the direction perpendicular to the multilayer superlattice layers were widely studied in long-standing related papers [7–9]. Theoretical results on the study of the acoustic phonons spectra in single-well nitride semiconductor nanostructures and nanowires, which were obtained in [10–16], cannot be applied to multilayer resonant tunneling structures (RTS) for the following reason: single-well nanostructures in [10–12] were considered to be placed in the external environment of the sapphire substrate, which made it possible to take the components of the elastic displacement vector and the components of the stress tensor equal to zero at the external boundaries of the nanostructure. Taking into account the fact, that the multilayer QCL cascades and QCD should be consistent with each other to ensure coherent tunneling mode [17], the above conditions cannot be used for the boundaries of the RTS with the external environment, and at the boundaries of its internal layers.
For an adequate description of physical processes in resonant tunneling structures, they should be considered to be placed in an external semiconductor medium. So, the active use of nanodevices, such as QCL and QCD, causes considerable interest in the physical processes that occur in their precision elements, this direction is the study of acoustic phonons in particular. By virtue of the facts indicated by us, features of the functioning the nanodevice active bands and cascades determine the formulation of a different model for the study of acoustic phonons. The problem, which is associated with the application of nonzero boundary conditions on the nanostructures heteroboundaries, as far as it is known, is not still an unresolved problem.

In the proposed paper the components of the displacement field \( u = (u_1, u_2, u_3) \), spectrum, phonon modes for shear, flexural and dilatational phonons are obtained by solving the equation of motion for the elastic continuum, using the boundary conditions for the elastic displacement components \( u_1, u_2, u_3 \) and components of the stress tensor \( \sigma_{ij} \), \( i, j = 1, 2, 3 \) on all heteroboundaries of the nanosystem. Using the developed theory for the geometric and physical parameters of a typical nitride-based RTS, which can function as an active zone of the near infrared QCD, the spectrum and components of the elastic displacement for acoustic phonons were studied. Their dependence on the geometric parameters of the investigated RTS is established.

2. Methods

2.1. Analytical solutions of equations for the elastic displacement of a nanosystem medium

In the statement of the problem we assume that the investigated RTS, which contains \( N \) semiconductor layers being in the external AlN semiconductor medium, is placed so, that the \( Oz \) axis is perpendicular to the interfaces of the layers of the nanosystem (Figure 1). Taking into account the notation introduced in figure 1, the density \( \rho(z) \) and elastic coefficients \( C_{iklm}(z) \) of the RTS layers are dependent on the coordinate \( z \) and can be presented correspondingly as follows:

\[
\rho(z) = \sum_{p=1}^{N} \rho^{(p)}[\theta(z_p - z_{p-1}) - \theta(z_p - z_{p+1})];
\]

\[
C_{iklm}(z) = \sum_{p=1}^{N} C_{iklm}^{(p)}[\theta(z_p - z_{p-1}) - \theta(z_p - z_{p+1})],
\]

where \( \theta(z) \) is a unit step function.

Acoustic phonon modes arising in a multilayer AlN/GaN RTS are obtained by solving the equation of motion for the elastic displacement of the medium of the RTS layers, which, taking into account (1), (2), can be presented as:

\[
\rho(z) \frac{\partial^2 u_i(r, t)}{\partial t^2} = \frac{\partial \sigma_{ik}(r)}{\partial x_k}; i, k = (1; 2; 3)
\]

where \( x_1 = x_2 = y; x_3 = z \), and \( u_i = u_i(x, y, z, t) \) are components of the displacement vector at the point \( r = (x_1, x_2, x_3) = (x, y, z) \) for time \( t \), and

\[
\sigma_{ik}(r) = C_{iklm}(z) u_{lm}(r), \quad l, m = (1; 2; 3)
\]

- stress tensor,

\[
u_{lm}(r) = \frac{1}{2} \left( \frac{\partial u_l(r)}{\partial x_m} + \frac{\partial u_m(r)}{\partial x_l} \right)
\]

- strain tensor components.
For the case of the investigated RTS, we assume that the propagation of acoustic phonons occurs within the Ox axis. Since for an arbitrarily chosen RTS p-th layer, it is uniform in the plane Ox,y, and the elastic displacement vector \( u_r(t, z) \) is independent on coordinate \( y \), this makes it possible to search for solutions of equation (3) as follows:

\[
u_r(t, z) = \sum_{p=1}^{N} u_i^{(p)}(x, z, t)[\theta(z_p - z_{p-1}) - \theta(z_p - z_{p+1})]
\]

\[
= \sum_{p=1}^{N} \left( \frac{u_1^{(p)}(z)}{u_2^{(p)}(z)} \right) [\theta(z_p - z_{p-1}) - \theta(z_p - z_{p+1})] e^{i(\omega t - qz)}.
\]

where \( u_1^{(p)}(z) \), \( u_2^{(p)}(z) \), \( u_3^{(p)}(z) \) - components of the displacement vector within the arbitrary nanostructure p-th layer.

