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I.V. Boyko[1], M.V. Tkach[2], Ju.O. Seti[2]

Self-Consistent Calculation of Potential Profile of GaN/AlN Resonace Tunnelling Structures

[1]*Ternopil Ivan Pul'uj National Technical University, Ruska str., 56, Ternopol, 46001, e-mail: boyko.i.v.theory@gmail.com*
[2]*Chernivtsi National University, Kotsubynsky str., 2, Chernivtsi, 58012, e-mail: ktf@chnu.edu.ua*

For resonant tunneling structure with GaN – potential wells and AlN – potential barriers, calculation of internal fields caused by piezoelectric and spontaneous polarization was carried.

In the model the effective mass of an electron and a dielectric continuum model using finite difference method self-consistent solutions of the Schrödinger and Poisson system of equations taking into account the contribution of piezoelectric and spontaneous polarizations was found.

Based on the found solutions of the Schrödinger and Poisson system of equations for resonance tunneling structure, which functioned as a cascade experimentally realized a quantum cascade detector, calculation of the potential profile and the electron energy spectrum was carried. It was found, that calculated value of detected energy is different from the experimentally obtained not more than 3 %.

Keywords: quantum cascade detector, resonance tunnel structure, piezoelectric polarization, spontaneous polarization, potential profile.

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Introduction

Significant scientific progress in the modern physics of semiconductors is the study of the work of quantum cascade detectors (QCD) [1-3], and the study of physical processes occurring in semiconductor resonance tunneling structures (RTS), which are their active elements. Currently, in relation to the physical nature of the processes occurring in the QCD can be distinguished two of their types.

The first type QCD, the layers of which RTS are based on arsenide compounds: GaAs, InAs, AlAs, GaInAs etc., the crystalline lattices of which belong to the $A^{III}B^{V}$ group of symmetry. QCD of this type works in the medium and far infrared spectral bands of electromagnetic waves. Thus their work is possible only at maintenance of low temperatures (cooling by liquid nitrogen). The work of the QCD of this type is well investigated experimentally [1-3] and theoretically [4-6].

The second type includes the QCD, the layers of which RTS are based on anisotropic semiconductor media, formed by nitride compounds GaN, AlN [7-9], the crystalline lattices of which also belong to the $A^{III}B^{V}$ symmetry group. An essential feature of the $A^{III}B^{V}$ group of nitrides is that in the work of the QCD on their basis it is necessary to take into account their anisotropic properties. Since in elemental lattices of wurtzite type, which usually have nitrides of the $A^{III}B^{V}$ group, the total dipole moment of each lattice is uncompensated, as well as on the heteroboundaries of multilayer RTS there is inconsistency of lattice constants, which leads to the emergence of spontaneous and piezoelectric polarizations. Thus, the total macroscopic polarization that occurs in the RTS layers creates an internal electric field that substantially deforms the potential profile of the nanostructure. Deep potential wells in the RTS layers that provide the work of nanoscale devices in the near infrared spectral bands of electromagnetic waves and their efficient functioning at significantly higher temperatures determine the considerable scientific and applied interest to the QCD based on the nitrides of the $A^{III}B^{V}$ group. However, despite a number of papers [10-15] on the investigation of mechanisms of internal fields occurrence in the RTS, at the moment there is no consistent theory, which would allow to perform calculations of potential profiles for multilayer RTS of cascades of QCD taking into account the contribution of piezoelectric and spontaneous polarizations. This is due to the fact that the approach to calculating the potential RTS profiles proposed in the above-mentioned works is rather rough, since it allows only the contribution of internal fields to the magnitude of an effective potential profile [10-13] or based on numerical modeling of solutions of a self-consistent system Schrödinger and Poisson equations [14, 15]. It can also be implemented

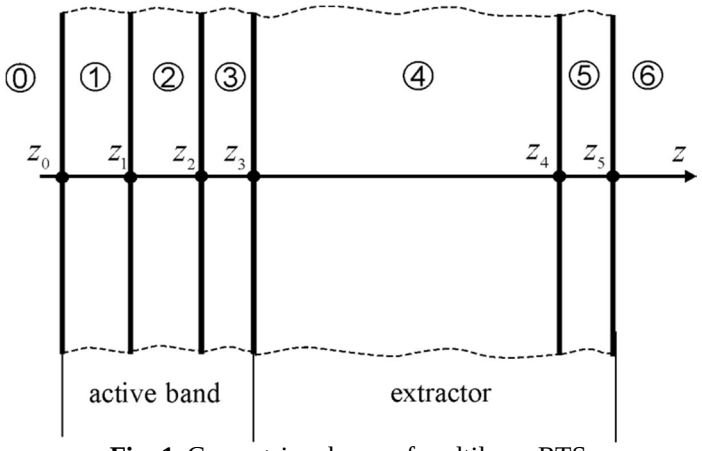

Fig. 1. Geometric scheme of multilayer RTS.

only on powerful computers.

