Concentration-size dependences for the electron energy in $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ nanofilms

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Abstract. Using approximation of dielectric continuum and the Green function method, studied in this work is the influence of electron-phonon interaction on position of the bottom of the ground energy band for electron in the quantum well of a finite depth. Considering the example of a plain nano-heterostructure with a quantum well based on the double heterojunction $Al_xGa_{1-x}As/GaAs$ (nanofilm), the authors have calculated the electron energy for a varied thickness of the film. It has been studied the influence of barrier material composition as well as electron-phonon interaction on the electron energy.

Keywords: nano-heterostructure, quantum well, spectrum, electron-phonon interaction.

1. Introduction

Quasi-two-dimensional semiconductor structures possess a number of unique properties, which allows creation of fast-response transistors based on them, electro-optical re-switchers, detectors and sources of radiation as well as devices of spintronics [1]. Investigation of these properties acquired hasty development in relation with new opportunities arising due to implementation of technologies for preparation of extraordinary thin layers between contacting crystals [2–4].

An important reason for growing scientific interest to the above structures is also creation of novelty efficient theoretical models capable to explain the observed phenomena or to predict new ones related with motion peculiarities of quasi-particles as well as their interaction, which are caused by spatial limitations.

Up to date, there are rather many semiconductor compounds suitable for creation of a new electron, optoelectronic, quantum-optic, and other devices based on the well-known heterojunction $Al_xGa_{1-x}As/GaAs$ [5–8] and in-depth studying the low-dimensional nano-systems on its base [9-11]. In particular, they ascertained the

opportunity to tune the energy spectrum of 2D electrons in quantum wells (QW) GaAs with $Al_xGa_{1-x}As$ barrier layers. For example, this tuning can be applied for creation of quantum cascade lasers of photo-detectors [12], which can be provided by changing the thickness or height of the barrier [13] that is determined by composition of barrier material.

Enlightened in works [14, 15] are theoretical backgrounds and the method for theoretical investigations of the influence of interaction between electron states and polarization optical vibrations on the energy of the ground electron level in plain nano-heterostructures with a single QW – in nano-films (NF). This method enabled us to perform calculations of the energy spectrum for electron in NF of various thicknesses. Concentration dependences of the electron energy in NF were not investigated, but this task seems rather topical from the viewpoint to find nano-heterostructures with necessary properties.

This paper is devoted to calculations of dependences of the electron energy on the thickness of the $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ NF with a varied concentration of aluminium in the barrier surroundings.

Analyzed were partial contributions of all the intermediate electron states from the discrete and continual spectrum parts to the electron energy with account of its interaction with spatially confined (LO) in the well material and semi-cconfined (L1) – in the barrier one, as well as interface (I) longitudinal polarization optical phonons and their dependence on the film thickness a and concentration x. It has been shown that, with exception of the very thin (down to 20 nm) films, topical is interaction between the states of the ground band with LO phonons and simultaneous participation of all the states from the discrete part of the electron energy spectrum. Growth of x from 0.2 up to 0.4 results in the 23-% shift of the value inherent to the position of the ground electron miniband in super-thin NF (down to 20 nm), and the shift by 5% – in NF with the thickness 20 to 50 nm. For the thicknesses higher than 80 nm, the dependence of the electron energy on composition of the barrier medium is considerably weaker.

2. Model and method for calculations

Let us consider electron that moves almost free inside QW created by two sequential $Al_xGa_{1-x}As$ /GaAs heterojunctions placed in the planes $z = \pm a/2$ of the Cartesian coordinate system.