Substituting (6) into the equation of motion (3) and taking into account relations (4), (5), we obtain:

\[
\begin{bmatrix}
\rho^{(p)} \omega^2 \delta_{ki} - C^{(p)}_{akl} \frac{\partial^2}{\partial x_k \partial x_l} & \rho^{(p)} \omega^2 \delta_{ki} & \rho^{(p)} \omega^2 \delta_{ki} \\
0 & -C^{(p)}_{444} \delta_{jij} + q^2 C^{(p)}_{66} & 0 \\
0 & 0 & -C^{(p)}_{333} \delta_{jij} + q^2 C^{(p)}_{444}
\end{bmatrix}
\begin{bmatrix}
\frac{du_1^{(p)}(z)}{dz} \\
\frac{du_2^{(p)}(z)}{dz} \\
\frac{du_3^{(p)}(z)}{dz}
\end{bmatrix}
\]

\[= 0.
\]

(7)

Taking into account the fact, that the semiconductor materials of the RTS layers are of the wurtzite crystal structure, it is worth to make the transition from the designations \( C_{\text{a44}}^{(p)} \) to the Voigt two-index designations \( C_{\alpha \beta} \) for elastic constants. Now, taking into account the explicit form of the tensor \([12]\), we obtain the matrix equation for the components \( u_1^{(p)}(z) \), \( u_2^{(p)}(z) \), \( u_3^{(p)}(z) \):

\[
\begin{bmatrix}
-C^{(p)}_{44} \frac{d^2}{dz^2} + q^2 C^{(p)}_{11} & 0 & \rho^{(p)} \omega^2 \\
0 & -C^{(p)}_{44} \frac{d^2}{dz^2} + q^2 C^{(p)}_{66} & 0 \\
0 & 0 & -C^{(p)}_{33} \frac{d^2}{dz^2} + q^2 C^{(p)}_{444}
\end{bmatrix}
\begin{bmatrix}
\frac{du_1^{(p)}(z)}{dz} \\
\frac{du_2^{(p)}(z)}{dz} \\
\frac{du_3^{(p)}(z)}{dz}
\end{bmatrix}
\]

\[= 0.
\]

(8)

which splits into three equations, respectively:

\[
\frac{d^2 u_1^{(p)}(z)}{dz^2} - i q \xi_1 \frac{du_3^{(p)}(z)}{dz} + k_1(q, \omega) u_1^{(p)}(z) = 0;
\]

\[
\xi_1 = \frac{-C^{(p)}_{11} + C^{(p)}_{44}}{C^{(p)}_{44}}; \quad k_1(q, \omega) = \sqrt{\rho^{(p)} \omega^2 - q^2 C^{(p)}_{11}}
\]

(9)

\[
\frac{d^2 u_2^{(p)}(z)}{dz^2} - \chi_2(q, \omega) u_2^{(p)}(z) = 0; \quad \chi_2(q, \omega) = \sqrt{q^2 C^{(p)}_{66} - \rho^{(p)} \omega^2} \sqrt{C^{(p)}_{44}}
\]

(10)

\[
\frac{d^2 u_3^{(p)}(z)}{dz^2} - \chi_3(q, \omega) u_3^{(p)}(z) = 0; \quad \chi_3(q, \omega) = \sqrt{\rho^{(p)} \omega^2 - q^2 C^{(p)}_{44}} \sqrt{C^{(p)}_{33}}
\]

(11)

and, as it can be seen from the equations (9) and (11), they form a system relatively \( u_1^{(p)}(z) \) and \( u_3^{(p)}(z) \). Formally, following the terminology for the classification introduced in [7, 8], the types of phonons arising in a separate p-th layer of the nanosystem are as follows. The solutions of equation (10) describe shear (SH) phonons. The solutions of the system of equations (9) and (11) determine the flexural (FL) and dilatational (DL) acoustic phonons, which are defined respectively as: \( u_1^{(p)}(z) = u^{(p)}(u_1^{(p)}(z)), \ u_3^{(p)}(z) \) and \( u_2^{(p)}(z) = u^{(p)}(u_2^{(p)}(z)), \ u_3^{(p)}(z) \), where the indices 'S' and 'A' denote the symmetric and antisymmetric functions of \( z \) correspondingly.
First let's find solutions for equation (10) that describe shear (SH) acoustic phonons. They look like:

\[ u_2(q, \omega, z) = u_2^{(0)}(q, \omega, z)\theta(-z) + u_2^{(N+1)}(q, \omega, z)\theta(z - z_N) \]

\[ + \sum_{p=1}^{N} u_2^{(p)}(q, \omega, z)[\theta(z - z_{p-1}) - \theta(z - z_p)] \]

\[ = B_2^{(0)}e^{\gamma_2 z}\theta(-z) + A_2^{(N+1)}e^{-\chi_2(z - z_N)}\theta(z - z_N) \]

\[ + \sum_{p=1}^{N} [A_2^{(p)}e^{-\gamma_2(z - z_{p-1})} + B_2^{(p)}e^{\gamma_2(z - z_{p-1})}][\theta(z - z_{p-1}) - \theta(z - z_p)]. \]

(12)

In relation (12), it is taken into account, that \( B_2^{(0)} = A_2^{(N+1)} = 0 \), since the displacements \( u_2(q, \omega, z) \) cannot be increased indefinitely in a semiconductor medium AlN to the left and right of the RTS, according to the condition:

\[ u_2(q, \omega, z)|_{z \rightarrow \pm \infty} \rightarrow 0. \]

