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Temperature Dependences of the Electron Energy in $Al_xGa_{1-x}As$ / GaAs / $Al_xGa_{1-x}As$ Nanofilms of Different Thickness and Composition of the Barrier Material

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Temperature dependences of the energy of electron ground state in $Al_xGa_{1-x}As$ / GaAs / $Al_xGa_{1-x}As$ nanofilms of different thickness and concentrations (x) of the barrier material were calculated. Calculations were performed by using the Green functions method, approximation of the effective masses for the electronic system and model of the dielectric continuum – for phonons. The interaction of all branches of the optical phonons: confined in the well material, semi-spaced – in barrier medium and interface has been taken into account. It is shown that the increase in the temperature from 0 to 300 K can cause the increase in the magnitude of long-wave shift of the electron energy about 25-30 % depending on the nanofilm thickness and concentration x.

Keywords: Nanoheterostructure, Quantum well, Electron, Energy.

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1. INTRODUCTION

Low-dimensional semiconductor structures possess unique properties allowing to create new devices of opto- and nanoelectronics on their basis [1]. This possibility is conditioned by the development and implementation of the production technologies of nanoscale crystal structures of different dimensions [2-4].

The persistent attention of researchers in the field of semiconductor physics to the study of the properties of the mentioned structures is explained by the necessity of creation of adequate models and consistent theoretical methods, which explain observed or predict new phenomena connected with the features of quasiparticle motion and their interaction caused by the presence of spatial restrictions.

A number of works devoted to the investigation of the formation mechanisms of energy and optical spectra of nanoheterostructures with quantum wells (QW) has been published up to now. In particular, the authors of [5] present the technique and results of calculations of the dependence of the electron energy spectrum in plane semiconductor nanostructures with double heterojunction – $Al_xGa_{1-x}As$ / GaAs / $Al_xGa_{1-x}As$ nanofilms (NF) on their thickness and composition of barrier medium. However, temperature changes of the spectra of these nanosystems have not been considered.

Investigation of the temperature dependence of the energy of charge carriers in nanosystems is possible in the framework of the Green function method [6]. In the work we present the calculation results performed by the specified method of the dependence of the electron ground state energy on the temperature and thickness of $Al_xGa_{1-x}As$ / GaAs / $Al_xGa_{1-x}As$ NF with different concentrations of aluminum in barrier medium.

Specific calculations are carried out using the values of the lattice constants a_0 of GaAs (5.653 Å) and AlAs (5.661 Å) and permittivities ε_0 (13.18 and 10.06) and ε_∞ (10.89 and 8.16, respectively) [7] and concentration of aluminum $x = 0.2$; 0.3; 0.4. The mentioned parameters determine the value of the limiting potential of a carrier in a QW, its effective mass in barrier medium and energy of semi-spaced and interface phonons [8, 9].

Calculation results imply that the interaction with optical polarization phonons induces the shift of the main minizone bottom of an electron in a QW towards smaller energy values. In the low temperature region, the shift, depending on the NF thickness, is equal to $a = Na_0$ (here N is the number of GaAs layers in the film) and concentration x, 2.75 – 4 meV. Increase in the nanosystem temperature from 0 to 300 K induces the increase in the shift value by approximately 25-30 %. The reason of the mentioned temperature changes is the interaction of an electron with phonons mainly confined in NF of the thickness more than 60 nm and with interface phonons – in thinner films (to 10 nm).

2. ANALYSIS OF THE CALCULATION RESULTS

Calculation results of the dependence of the shift Δ of the main minizone bottom of an electron in a QW [5, 6] on the temperature T for the fixed values of the NF thickness and concentration are represented in Fig. 1. As seen, behavior of this dependence is different for NF of different thicknesses at different values of x. In NF consisting of more than 70 GaAs layers, temperature increase induces a monotonic nonlinear increase in the shift value of the main minizone bottom of an electron towards smaller energy values; in thinner films – its increment can be almost absent (curve $N = 1$ in Fig. 1b) or have the opposite sign (curves $N = 5$ in Fig. 1a; $N = 1$ and $N = 20$ in Fig. 1c). Sign change of the shift increment with the temperature change in ultrathin films is explained by the peculiarities of the interaction between an electron and interface phonons [6].

Dependences of the shifts of the main minizone bottom of an electron on the NF thickness a at the fixed values of the temperature T and concentration x are illustrated in Fig. 2. It is seen that with increasing NF thickness, main minizone bottom is non-monotonously shifted towards smaller energies (and the stronger, the higher temperature is) achieving the maximum in ultrathin (5-7 nm depending on the value of x) films. At $a > 20$ nm increase in the NF thickness leads to a slow decrease in the long-wavelength shift of the main minizone bottom of an electron in a QW to the value typical