GaAs and AlAs compounds possess close values of lattice parameters (5.653 and 5.661 Å, respectively) as well as dielectric permittivity ε_0 (13.18 and 10.06) and ε_∞ (10.89 and 8.16) [16]. It allows considering the heterojunction as non-strained and neglecting its self-polarization, and QW – as the rectangular one. The electron energy value in the states of the discrete part of the spectrum are defined by the following relation

$$E_n\left(\vec{k}_\parallel\right) = E_n + \frac{\hbar^2 k_\parallel^2}{2m^{(0)}} . \tag{1}$$

Here, $\vec{k}_\parallel = (k_x, k_y)$ is the longitudinal component of the electron quasi-impulse that defines the state of its motion inside the plane of NF; $m^{(0)}$, $m^{(1)}$ – electron effective mass in well (GaAs) and barrier ($Al_xGa_{1-x}As$) media, respectively. Without account of interaction with phonons, the electron energy at the n-th level (E_n) in QW with a finite depth V can be found from the equation

$$\left\{tg\left(\frac{a}{2}\frac{\sqrt{2m^{(0)}E_n}}{\hbar}\right)\right\}^{\pm 1} = \pm\sqrt{\frac{m^{(0)}(V - E_n)}{m^{(1)}E_n}} , \tag{2}$$

where the sign (+ or −) should be chosen in accord to state symmetry – "plus" in the case of symmetrical states (odd n) and "minus" for the anti-symmetric ones (even n) [17]. The depth of QW, V, energy of semi-confined phonons Ω_{L1} and value of the effective mass of electron in barrier medium $m^{(1)}$ are related with the aluminium concentration x:

$$V = 0.6 \cdot (1.115\,x + 0.37x^2) \text{ (eV)},$$

$$\Omega_{L1} = 36.25 + 1.83x + 17.12x^2 - 5.11x^3 \text{ (meV)},$$

$$m^{(1)} = (0.067 + 0.083\,x)\,m_e ,$$

where m_e is the free-electron mass [17].

Electron-phonon interaction (EPI) changes the electron energy in QW. In particular, in the approach of weak interaction between electrons and polarization optical phonons, the shift of the bottom of the electron ground band can be represented as a sum [16]

$$\Delta = \Delta_{LO} + \Delta_{L1} + \Delta_I \tag{3}$$

of partial shifts Δ_{LO}, Δ_{L1} and Δ_I caused by interaction with confined, semi-confined and interface phonons, respectively. The value of each this quantity is defined by interaction between electrons and phonons through the states of the ground and all higher bands from the discrete and continual parts of the spectrum. The formulas for calculation of these quantities were obtained within the framework of the Green function method and represented in [16].

Contributions of each EPI mechanism to the value of a partial shift of the band bottom change with varying the NF thickness and can, obviously, be dependent on composition of barrier medium. Adduced below are the results of calculations for the dependence of the electron energy in GaAs NF on its thickness and aluminium concentration in barrier medium $Al_xGa_{1-x}As$.

3. Results of calculations

Specific calculations were performed for GaAs NF embedded into barrier medium $Al_xGa_{1-x}As$ at low temperatures (formally, $T = 0$ K) and x values equal to 0.2, 0.3 and 0.4. The results of calculations performed for the energy of levels on the NF thickness НП $a = Na_0$ (where N is the amount of GaAs layers in NF) are depicted in Fig. 1.

With growing the thickness of NF, the energy of levels in QW decreases, while their amount grows. In the case of small NF thickness ($a < 20$ nm or $N \leq 35$), when x grows, the amount of levels in QW and their energy values increase considerably. It can be explained by respective growth of the QW depth as well as by lowering the electron energy in barrier material (due to the increase in the electron effective mass) with the increase in x. In NF with the thickness higher than 60 GaAs layers ($a > 34$ nm), the dependence of the level energy in QW on the x value becomes essentially weaker, which is caused by weakening the influence of surroundings on the electron state in well material.

Fig. 2 shows dependences of the partial shift Δ_{LO} of the bottom of the ground electron miniband in QW on the NF thickness. This shift is caused by interaction of electrons with confined phonons as well as changes in its components due to EPI with account of the ground state ($\Delta^{(d)}_1$) and all the states of discrete ($\Delta^{(d)}$) and continual parts in the electron spectrum ($\Delta^{(c)}$).