(13)

Solutions \( u_1(z) \) and \( u_3(z) \) of the system of equations (9) and (11) are obtained as follows. If the following notation is introduced,

\[ A^{(p)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad B^{(p)} = \begin{pmatrix} 0 & -iqc_1 \\ -iqc_3 & 0 \end{pmatrix}; \quad C^{(p)} = \begin{pmatrix} k^2 & 0 \\ 0 & k^2 \end{pmatrix} \]

(14)

then the system of equations \( u_1(z), u_3(z) \) is equivalent to the following differential equation:

\[ A^{(p)}\frac{d^2 u^{(p)}(z)}{dz^2} + B^{(p)}\frac{du^{(p)}(z)}{dz} + C^{(p)}u^{(p)}(z) = 0; \quad u^{(p)}(z) = \begin{pmatrix} u_1^{(p)}(z) \\ u_3^{(p)}(z) \end{pmatrix} \]

(15)

Searching for solutions of equation (15) in following form

\[ u^{(p)}(z) = \begin{pmatrix} \alpha_1^{(p)} \\ \alpha_3^{(p)} \end{pmatrix}e^{\lambda z} \]

we obtain an equation, that makes it possible to determine the eigenvalues \( \lambda \) and functions \( \alpha_1^{(p)}, \alpha_2^{(p)} \):

\[ (A^{(p)})^2\lambda^2 + (B^{(p)}\lambda + C^{(p)})\frac{\alpha_1^{(p)}}{\alpha_3^{(p)}} = 0 \]

(17)

From expression (17) the biquadratic equation for the eigenvalues is obtained:

\[ \lambda^4 + (k_1^2 + k_3^2 + \alpha_1 c_3 q^2)\lambda^2 + k_1^2 k_3^2 = 0 \]

(18)

its solutions, taking into account the notation in the equations (9), (11):

\[ \lambda_{1,2,3,4} = \pm \sqrt{-\frac{1}{2}(k_1^2 + k_3^2 + \alpha_1 c_3 q^2) \pm \sqrt{\frac{1}{4}(k_1^2 + k_3^2 + \alpha_1 c_3 q^2)^2 - k_1^2 k_3^2}} \]

\[ = \pm \frac{q^2[(C^{(p)}_{11})^2 - C^{(p)}_{11}C^{(p)}_{13} + 2C^{(p)}_{11}C^{(p)}_{14}] + (C^{(p)}_{13} + C^{(p)}_{14})^2\omega^2}{2C^{(p)}_{33}C^{(p)}_{44}} \]

\[ \pm \frac{q^2[(C^{(p)}_{13})^2 - C^{(p)}_{11}C^{(p)}_{13} + 2C^{(p)}_{13}C^{(p)}_{24}] + (C^{(p)}_{13} + C^{(p)}_{24})^2\omega^2}{2C^{(p)}_{33}C^{(p)}_{44}} \]

\[ - (\rho^{(p)}\omega^2 - q^2C^{(p)}_{11}C^{(p)}_{24} - q^2C^{(p)}_{14}C^{(p)}_{24})^{1/2} \] \( C^{(p)}_{33}C^{(p)}_{44} \}

\[ , \lambda_1 = -\lambda_3; \quad \lambda_2 = -\lambda_4 \]

(19)

Next, the eigenfunctions \( \alpha^{(p)} \) are obtained from equation (17):

\[ \left\{ \frac{\lambda_n^2 + k_1^2}{\lambda_n^2 + k_3^2} - iqc_1\lambda_n \mid \alpha_n^{(p)} \right\} = 0; \quad n = 1-4 \]

(20)

whence follows:

\[ \alpha_{1,n}^{(p)} = -iqc_1\lambda_n; \quad \alpha_{3,n}^{(p)} = -(\lambda_n^2 + k_3^2). \]

(21)
For the norm of the vector \( \alpha{\ell}\) we have:
\[
\|\alpha{\ell}\| = \sqrt{|\alpha{\ell}{x}\|} + |\alpha{\ell}{x}\| = \sqrt{q^2 \lambda^2_n c^2_n + (\lambda^2_n + k^2_n)^2}
\]
(22)

Therefore, the general solutions of system (9), (11) look like
\[
\begin{align*}
\alpha{1}(z) &= \frac{\alpha{1}{x}}{\|\alpha{1}\|} A_1 e^{\lambda_1 z} + \frac{\alpha{1}{x}}{\|\alpha{1}\|} B_1 e^{\lambda_2 z} + \frac{\alpha{1}{x}}{\|\alpha{1}\|} C_1 e^{\lambda_3 z} + \frac{\alpha{1}{x}}{\|\alpha{1}\|} D_1 e^{\lambda_4 z} \\
\alpha{2}(z) &= \frac{\alpha{2}{x}}{\|\alpha{2}\|} A_2 e^{\lambda_1 z} + \frac{\alpha{2}{x}}{\|\alpha{2}\|} B_2 e^{\lambda_2 z} + \frac{\alpha{2}{x}}{\|\alpha{2}\|} C_2 e^{\lambda_3 z} + \frac{\alpha{2}{x}}{\|\alpha{2}\|} D_2 e^{\lambda_4 z}
\end{align*}
\]
(23)
where \( \lambda_1, \lambda_2 \) - roots of the characteristic equation of system (9), (11). Besides, there should be 
\[
C_1^{(0)} = B_1^{(0)} = A_2^{(N+1)} = B_2^{(N+1)} = 0,
\]
according to the condition similar to condition (13), i.e.: 
\[
u_{i j k}(q, \omega) \big|_{\gamma = \pm \infty} \to 0
\]
(24)