In the proposed paper, taking into account the contribution of piezoelectric and spontaneous polarizations, self-consistent solutions of the Schrödinger and Poisson equations are found. With their use, the quantum-mechanical theory of stationary electronic states in a flat RTS as an active band of QCD is developed.

For the RTS of the experimentally investigated QCD with GaN-potential wells and AlN-potential barriers, functionalized in the near infrared range, the self-consistent calculation of the electronic potential profile, the stationary energy spectrum and the value of the detected energy was performed.

I. Self-consistent solutons of Shrodinger and Poisson's equations

A multilayer RTS, which is located so that in the Cartesian coordinate system, the OZ axis is perpendicular to the boundaries of the separation of nanostructure layers, is considered (Fig. 1). It is assumed that the medium (0), (1), (3), (5), (6) correspond to the semiconductor material AlN, medium (2) – GaN, medium (4) – $Al_{0.58}Ga_{0.42}N$.

Using for an electron the model of effective masses we have:

$$m(z) = m_0\left\{q(-z)+q(z-z_5)+\sum_{p=0}^{2}\left[q(z-z_{2p})-q(z-z_{2p+1})\right]\right\}+m_1[q(z-z_1)+q(z-z_2)]+ \\ +m_2[q(z-z_3)+q(z-z_4)], \quad (1)$$

where $q(z)$ - Heaviside step function, $z_{-1}\to-\infty$, $z_6\to\infty$, a $m_0 = m^{(0)} = m^{(1)} = m^{(3)} = m^{(5)} = m^{(6)}$, $m_1 = m^{(2)}$ i $m_2 = m^{(4)}$ - effective electron masses in potential barriers and wells of RTS, respectively.

Similarly, for dielectric permittivity, RTS can be written:

$$e(z) = e^{(0)}\left\{q(-z)+q(z-z_5)+\sum_{p=0}^{2}\left[q(z-z_{2p})-q(z-z_{2p+1})\right]\right\}+e^{(1)}[q(z-z_1)+q(z-z_2)]+ \\ +e^{(2)}[q(z-z_3)+q(z-z_4)], \quad (2)$$

$e^{(0)} = e^{(1)} = e^{(3)} = e^{(5)} = e^{(6)}$, $e_1 = e^{(2)}$ i $e_2 = e^{(4)}$ - dielectric permeability of RTS layers material.

Energy spectrum of an electron E_n and its wave functions $\Psi_n(E_n, z)$ are determined by solving a self-consistent system of Schrödinger and Poisson equations:

$$\begin{cases} -\dfrac{\mathbf{h}^2}{2}\dfrac{d}{dz}\left(\dfrac{1}{m(z)}\dfrac{d\Psi(z)}{dz}\right)+V(z)\Psi(z)=E\Psi(z), \\ \dfrac{d}{dz}\left(e(z)\dfrac{dj_H(z)}{dz}\right)=-r(z) \end{cases}, \quad (3)$$

where $r(z)$ - free charge density inside RTS, and the effective potential for an electron is found as:

$$V(z) = \Delta E_C(z)+V_H(z)+V_{ex}(z)+V_E(z), \quad (4)$$

In the ratio (4):

$$\Delta E_C(z)=\begin{cases}0.719(E_g(\mathrm{AlN})-E_g(\mathrm{GaN})),\ z<0,\ 0\le z<z_1,\ z_2\le z<z_3, z_4\le z<z_5,\ z>z_5\\ 0,\ z_1\le z<z_2\\ 0.719(E_g(\mathrm{Al_{0.58}Ga_{0.42}N})-E_g(\mathrm{GaN})),\ z_3\le z<z_4\end{cases}, \quad (5)$$

- potential RTS profile for the electron, calculated without taking into account the electric field of piezoelectric and spontaneous polarizations, where the dependence of the band gap width on temperature T for a $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{N}$ semiconductor is given by the Varshni empirical relation [13-15]:

$$E_g(x,T)=E_g(x,0)-\frac{a(x)T^2}{b(x)+T}, \quad (6)$$

and the dependence on the value of x:

$$E_g(x,0)=x^2+1.59x+3.51;$$
$$a(x)=(2.15x^2-0{,}46x+0.94)\cdot 10^{-3}, \quad (7)$$
$$b(x)=1561x^2-270x+791$$

In the ratio (4):

$$V_H(z)=e\,j_H(z) \quad (8)$$

- the potential which is the solution of the Poisson equation in the system of equations (3).