It is seen that this interaction causes shift of the bottom of the ground miniband to the side of lower energies. In the case of thin films ($a < 20$ nm), the contribution $\Delta^{(d_1)}$ is dominant, its value sharply grows with the growing NF thickness up to $a \approx 15$ nm and then gradually decreases. The higher is the concentration x, the higher is the rate of $\Delta^{(d_1)}$ growth. Its behavior can be explained using the apparent dependence of the electron–L0-phonons connection function on a [9] as well as non-apparent – via the electron quasi-impulse change, the value of which depends on the ground level energy, i.e., on x.

Interaction with L0-phonons accompanied by excitation of states in the discrete part of the spectrum results in the growth of the shift value. The larger is the NF thickness, the larger is the shift value. In the case of $a > 50$ nm, the total contribution of the states from the discrete part of the spectrum $\Delta^{(d)}$ exceeds the contribution of the states from the ground band $\Delta^{(d_1)}$. The value $\Delta^{(d)}$, like to $\Delta^{(d_1)}$, also grows with increasing the NF thickness. And the higher is the concentration value x in the solution $Al_xGa_{1-x}As$, the higher is the rate of $\Delta^{(d)}$ growth. It is explained by the concentration dependence both of values inherent to energy levels in QW and their amount there.
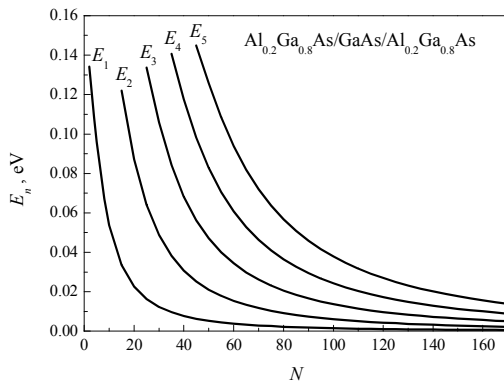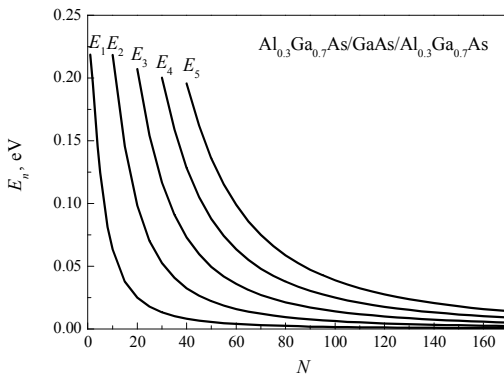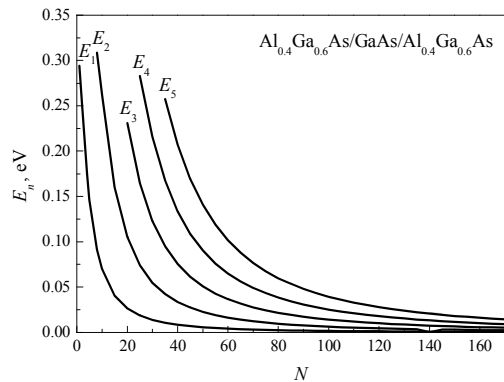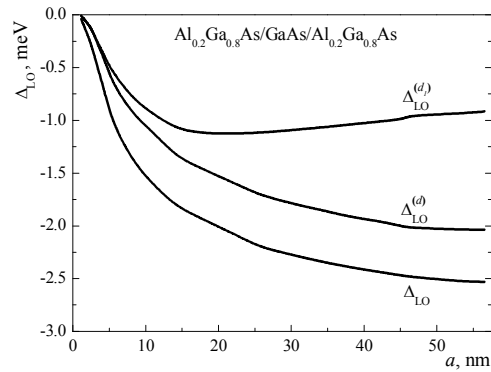