2.2. Theory of the acoustic phonons spectrum in multilayered nanostructures

The relation between the coefficients \( A_1^{(p)}, B_1^{(p)} \) of the \( p \)-th and \( p + 1 \)-th the nanostructure layers in solutions (12) can be established using the boundary conditions for the components \( u_2^{(p)}(q, \omega, z) \) and components \( \sigma_{zz}(q, \omega, z) = \sigma_{zz}^{(p)}(q, \omega, z) \) of the stress tensor:
\[
\begin{align*}
&\left\{ \begin{array}{l}
 u_2^{(p)}(q, \omega, z) \big|_{z = \pm \infty} = u_2^{(p+1)}(q, \omega, z) \big|_{z = \pm \infty} \\
 \sigma_{zz}^{(p)}(q, \omega, z) \big|_{z = \pm \infty} = \sigma_{zz}^{(p+1)}(q, \omega, z) \big|_{z = \pm \infty}
\end{array} \right.
\end{align*}
\]
(25)
which are found as follows:
\[
\sigma_{zz}^{(p)}(q, \omega, z) = \frac{1}{2} C_{44}^{(p)} \left( \frac{\partial u_1^{(p)}(x, z)}{\partial y} + \frac{\partial u_1^{(p)}(x, z)}{\partial z} \right) = \frac{1}{2} C_{44}^{(p)} \left( \frac{\partial u_1^{(p)}(x, z)}{\partial y} + \frac{\partial u_1^{(p)}(x, z)}{\partial z} \right) e^{i(\omega t - q x)}
\]
(26)

Using the transfer matrix method [15] for conditions (25), the coefficients in solutions (12) can be sequentially expressed for RTS layers from the left to right:
\[
\begin{align*}
&T_0^{(p+1)}(q, \omega) = \left[ \begin{array}{c} A_2^{(N+1)} \\ 0 \end{array} \right] \\
&T_2^{(0,N+1)}(q, \omega) = \prod_{p=0}^{N} T_2^{(p,p+1)}(q, \omega) ;
\end{align*}
\]
(27)
Since the transfer matrix \( T_2^{(0,N+1)}(q, \omega) \) of the investigated nanosystem is now defined, the spectrum of shear acoustic phonons \( \Omega^{SH}(q) = \text{Im}(\omega) \) is obtained from the dispersion equation:
\[
|T_2^{(0,N+1)}(q, \omega)| = 0
\]
(28)
Similarly, as it was done above, for the coefficients \( A_1^{(p)}, B_1^{(p)}, C_1^{(p)}, D_1^{(p)} \) of solutions in the \( p \)-th and \( p + 1 \)-th layers of the nanosystem, the relation is established using the boundary conditions for the components of the displacement vector \( u_{\ell}^{(p)}(q, \omega, z) \) and the stress tensor components \( \sigma_{zz}(q, \omega, z) = \sigma_{zz}^{(p)}(q, \omega, z) ; \sigma_{zz}(q, \omega, z) = \sigma_{zz}^{(p)}(q, \omega, z) ; \)}
where

\[
\sigma_{xx}^{(p)}(q, \omega, z) = \frac{1}{2} C_{44}^{(p)} \left( \frac{\partial u_{y}^{(p)}(x, z)}{\partial x} + \frac{\partial u_{x}^{(p)}(x, z)}{\partial z} \right) e^{i(\omega - q)z} = \frac{1}{2} C_{44}^{(p)} \left( -i q u_{y}^{(p)}(z) + \frac{du_{x}^{(p)}(z)}{dz} \right) e^{i(\omega - q)z}, \quad z < 0;
\]

and

\[
\sigma_{xx}^{(p)}(q, \omega, z) = C_{13}^{(p)} \nabla \cdot u_{l}^{(p)}(x, z) + (C_{33}^{(p)} - C_{13}^{(p)}) \frac{\partial u_{l}^{(p)}(x, z)}{\partial z} = -i q C_{13}^{(p)} u_{l}^{(p)}(z) + C_{33}^{(p)} \frac{du_{l}^{(p)}(z)}{dz} \times e^{i(\omega - q)z}, \quad z > z_{N}.
\]