Further in the expression (4):

$$V_{ex}(z)=-\left(\frac{9}{4p^2}\right)^{1/3}\left[1+\frac{0{,}6213r_s}{21}\ln\left(1+\frac{21}{r_s(z)}\right)\right]\frac{e^2}{4pe_0r_s(z)e(z)a_B^*(z)}, \quad (9)$$

exchange-correlation potential, calculated in the Hedin and Lundqvist approximation, where - $r_s(z)=\left(\frac{4p}{3}a_B^{*3}n(z)\right)^{-1/3}$ dimensionless function that characterizes the electron gas in the nanostructure, In relation to the effective Bohr radius $a_B^*(z)=\frac{e(z)}{m(z)a_B}$, a_B - Bohr radius, $n(z)$ - is the concentration of carriers that create a static spatial charge.

The potential energy $V_E(z)$ of the interaction of an electron with fields of spontaneous and piezoelectric polarization inside the RTS is found as:

$$V_E(z)=\begin{cases}0,\ z<0,\\ eF_1z;\ 0\le z<z_1,\\ eF_1z_1-eF_2z,\ z_1\le z<z_2,\\ -eF_2z_2+eF_3z,\ z_2\le z<z_3,\\ eF_3z_3-eF_4z,\ z_3\le z<z_4,\\ -eF_4z_4+eF_5z,\ z_4\le z<z_5,\\ 0\ ,z\ge z_5\end{cases} \quad (10)$$

The values of internal fields F_p, $p=0..5$, are determined from the condition of continuity of the vector of electrical displacement $\overline{D}_p=e^{(p)}\overline{F}_p+\overline{P}_p$ on all the RTS heteroboundaries, i.e. :

$$\overline{D}_p=\overline{D}_{p+1}, \quad (11)$$

without taking into account the availability of free charges within the RTS [12-14], which gives the condition:

$$\sum_{p=0}^{5}F_pd_p=0, \quad (12)$$

Then, from the relations (10) and (11) we have:

$$F_p=\frac{\sum_{k=0}^{5}\left(P_k-P_p\right)\frac{d_k}{e^{(k)}}}{e^{(p)}\sum_{k=0}^{5}\frac{d_k}{e^{(k)}}}, \quad (13)$$

d_k - the thickness of the corresponding layer of the RTS.

The magnitude of the macroscopic polarization $P^{(p)}$ in expression (13), formed in random *p*-th RTS layer, is expressed as the sum of spontaneous $P_{SP}^{(p)}$ and piezoelectric $P_{PZ}^{(p)}$ polarizations:

$$P^{(p)}=P_{SP}^{(p)}+P_{PZ}^{(p)}, \quad (14)$$

Spontaneous polarization in hexagonal wurtzite-type crystals is given as:

$$\overline{P}_{SP}^{(p)}=P_{SP}^{(p)}\overline{k}, \quad (15)$$

where $\overline{k}$ - unit vector along the Oz axis, which determines the orientation of the crystallographic axis.

Piezoelectric polarization for a three-component semiconductor layer of $A_xB_{1-x}N$ -type, depending on the concentration x of the component A is determined by linear approximation:

$$P_{PZ(SP)}^{(p)}(x) = P_{PZ(SP)}^{AN(p)}(h^{(p)}(x)) + \\ + (1-x)P_{PZ(SP)}^{BN(p)}(h^{(p)}(x)) \quad , \qquad (16)$$

where $P_{PZ(SP)}^{AN(p)}(h^{(p)}(x))$ i $P_{PZ(SP)}^{BN(p)}(h^{(p)}(x))$ - due to the inconsistency of the lattice constants of the RTS layers, depend on the magnitude of the basal deformation $h^{(p)} = h^{(p)}(x) = \frac{a_{\text{subs}} - a(x)}{a(x)}$, where $a(x)$ and a_{subs} - lattice constants of material of the nanostructure and substrate layers respectively, and:

$$a(x) = 0.31986 - 0.00891x,$$

$$a_{\text{buf}} = \frac{\sum_{p=1}^{5} A^{(p)} \frac{d_p}{a^{(p)}}}{\sum_{k=1}^{5} \frac{d_p}{(a^{(p)})^2}}; \qquad ,[13] \qquad (17)$$

$$A^{(p)} = C_{11}^{(p)} + C_{12}^{(p)} - 2\frac{(C_{13}^{(p)})^2}{C_{33}^{(p)}}$$

where $a^{(p)}$ - lattice constant of material, d_p - thickness, $C_{11}^{(p)}, C_{12}^{(p)}, C_{13}^{(p)}, C_{33}^{(p)}$ - elastic constants of the RTS the p-th layer.