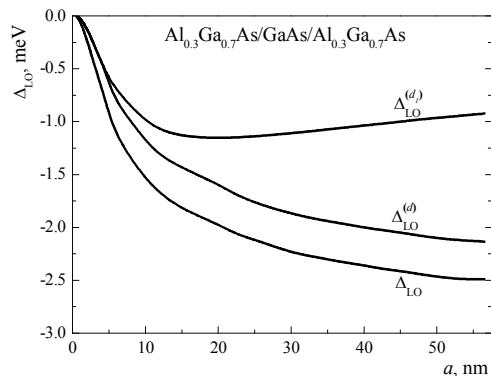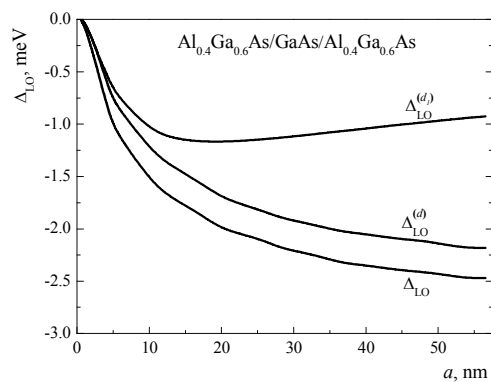**Fig. 1.** Dependence of the energy for electron levels in QW on the thickness of $Al_xGa_{1-x}As$ /GaAs/ $Al_xGa_{1-x}As$ nanofilms (N is the amount of GaAs layers) for the values of concentration x: 0.2 (*a*), 0.3 (*b*), 0.4 (*c*).

Fig. 2. NF thickness dependence of the shift Δ_{LO} for the bottom of the ground electron miniband in QW, which is caused by its interaction with confined phonons at the concentration x values: 0.2 (*a*), 0.3 (*b*), 0.4 (*c*).

With increasing the thickness of NF, the influence of states from the continual part of electron energy spectrum in QW is increased, too. Their contribution ($\Delta_{LO}^{(c)}$) in combination with the states from the discrete part of the spectrum ($\Delta_{LO}^{(d)}$) forms the value of partial shift

$$\Delta_{LO} = \Delta_{LO}^{(d)} + \Delta_{LO}^{(c)}.$$

Thus, the total shift of the electron ground miniband caused by its interaction with confined phonons is a monotonic non-linear growing function of the thickness of $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ heterosystem. The rate of this function growth has its maximum in the range $a < 20$ nm. This rate becomes higher when the concentration x grows. In NF possessing the thickness above 50 nm, the shift Δ_{LO} becomes insensitive to x changes and reaches saturation. For $a \geq 100$ nm, it gradually acquires the value 2.9 meV, which is typical to bulk GaAs crystal.
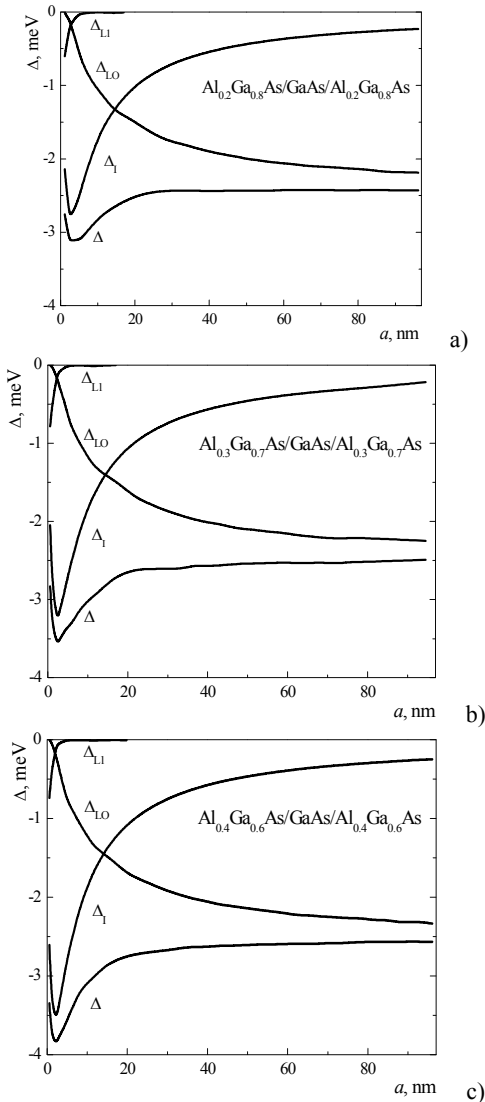