From conditions (29), using the transfer matrix method [15], we obtain:

\[
\begin{pmatrix}
A_{l}^{(0)} \\
B_{l}^{(0)} \\
0 \\
0
\end{pmatrix} = T_{1,3}^{(0,N+1)}(q, \omega)
\begin{pmatrix}
0 \\
0 \\
C_{i}^{(N+1)} \\
D_{i}^{(N+1)}
\end{pmatrix};
\]

\[
T_{1,3}^{(0,N+1)}(q, \omega) = \prod_{p=0}^{N} T_{1,3}^{(p,p+1)}(q, \omega),
\]

\[
T_{1,3}^{(p,p+1)}(q, \omega) = (t_{1,3}^{(p)})^{-1} t_{1,3}^{(p+1)};
\]

\[
\begin{pmatrix}
\eta_{1,1}^{(p)} e^{\lambda_{1}z} \\
\eta_{1,2}^{(p)} e^{\lambda_{2}z} \\
-\eta_{1,1}^{(p)} e^{-\lambda_{1}z} \\
-\eta_{1,2}^{(p)} e^{-\lambda_{2}z}
\end{pmatrix} = \begin{pmatrix}
\beta_{1,1}^{(p)} e^{\lambda_{1}z} \\
\beta_{1,2}^{(p)} e^{\lambda_{2}z} \\
-\beta_{1,1}^{(p)} e^{-\lambda_{1}z} \\
-\beta_{1,2}^{(p)} e^{-\lambda_{2}z}
\end{pmatrix};
\]

\[
\begin{pmatrix}
\gamma_{1,1}^{(p)} e^{\lambda_{1}z} \\
\gamma_{1,2}^{(p)} e^{\lambda_{2}z} \\
\gamma_{1,1}^{(p)} e^{-\lambda_{1}z} \\
\gamma_{1,2}^{(p)} e^{-\lambda_{2}z}
\end{pmatrix} = \begin{pmatrix}
\gamma_{2,1}^{(p)} e^{\lambda_{1}z} \\
\gamma_{2,2}^{(p)} e^{\lambda_{2}z} \\
\gamma_{2,1}^{(p)} e^{-\lambda_{1}z} \\
\gamma_{2,2}^{(p)} e^{-\lambda_{2}z}
\end{pmatrix} = \begin{pmatrix}
\gamma_{3,1}^{(p)} e^{\lambda_{1}z} \\
\gamma_{3,2}^{(p)} e^{\lambda_{2}z} \\
\gamma_{3,1}^{(p)} e^{-\lambda_{1}z} \\
\gamma_{3,2}^{(p)} e^{-\lambda_{2}z}
\end{pmatrix} = \begin{pmatrix}
\gamma_{4,1}^{(p)} e^{\lambda_{1}z} \\
\gamma_{4,2}^{(p)} e^{\lambda_{2}z} \\
\gamma_{4,1}^{(p)} e^{-\lambda_{1}z} \\
\gamma_{4,2}^{(p)} e^{-\lambda_{2}z}
\end{pmatrix}.
\]
where the following notation is introduced:

\[
\eta^{(p)}_{l,n} = -iqc_1\lambda_n/\sqrt{q^2\lambda_n^2c_l^2 + (\lambda_n^2 + k_f^2)^2};
\]

\[
\eta^{(p)}_{l,n} = -(\lambda_n^2 + k_f^2)/\sqrt{q^2\lambda_n^2c_l^2 + (\lambda_n^2 + k_f^2)^2};
\]

\[
\beta^{(p)}_{l,n} = \frac{1}{2}iqc_{id}^{(p)}k_f^2/\sqrt{q^2\lambda_n^2c_l^2 + (\lambda_n^2 + k_f^2)^2};
\]

\[
\gamma^{(p)}_{l,n} = -\lambda_n(C_{12}^{(p)}q^2 + C_{13}^{(p)}(\lambda_n^2 + k_f^2))/\sqrt{q^2\lambda_n^2c_l^2 + (\lambda_n^2 + k_f^2)^2}, \quad n = 1, 2.
\]

(33)

The flexural and dilatational acoustic phonons spectrum dependences \(\Omega^{(F,D,L)}(q)\) are determined from the dispersion equation:

\[
|T_{13}^{(0,N+1)}(q, \omega)| = 0
\]

(34)

Further the following coefficients are introduced:

\[
B_1^{(0)} = A_1^{(0)}/A_1^{(0)}; \quad A_1^{(p+1)} = A_1^{(p+1)}/A_1^{(0)}; \quad B_1^{(p+1)} = B_1^{(p)}/A_1^{(0)};
\]

\[
c_1^{(p+1)} = C_1^{(p)}/A_1^{(0)}; \quad d_1^{(p+1)} = D_1^{(p)}/A_1^{(0)};
\]

\[
c_2^{(p+1)} = A_2^{(p+1)}/B_2^{(0)}; \quad b_2^{(p+1)} = B_2^{(p+1)}/B_2^{(0)}, \quad p = 0 \ldots N
\]

(35)

For each nanosystem layer the coefficients \(a^{(p+1)}\), \(b^{(p+1)}\) are likely to be found using the boundary conditions (25) for relations (12), (26). Thus, the coefficients \(A_1^{(p+1)}, B_1^{(p+1)}\) can be expressed in terms of the coefficient \(B_2^{(0)}\), which is determined from the normalization condition for shear phonons [19]:

\[
\int_{-\infty}^{+\infty} \rho(z)\left|u_2(q, \omega, z)\right|^2 \, dz = \frac{\hbar}{2I_x I_y \omega}
\]

(36)

which uniquely determines the components \(u_2(q, \omega, z)\).