The value of piezoelectric polarization within a separate RTS layer is defined as:

$$P_{PZ}^{(p)} = 2h^{(p)}e_{31}^{(p)} + h_z^{(p)}e_{33}^{(p)} = 2h^{(p)}e_{31}^{(p)} + \left(-\frac{2C_{13}^{(p)}}{C_{33}^{(p)}}h^{(p)}\right)e_{33}^{(p)} = 2h^{(p)}\left(e_{31}^{(p)} - e_{33}^{(p)}\frac{C_{13}^{(p)}}{C_{13}^{(p)}}\right) h_z^{(p)} = -\frac{2C_{13}^{(p)}}{C_{33}^{(p)}}h^{(p)}, \quad (18)$$

where $e_{31}^{(p)}$, $e_{33}^{(p)}$ - piezoelectric constants.

On the heteroboundaries of the investigated system we obtain the conditions of the continuity for the wave function and the flows of its probabilities, which is the solution of the first equation of the self-consistent system (3):

$$\begin{cases} \Psi_n^{(p)}(E_n, z_p) = \Psi_n^{(p+1)}(E_n, z_p) \\ \frac{1}{m^{(p)}(z)} \frac{d\Psi_n^{(p)}(E_n, z)}{dz}\Big|_{z=z_p} = \frac{1}{m^{(p+1)}(z)} \frac{d\Psi_n^{(p+1)}(E_n, z)}{dz}\Big|_{z=z_p} \end{cases} p = 0,.5 \quad , \qquad (19)$$

and conditions for the continuity of the potential $j_H(z)$ and the vector of electric displacement field:

$$\begin{cases} j_H^{(p)}(z_p) = j_H^{(p)}(z_p) \\ e^{(p)}(z)\frac{dj_H^{(p)}(z)}{dz}\Big|_{z=z_p} - e^{(p+1)}(z)\frac{dj_H^{(p+1)}(z)}{dz}\Big|_{z=z_p} = -s(z_p) \end{cases}; \; p = 0,.5, \qquad (20)$$

where the second condition takes into account the presence of surface charges on the nanosystem heteroboundaries.

It is believed that for the potential outside of the RTS, the conditions for its disappearance are fulfilled:

$$j_H(z)\big|_{z\to 0} \to 0; \; j_H(z)\big|_{z\to z_5} \to 0. \qquad (21)$$

Solutions of the self-consistent system (3) are searched on a uniform grid [16]:

$$\overline{w} = \left\{ z_s = sh, \; s = 0, 1, ...N, \; h = \frac{l}{N} \right\}, \qquad (22)$$

where $l = d_1 + d_2 + d_3 + d_4 + d_5 = z_5$ - total RTS thickness.

According to the finite difference method, the first and second derivatives are approximated as [16] (for convenience, the index "*n*" is omitted):

$$\frac{d\Psi^{(s)}(z)}{dz}\Big|_{z=z_s} = \frac{\Psi_{s+1} - \Psi_s}{h}; \\ \frac{d^2\Psi^{(s)}(z)}{dz^2}\Big|_{z=z_s} = \frac{\Psi_{s+1} - 2\Psi_s + \Psi_{s-1}}{h^2} \quad , \qquad (23)$$

In addition, for wave functions, conditions of periodicity similar to those of Born–von Karman boundary condition must be fulfilled. This gives the condition:

$$\Psi_0 = \Psi_N; \; \Psi_1 = \Psi_{N+1}, \qquad (24)$$

Then the wave functions of the electron are determined by solutions of the matrix equation:

$$\sum_{r=1}^{N} A_{sr}\Psi_s = f_s, ; \Psi_s = \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \\ \Psi_s \\ \text{M} \\ \Psi_N \end{pmatrix};$$

$$f_s = \begin{pmatrix} c_s h \\ 0 \\ 0 \\ 0 \\ 0 \\ \text{M} \\ 0 \end{pmatrix}; \; c_s = \frac{\sqrt{2m_1(\Delta E_C(z_s) - E)}}{\mathbf{h}} \qquad (25)$$

where A_{sr} $(s = \overline{1...N}, r = \overline{1...N})$ - matrix, for which elements we have:

$$A_{sr} = \begin{cases} 1, & r = s-1, \\ -\left(1 + \dfrac{m_s}{m_{s+1}}\right), & r = s, \\ \dfrac{m_s}{m_{s+1}}, & r = s+1, \\ 0, & \text{other elements} \end{cases}$$