Fig. 3. NF thickness dependence of the partial shifts (Δ_{LO}, Δ_{L1}, Δ_I) and the total one (Δ) for the bottom of the ground electron miniband in QW at the concentration x values: 0.2 (*a*), 0.3 (*b*), 0.4 (*c*).

The influence of changes in the NF thickness and composition of barrier material on the value of partial shifts caused by EPI with semi-confined and interface phonons can be naturally observed in ultra-thin films with the thickness up to 10 and 20 nm, respectively (Fig. 3).

The wave-function of the ground electron state in QW is symmetrical, therefore it interacts only with the symmetric branch of I-phonons. Interaction with these phonons through the states of higher minibands from the discrete part of the spectrum gives a contribution that does not exceed 5% of $\Delta_I^{(d_1)}$, while the contribution of the states from the continual part is negligible. Growth of the aluminium concentration in barrier material enhances interaction with I-phonons as result of growth in their energy and in the magnitude of electron-I-phonons connection function (due to increasing the difference between the values of dielectric permittivities inherent to well and barrier material).

The value Δ_{L1} is also formed due to interaction of semi-confined phonons with the states of the ground miniband; the total contribution of interband contributions [16] with participation of higher states in the discrete part of the spectrum is low as compared with $\Delta_{L1}^{(d_1)}$, while through the continual states ($\Delta_{L1}^{(c)}$) it does not exceed 1% of $\Delta_{L1}^{(d_1)}$.

The values Δ_I and Δ_{L1} sharply drop with increasing the NF thickness. In this case, the dependence of the value Δ_{L1} on a, contrary to that of Δ_I, monotonically slows down, and its initial values are considerably lower than those of Δ_I. Unlike the partial contributions of L0- and I-phonons to the value of the total shift observed for the bottom of the electron ground miniband in QW, the contribution of L1-phonons is decreased with increasing the concentration x. It is explained by the growth of the potential barrier height for electron in QW and, respectively, by decreasing the probability for electron to penetrate into barrier medium, which results in decreasing the values of its electron–phonons connection function [16].

4. Conclusions

The above mentioned results of calculations show that long-wave shifts of the bottom for the electron ground miniband in super-thin (up to 10 nm) $Al_xGa_{1-x}As / GaAs/ Al_xGa_{1-x}As$ films are predominantly caused by interaction with I-phonons, while with increasing their thickness above 60 nm – with L0-phonons. In the case of essential growth of the NF thickness above 100 nm, the influence of I-phonons drops down to zero, while the value Δ_{LO} approaches to that typical for bulk GaAs (2.9 meV). This behavior is fully understandable, since with the growth of the NF thickness the probability to find electron at the hetero-junction boundaries is decreased, and in the middle of the quantum well it increases.

Growth of the aluminium concentration in barrier material results in growth of the value corresponding to the total shift of the bottom of the electron ground miniband in QW. In super-thin films ($a \leq 10$ nm), this augmentation reaches 0.73 meV (23%) for x changing from 0.2 up to 0.4, mainly due to increased interaction with interface phonons; in NF with the thickness between 20 to 50 nm, it reaches 0.1 meV (5%) due to interaction with confined and interface phonons.

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