Similarly, the coefficients \(A_1^{(p+1)}, B_1^{(p+1)}, c_1^{(p+1)}, d_1^{(p+1)}\) are obtained using the boundary conditions (29) for relations (23), (30), (31). The coefficients \(A_1^{(p+1)}, B_1^{(p+1)}, C_1^{(p+1)}, D_1^{(p+1)}\) are expressed in terms of the coefficient \(A_1^{(0)}\), which is now found from the normalization conditions for flexural and dilatational acoustic phonons [19]:

\[
\int_{-\infty}^{+\infty} \rho(z)\left|u_3(q, \omega, z)\right|^2 + \left|u_5(q, \omega, z)\right|^2 \, dz = \frac{\hbar}{2I_x I_y \omega}
\]

(37)

which allows to determine the displacement components \(u_2(q, \omega, z)\) and \(u_5(q, \omega, z)\) uniquely. Besides, in expressions (36), (37) \(I_x, I_y\) are the geometric dimensions of the studied nanosystem cross-sectional area by the \(xy\) plane.

### 3. Results and discussion

The spectrum of various types of acoustic phonons arising in the studied multilayered nanostructure and the corresponding normalized components of the elastic displacement were calculated using the theory developed above. The calculations were carried out on the example of a two-well AlN/GaN nanosystem - active band of quantum cascade detector. Geometric parameters used for calculation are as follows: the widths of the potential wells are \(d_1 = 5\) nm; \(d_2 = 5\) nm, the width of the potential barrier is \(b = 3\) nm. The values of the geometric parameters of the cross section of the nanosystem along the \(Ox\) and \(Oy\) axes were chosen such as in the paper [20]: \(I_x = I_y = 10^{-5}\) m. The values of the nanosystem physical parameters used in the calculations, taken from papers [21, 22], are presented on table 1.

The value of the spectrum energy of acoustic phonons within the proposed theory is limited to the first Brillouin zone and, as it is known from the papers [23–25], reaches a maximum value of the order of 25meV. With this in mind and to compare the numerical results of our calculations with other papers [10–12] the maximum value of the energy range of acoustic phonons, the calculation of which is given below, it is advisable to choose a value of 20 meV.

#### 3.1. Spectrum characteristics and displacement field components for shear acoustic phonons

In figures 2(a), (b) are shown the dependencies of the shear acoustic phonon spectrum energy levels \(\Omega_{n}^{SH}\) (Figure 2(a)) on the wave vector \(q\), as well as the dependences of this spectrum (figure 2(b)) on the position of the internal potential barrier relatively the external boundaries of the nanosystem \((0 \leq d \leq d_1 + d_2)\), calculated at \(q = 3\pi/(d_1 + d_2 + b)\). As it is seen from figure 2(a), the spectral dependences on \(q\) for the shear acoustic phonons in the nanostructure are formed in the interval \(\Omega_{n}^{SH}(q) \leq \Omega_{n}^{SH}(q) \leq \Omega_{n}^{ALNI}(q)\), where \(\Omega_{n}^{SH}(q)\) and \(\Omega_{n}^{ALNI}(q)\) are the corresponding limiting dependences on \(q\) for bulk GaN and AlN crystals [10, 11, 26].
means, that the values of the calculated energies for shear acoustic phonons are in the same range as in papers [10–12, 15, 16]. It can be seen from the figure, that the spectrum dependencies \( \Omega_{\text{SH}}^n(q) \) are formed at energy values \( \Omega = \Omega_{\text{SH}}^{\text{AlN}}(q) \), forming dependency branches, which consist of two dependencies with close energies values. Besides, as it can be seen from the callout in figure 2(a), the distances between the initial energies for neighboring branches are almost equidistant. When \( q \) values increase, the values of the \( \Omega_{\text{SH}}^n(q) \) energies grow quasi-quadratically at first, and then, they grow in such a way, that the curves \( \Omega_{\text{SH}}^n(q) \) become actually parallel to curve \( \Omega_{\text{Galn}}(q) \).

As it can be seen from figure 2(b), where the dependencies of the energies \( \Omega_{\text{SH}}^n \) on the value of \( d \) are shown, with the increase of \( d \), a certain number of maxima and minima are formed in them, associated with number of the level \( n \). That is, as it can be seen from the figure, each level of dependence \( \Omega_{\text{SH}}^n(d) \) is characterized by the presence of \( n - 1 \) minima and \( n \) maxima. It is also worth noting the occurrence of an anticrossing effect between adjacent energy levels \( \Omega_{\text{SH}}^n(d) \) and \( \Omega_{\text{SH}}^{n+1}(d) \).

In figure 3 the dependencies of the displacement field components \( u_2(q, \omega, z) \) on the geometric dimensions of the nanostructure, calculated for all values of the shear phonon spectrum \( \Omega_{\text{SH}}^n \) at \( q = 39/(d_1 + d_2 + b) \) and normalized with the condition (36), are presented. As it can be seen from the above dependencies, the maximum values of the function \( u_2(q, \omega, z) \) are formed for odd values of the energy level number \( n \) in the left potential well, and for even values of \( n \) in the right potential well. Besides, as it can be seen from the figure, the absolute values of the maxima \( \max u_2(q, \omega, z) \) for even values of \( n \) are much larger than the corresponding values for odd \( n \). It should also be noted, that with an increase in the number \( n \), the maxima for odd \( n \) decreases slowly, while, for example, for \( n = 2 \) and \( n = 10 \), the values \( \max u_2(q, \omega, z) \) actually differ by two orders.