, if the grid nodes z_s coincide with RTS heteroboundaries and

$$A_{sr} = \begin{cases} 1, & r = s-1, \\ (k_s^2 - c_s^2)h^2 - 2, & r = s \\ -1, & r = s+1 \\ 0, & \text{other elements} \end{cases} \text{ otherwise.}$$

The stationary energy spectrum $E_n^{(s)}$ of electron is determined from the dispersion equation:

$$\det\left|A_{NN} - lI\right| = 0, \qquad (26)$$

i.e., for each eigenvalue l_n of a matrix A_{NN}, the energy value of the discrete spectrum is defined as:

$$E_n^{(s)} = \frac{(l_n + 2)\mathbf{h}^2}{2m_s h^2} + \frac{c_s^2 h^2}{2m_s}, \qquad (27)$$

$n = 1, 2, ...$ - number of the energy level of the stationary electronic spectrum.

Similarly, we find that solutions of the Poisson equation, taking into account the boundary conditions for it (20), and with the approximation of derivatives in accordance with (23), are determined by solutions of the matrix equation:

$$\sum_{r=1}^{N} B_{sr} j_s = F_s, ; j_s = \begin{pmatrix} j_1 \\ j_2 \\ j_3 \\ j_4 \\ j_s \\ \text{M} \\ j_N \end{pmatrix}; \; j_0 = j_{N+1} = 0; \; F_s = \begin{pmatrix} -r_1 h \\ P_2 - P_1 \\ \text{M} \\ -r_{s-1} h \\ P_s - P_{s-1} \\ \text{M} \\ -r_N h \\ P_{N+1} - P_N \end{pmatrix}, \qquad (28)$$

where B_{sr} $(s = \overline{1...N}, r = \overline{1...N})$ - matrix, for which elements we have:

$$B_{sr} = \begin{cases} e^{(s-1)}, & r = s-1, \\ -(e^{(s-1)} + e^{(s)}), & r = s, \\ e^{(s)}, & r = s+1, \\ 0, & \text{other elements} \end{cases}$$

, if the grid nodes z_s coincide with RTS heteroboundaries and

$$B_{sr} = \begin{cases} e^{(s)}, & r = s-1, \\ -(e^{(s)} + e^{(s+1)}), & r = s \\ e^{(s+1)}, & r = s+1 \\ 0, & \text{other elements} \end{cases} \text{ otherwise.}$$

In the ratio (28):

$$r_s = r(z) = s(z_s)d(z_{s+1} - z_s) + e(N_D^+ - n(z_s)) =$$
$$= (P(z)\big|_{z=z_s+0} - P(z)\big|_{z=z_s-0})/h + e(N_D^+ - n(z_s)) = (P_{s+1} - P_s)/h + e(N_D^+ - n(z_s));$$

$$N_D^+ = \frac{N_D}{1 + 2\exp\left(\frac{E_F - E_n^{(s)}}{kT}\right)}; \qquad (29)$$

$$n(z_s) = n(E, z_s) = \sum_m n_0 \left|\Psi(E_n^{(s)}, z_s)\right|^2 = \frac{m_p k_B T}{p\mathbf{h}^2} \sum_m \left|\Psi(E_n^{(s)}, z_s)\right|^2 \ln\left|1 + \exp\left(\frac{E_F - E_n^{(s)}}{k_B T}\right)\right|,$$

E_F - Fermi level of the RTS material layers, N_D, N_D^+ - concentration of donor and ionized donor impurities, respectively, n_0 - free carriers concentration in the RTS.

Now the self-consistent solution of the system of Schrödinger and Poisson equations (3) is based on the method of successive iterations l according to the scheme:

$$\begin{cases} -\frac{\mathbf{h}^2}{2}\frac{\partial}{\partial z}\left(\frac{1}{m(z)}\frac{\partial \Psi_n^{(l+1)}(z)}{\partial z}\right) + V^{(l+1)}(z)\Psi_n^{(l+1)}(z) = \\ = E_n^{(l+1)}\Psi_n^{(l+1)}(z); \\ \frac{\partial}{\partial z}\left(e(z)\frac{\partial j_H^{(l)}(z)}{\partial z}\right) = -r^{(l)}(z) \end{cases}, \qquad (30)$$

where the effective potential in the first order of iterations is calculated as:

$$V^{(1)}(z) = \Delta E_C(z) + V_E(z). \qquad (31)$$

The accuracy of calculations by the scheme (29) given the obvious conditions:

$$\frac{\left|\left|\Psi_n^{(l+1)}(z)\right|^2 - \left|\Psi_n^{(l)}(z)\right|^2\right|}{\left|\Psi_n^{(l)}(z)\right|^2} << 1; \quad , \qquad (32)$$
$$\frac{\left|j_H^{(l)}(z) - j_H^{(l-1)}(z)\right|}{j_H^{(l)}(z)} << 1$$

In direct calculations the accuracy of the calculations according to conditions (32) was considered equal to 10^{-6}, which was provided by 7-10 iterations according to the scheme (30).