### 3.2. Spectral characteristics and the displacement field components for dilatational and flexural acoustic phonons

In figures 4(a), (b) the dependencies of the energy levels for the mixed spectrum \( \Omega_{\text{FL,DL}}^n \) of flexural and dilatational acoustic phonons on the wave vector \( q \) (Figure 4(a)) are presented, as well as the dependencies of this spectrum (figure 4(b)) on the position of the internal potential barrier relatively the external boundaries of the nanosystem \( (0 \leq d \leq d_1 + d_2) \), calculated at a fixed value \( q = 26/(d_1 + d_2 + b) \). Here, the value of the wave vector differs from its value used in the calculations for shear acoustic phonons. It means, that we want the number of given dependences \( u_1(q, \omega, z) \), \( u_2(q, \omega, z) \) and \( u_2(q, \omega, z) \) to be approximately the same, and since the

| Table 1. Physical parameters of the nanosystem layers material. |
|---------------------------------------------------------------|
| \( \alpha \) (kg/m\(^3\))   | 6150  | 3255 |
| \( C_{11} \) (GPa)       | 390   | 396  |
| \( C_{12} \) (GPa)       | 145   | 137  |
| \( C_{13} \) (GPa)       | 106   | 108  |
| \( C_{33} \) (GPa)       | 398   | 373  |
| \( C_{44} \) (GPa)       | 105   | 116  |
| \( C_{66} \) (GPa)       | 122.5 | 129.5|

Figure 2. Dependencies of the shear acoustic phonons spectrum \( \Omega_{\text{SH}}^n \) on the wave vector \( q \) and \( d \).
spectra \( \Omega_n^{(FL,DL)} \) and \( \Omega_n^{(SH)} \) at the same values of \( q \) contain different number of dependency branches, we had to choose different values of the wave vector \( q \).

The dependence spectrum \( \Omega_n^{(FL,DL)}(q) \) is inherently a mixed spectrum of dilatational and flexural acoustic phonons modes of a nanosystem, and as it can be seen from figure 4(a), consists of three groups of dependencies located within: for the first group (I): \( \Omega_n^{(DL)}(q) \leq \Omega_n^{(FL,DL)}(q) \leq \Omega_n^{(ALN)}(q) \), for the second group (II): \( \Omega_n^{(ALN)}(q) \leq \Omega_n^{(FL,DL)}(q) \leq \Omega_n^{(GaN)}(q) \), for the third group (III): \( \Omega_n^{(GaN)}(q) \leq \Omega_n^{(FL,DL)}(q) \leq \Omega_n^{(ALN)}(q) \), where \( \Omega_n^{(GaN)}(q) \), \( \Omega_n^{(ALN)}(q) \) and \( \Omega_n^{(GaN)}(q) \), \( \Omega_n^{(ALN)}(q) \) are corresponding limiting energy dependencies, which are determined by the propagation velocities of transverse and longitudinal acoustic phonons for bulk crystals [10, 11, 26]. This means, that the values of the calculated energies for spectrum of dilatational and flexural acoustic phonons are in the same range as in papers [10–12, 15, 16].

As it can be seen from figure 4(a), the dependence branches \( \Omega_n^{(FL,DL)}(q) \) are formed at values \( \Omega_n^{(ALN)}(q) \) and when \( q \) increases, they grow sequentially crossing the dependency branches \( \Omega_n^{(GaN)}(q), \Omega_n^{(ALN)}(q), \Omega_n^{(GaN)}(q) \), correspondingly. In this case, for the third group (III) dependence branches show a quasilinear dependence on \( q \), and for the second (II) and first group (I) such dependencies in the calculated range of \( q \) values are actually linear.

Figure 3. Dependencies of the elastic displacement components \( u_n(q, \omega, z) \) on \( z \) for the shear phonons energy spectrum values \( \Omega_n^{(SH)} = (8.402; 8.438; 8.755; 8.892; 9.312; 9.599; 10.039; 10.892; 11.578; 11.818) \) meV at \( q = 39/(d_1 + d_2 + b) \).
Figure 3. (Continued.)

Figure 4. Dependencies of the spectrum $\Omega_{\Delta n}\Omega_{\Delta d}$ on the wave vector $q$ (a) and on the $d$ values (b).
It should also be noted, that successive energy levels for odd and even values of \( n \), starting from the values of wave vector \( q \), become equidistant to each other. As it can be seen from figure 4 (b), depending on \( d \), three groups of the spectrum \( \Omega_n^{FL, DL} \) are formed, which are located in the following range: for the first group (I): \( \Omega_{GaN}^T \leq \Omega_n^{FL, DL} \leq \Omega_{AlN}^T \), for the second group (II): \( \Omega_{AlN}^T \leq \Omega_n^{FL, DL} \leq \Omega_{GaN}^T \), for the third group (III): \( \Omega_{GaN}^T \leq \Omega_n^{FL, DL} \leq \Omega_{AlN}^T \).