II. Discussion of results

On the basis of the developed theory, the calculation of the stationary energy spectrum of the electron E_n and its wave functions $\Psi_n(E_n, z)$ in RTS, and effective potential $V(z)$ and its components $\Delta E_C(z), V_H(z), V_{ex}(z), V_E(z)$ was performed.

Direct calculations were performed for the experimentally implemented RTS, which functioned as a cascade of QCD. [8]. The geometric parameters of the RTS are as follows: the thickness of potential barriers: $\Delta_1 = 2$ nm; $\Delta_2 = 1$ nm; $\Delta_3 = 1$ nm, the width of the potential wells: $d_1 = 2.08$ nm; $d_2 = 15$ nm. Physical parameters of RTS are as follows: Effective masses of the electron:

$$m_0 = m(\text{GaN}) = 0.186m_e;$$
$$m_1 = m(\text{AlN}) = 0.322m_e;$$
$$m_2 = m(\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}) = 0.265m_e;$$

dielectric permeability:

$$e_1 = e(\text{GaN}) = 10;$$
$$e_2 = e(\text{AlN}) = 8.5; \quad ;$$
$$e_3 = e(\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}) = 9.13$$

concentration of donor impurities: $N_D = 6 \cdot 10^{17}$ cm^{-3};

piezoelectric constants (C/m^2):

$$e_{31}^{(0)} = e_{31}(\text{GaN}) = -0.49;\ e_{31}^{(1)} = e_{31}(\text{AlN}) = -0.60;$$
$$e_{31}^{(2)} = e_{31}(\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}) = -0.554;$$
$$e_{33}^{(0)} = e_{33}(\text{GaN}) = 0.73;\ e_{33}^{(1)} = e_{33}(\text{AlN}) = 1.46;$$
$$e_{33}^{(2)} = e_{33}(\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}) = 1.327;$$

elastic constants (GPa):

$C_{11}^{(0)} = C_{11}(\text{GaN}) = 374;\ C_{11}^{(1)} = C_{11}(\text{AlN}) = 345;$

$C_{11}^{(2)} = C_{11}(\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}) = 357.18;$

$C_{12}^{(0)} = C_{12}(\text{GaN}) = 106;\ C_{12}^{(1)} = C_{12}(\text{AlN}) = 125;$

$C_{12}^{(2)} = C_{12}(\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}) = 117.02;$

$C_{13}^{(0)} = C_{13}(\text{GaN}) = 70;\ C_{13}^{(1)} = C_{13}(\text{AlN}) = 120;$

$C_{13}^{(2)} = C_{13}(\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}) = 99{,}00;$

$C_{33}^{(0)} = C_{33}(\text{GaN}) = 397;\ C_{33}^{(1)} = C_{33}(\text{AlN}) = 395;$

$C_{33}^{(2)} = C_{33}(\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}) = 388{,}28.$

spontaneous polarization (C/m^2):

$P^{SP(1)} = P^{SP}(\text{GaN}) = -0.029;$

$P^{SP(2)} = P^{SP}(\text{AlN}) = -0.081;$

$P^{SP(3)} = P^{SP}(\text{Al}_{0.58}\text{Ga}_{0.42}\text{N}) = -0.059.$

On Fig. 2 shows the energetic scheme of one cascade of QCD, the calculation of which was performed without taking into account the electric field of spontaneous and piezoelectric polarization according to the relations (5) - (7). From figure (2) it is seen that in comparison with cascades of QCD, operating in the middle and far infrared ranges of electromagnetic waves [1, 2], depths of the potential wells and height of the potential barriers are much larger, which represents significant prospects for the variation of the working characteristics of the QCD by varying of the parameters of the geometric design of the RTS [4, 5].

Calculations of the effective potential component

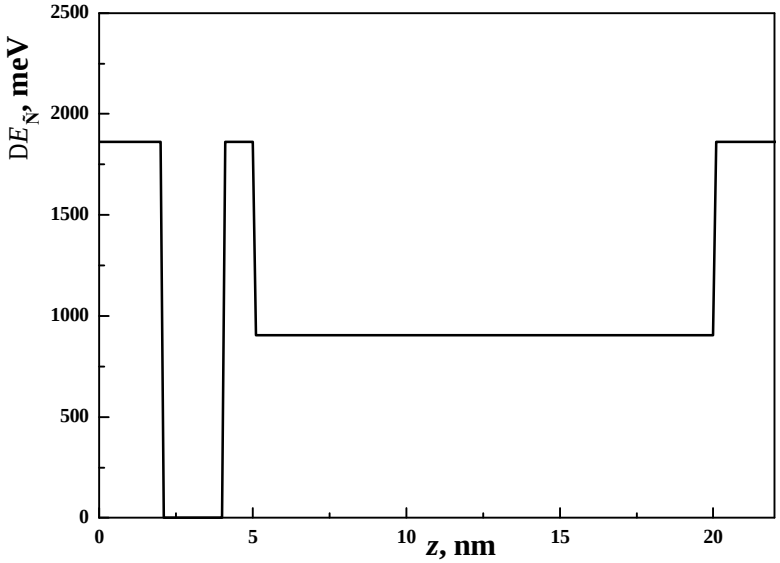

Fig. 2. Energetic scheme of one cascade of QCD without taking into account the electric field of spontaneous and piezoelectric polarization.

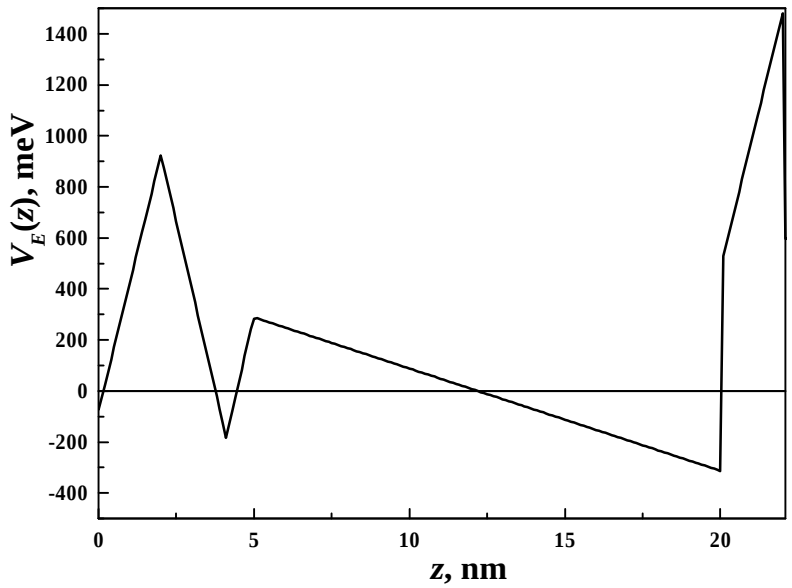

Fig. 3. Dependence on the value of z component of the effective potential determined by piezoelectric and spontaneous polarizations.

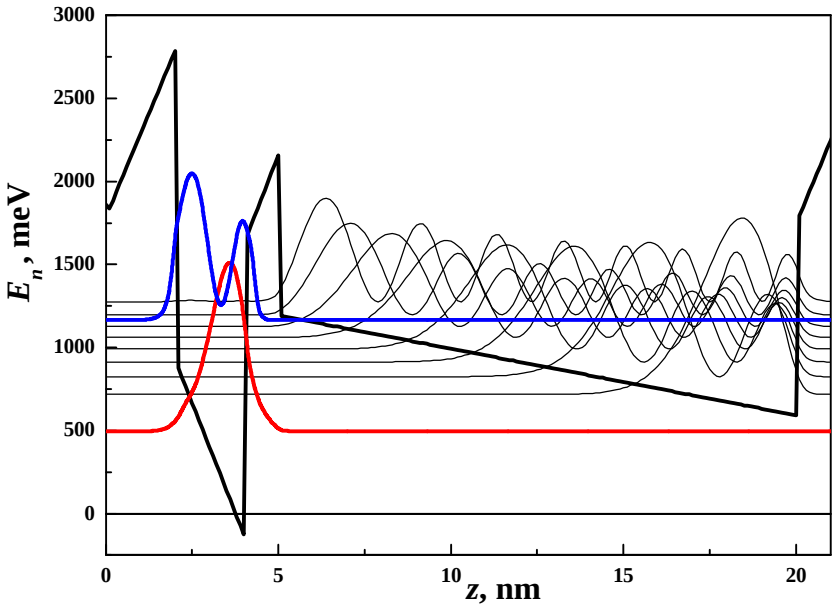

Fig. 4. The energy structure of the QCD cascade with the indicated energy levels of the electron stationary states and the corresponding distributions $|\Psi(E_n, z)|^2$ of the probability of its location within the RTS.

determined by piezoelectric and spontaneous polarizations were performed according to the relations (4), (8)-(10). The results of calculations, depending on the value of z, are given in Fig. 3. It is seen from Fig. 3 that the internal electric fields determined by piezoelectric and spontaneous polarizations are commensurable with the values of the heights and depths of the potential wells on the RTS barriers, respectively, which, as will be seen below, is the reason for their significant contribution in the total effective potential.