The energy dependencies for the first group (I) are characterized by the presence of \( n \) maxima and \( n - 1 \) minima for each number \( n \) of the energy level as it was established above for shear acoustic phonons. In the second group (II) of dependences the following features arise: the first energy level of this group is formed by dependencies, expressed only in four intervals of change of \( d \), that is: 1.25 nm \( \leq d \leq 2.50 \) nm; 3.35 nm \( \leq d \leq 4.60 \) nm; 5.50 nm \( \leq d \leq 6,75 \) nm; 7.65 nm \( \leq d \leq 8,90 \) nm. Besides, it should be noted that the minimum values for these dependences are \( \Omega_{GaN}^T \) values. The next two dependencies of this group form six maximums and five minimums, the dependence for the last level of this group has seven maximums and six minimums.

As it can be seen from the figure 4 (b), the energy dependences for the third group (III) are symmetric relatively the position of the internal potential barrier in the total potential well \( d \). Besides, the last level of this

Figure 5. Dependencies of the elastic displacement components \( u_1(q, \omega, z) \) and \( u_3(q, \omega, z) \) on \( z \) for energy values \( \Omega_n^{FL, DL} = (5.657; 5.961; 6.484; 7.270; 7.497; 8.475; 9.629; 10.528; 11.177; 12.786; 13.330; 14.050) \) meV at \( q = 2\pi/(d_1 + d_2 + b) \).
A group of dependencies is expressed in three intervals $d$: $0.0 \text{ nm} \leq d \leq 2.0 \text{ nm}$; $4.0 \text{ nm} \leq d \leq 6.0 \text{ nm}$; $8.0 \text{ nm} \leq d \leq 10.0 \text{ nm}$.

In figures 5(a)–(l) the dependencies of the elastic displacement components $u_1(q, \omega, z)$ and $u_3(q, \omega, z)$ are given for the values of the spectrum energies $\Omega_n^{FL, DL}$ obtained at $q = 26/(d_1 + d_2 + b)$, which allow to demonstrate properly the properties of the functions $u_1(q, \omega, z)$ and $u_3(q, \omega, z)$. As it can be seen from figure 5 with a change in $z$, the dependencies of the functions $u_1(q, \omega, z)$ and $u_3(q, \omega, z)$ are as follows. The calculated dependences alternately manifest themselves in the left and right potential wells of the nanosystem, while the absolute values of the maxima of these functions $u_1(q, \omega, z)$ and $u_3(q, \omega, z)$ with an increase in the energy values that are formed in both potential wells approach each other, reaching almost the same values for the dependences shown in figure 5(g) and figure 5(h). With a further increase of $\Omega_n^{FL, DL}$ energy, the maximum values of $|\max u_1(q, \omega, z)|$ and $|\max u_3(q, \omega, z)|$ with an increase in the energy values that are formed in both potential wells approach each other, reaching almost the same values for the dependences shown in figure 5(g) and figure 5(h). The main property of the $u_1(q, \omega, z)$ and $u_3(q, \omega, z)$ functions that should be distinguished is that they, within the limits of a single layer of a nanosystem, behave accordingly as the symmetric and antisymmetric functions relatively to the center of a given layer. It should also be noted, that with an increase in the energy value $\Omega_n^{FL, DL}$, the number of maxima and minima created by $u_1(q, \omega, z)$ and $u_3(q, \omega, z)$ functions with changing of $z$ within the layers of the nanosystem increases, and this feature is most
sufficient in the layers that coincide with the potential wells of the nanosystem, which is clearly seen from figures 5(g)–(k). The absolute values of the maxima \( |\max u_1(q, \omega, z)| \) and \( |\max u_2(q, \omega, z)| \) do not tend to decrease with the increase of energies \( \Omega_{n}^{FL,DL} \), as compared with the being established for the values \( |\max u_3(q, \omega, z)| \), calculated for shear acoustic phonons. Besides, it is seen from figure 5, that in the external semiconductor medium to the left and to the right of the studied nanosystem, the values of components \( u_1(q, \omega, z) \) and \( u_3(q, \omega, z) \) tend to zero according to relation (24).

4. Conclusions

An analytical theory of the elastic displacement field components and the spectrum of acoustic phonons, arising in a multilayer nitride-based semiconductor GaN/AlN resonant tunneling structure, is developed.

Using the geometric and physical parameters of a nanosystem, that can function as an active element of a quantum cascade detector, the spectrum of all types of acoustic phonons arising in the nanostructure and the elastic displacement field corresponding components, are calculated. The dependences of the spectrum of acoustic phonons on the wave vector and geometric parameters of the studied nanosystem are established, and their properties are investigated.

For the elastic displacement field components, their dependence on the geometric dimensions of the nanosystem is established. It has been established, that in the region of an arbitrary layer of the nanosystem, the dependencies \( u_1(z) \) and \( u_2(z) \) correspondingly have the properties of symmetric and antisymmetric functions relatively coordinate, that coincides with the middle of this nanosystem layer. The results can be directly used to study the processes of electron-acoustic phonon interaction in multilayer nitride-based nanosystems.

ORCID iDs

I V Boyko \( \odot \) https://orcid.org/0000-0003-2787-1845
M R Petryk \( \odot \) https://orcid.org/0000-0003-2787-1845
J Fraissard \( \odot \) https://orcid.org/0000-0002-9465-1933

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