The results of calculation of the total effective potential on the value of z for the investigated RTS are presented on Fig. 4. It is seen from the figure, that taking into account the effects in the components of the effective potential according to the relation (4), leads to a significant deformation of the output potential. It should be noted, that this effect is a consequence of the physical properties of the investigated RTS potential wells and barriers layers material and is of decisive importance for the electromagnetic waves detection process the by the QCL.

In addition, in Fig. 4 showed the calculated values of the resonant electron energies in the investigated RTS (left on the picture) and the corresponding distributions of the probability of finding electron within the nanosystem $|\Psi(E_n, z)|^2$ (reduced to scale of energy scale). The direct values of the resonant energies and information on the localization of the electron within the RTS for the corresponding energy state are given in Table. 1. It is seen from Fig. 4 that the calculated value of the detected energy corresponding to the energy transition between the electron states localized in the active band of QCD is as follows: $\Omega = \Omega^{(\text{theor})} = \mathrm{E}_8 - \mathrm{E}_1 = 670.7\ meV$. The calculated value of the value of the detected energy is well correlated with the experiment, since it differs from the experimentally obtained value $\Omega^{(\text{exp})} = 650.0\,meV$ by no more than 3.1 %.

Table 1

The values of the energies of the electron discrete spectrum in the closed RTS of QCD and their localization

Energy values (meV)	Localization
E_1= 496.2	active band
E_2= 717.4	extractor
E_3= 824.7	extractor
E_4= 912.5	extractor
E_5= 990.1	extractor
E_6= 1061.1	extractor
E_7= 1128.4	extractor
E_8= 1166.9	active band
E_9= 1197.6	extractor
E_{10}= 1276.1	extractor

Conclusions

On the basis of the self-consistent solutions of the Schrödinger-Poisson equations, taking into account the contribution of piezoelectric and spontaneous polarizations, a quantum-mechanical theory of stationary electronic states in a flat RTS as an active band of QCD was developed. For experimentally studied RTS on the basis of the developed theory, a self-consistent calculation of the electronic potential profile, the stationary energy spectrum and the value of the detected energy is performed. It is shown that the results of calculations are in good agreement with the experiment.

Boyko I.V. - Ph.D. in Physics and Mathematics, Associate Professor, Associate Professor of the Software Engineering Department;
Tkach M.V. - Doctor of Sciences in Physics and Mathematics, Professor, Head of the of Theoretical Physics and Computer Modelling Department;
Seti Ju.O. - Doctor of Sciences in Physics and Mathematics, Professor, professor of the Theoretical Physics and Computer Modelling Department.

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І.В. Бойко[1], М.В. Ткач[2], Ю.О. Сеті[2]

Самоузгоджений розрахунок потенціального профілю GaN/AlN резонансно-тунельних структур

[1]Тернопільський національний технічний університет імені Івана Пулюя, вул. Руська 56, м. Тернопіль, e-mail: boyko.i.v.theory@gmail.com
[2]Чернівецький національний університет імені Юрія Федьковича, вул. Коцюбинського, 2, м. Чернівці, e-mail: ktf@chnu.edu.ua

Для резонансно-тунельної структури з GaN – потенціальними ямами та AlN – потенціальними бар'єрами виконано розрахунок внутрішніх полів, спричинених виникаючими у наноструктурі п'єзоелектричною та спонтанною поляризаціями.

У моделі ефективних мас для електрона та моделі діелектричного континууму з використанням методу скінченних різниць знайдено самоузгоджені розв'язки системи рівнянь Шредінгера та Пуассона з урахуванням внеску п'єзоелектричної та спонтанної поляризацій.

На основі знайдених розв'язків системи рівнянь Шредінгера та Пуассона для резонансно-тунельної структури, що слугувала каскадом експериментально реалізованого квантового каскадного детектора, виконано розрахунок її потенціального профілю та електронного енергетичного спектру. Встановлено, що розрахована величина детектованої енергії відрізняється від експериментально отриманої не більше ніж на 3 %.

Ключові слова: квантовий каскадний детектор, резонансно-тунельна структура, п'єзоелектрична поляризація, спонтанна поляризація, потенціальний профіль.