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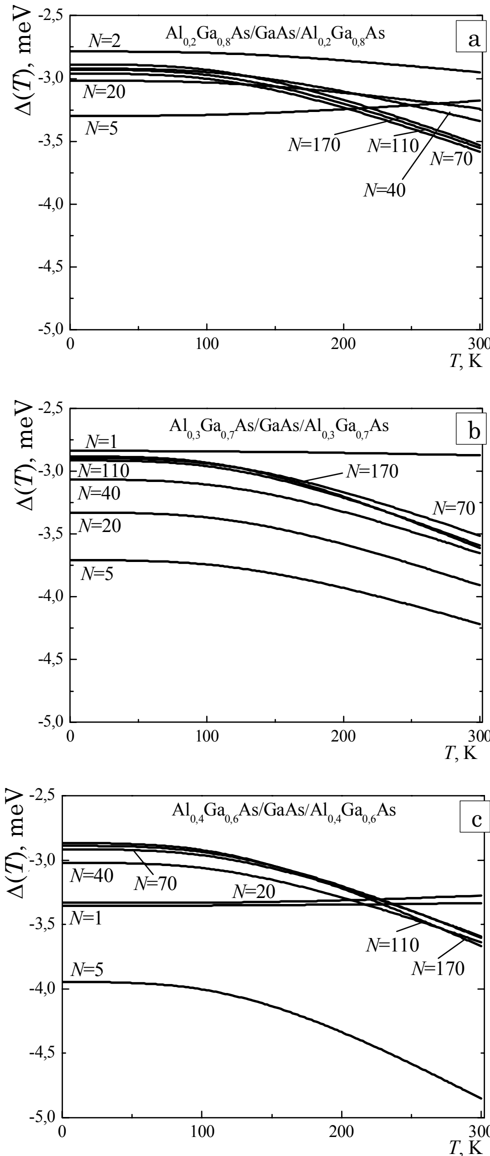

Fig. 1 – Dependences of the shift Δ of the main minizone bottom of an electron induced by the interaction with optical phonons on the temperature T at different values of the NF thickness N and concentration x: a) 0.2; b) 0.3; c) 0.4

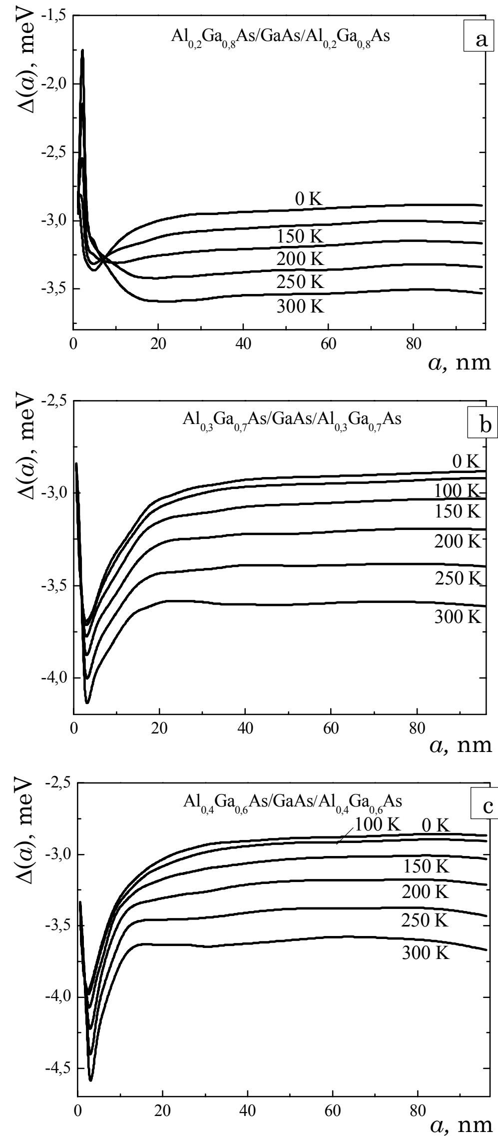

Fig. 2 – Dependences of the shift Δ of the main minizone bottom of an electron induced by the interaction with optical phonons on the NF thickness a at different values of the temperature (numbers near the curves) and concentration x: a) 0.2; б) 0.3; в) 0.4

for bulk GaAs. This is explained by the behavior of the corresponding changes in the partial shifts caused by the interaction with confined, semi-spaced and interface phonons – with the increase in the NF thickness the role of the first increases while of the latter – decreases.

Increase in the NF temperature induces both the increase in the maximum height and its shift towards larger thicknesses; location and initial (at $T = 0$) height of the maximum depend on x.

3. CONCLUSIONS

Analysis of the calculation results indicates that in $Al_xGa_{1-x}As$ / GaAs / $Al_xGa_{1-x}As$ films of the thickness to 10 nm the long-wavelength shifts of the main minizone bottom of an electron are induced mainly by the interaction with interface and with the increase in their thickness more than 60 nm – with confined phonons. In NF of the thickness from 10 to 60 nm (depending on x) the influence of both specified types of phonons is total: semi-spaced phonons make a small contribution to the value of the electron energy compared with the contribution of interface ones (to 25 %). With a considerable increase in the NF thickness (more than 100 nm) the influence of interface phonons decreases to zero and the value of the shift induced by confined phonons tends to the value typical for bulk GaAs (2.9 meV).

Increase in the concentration of aluminum in barrier medium leads to the increase in the value of the total shift of the main minizone bottom of an electron in a QW. In ultrathin films of the thickness to 10 nm, its increment achieves 0.73 meV (23 %) at the change in x from 0.2 to 0.4 mainly due to the strengthening of the interaction with interface phonons; in NF of the thickness from 20 to 50 nm – 0.1 meV (5 %), respectively, due to the interaction with confined and interface phonons.

Temperature increase from 0 to 300 K induces the

change in the long-wavelength shift of the main minizone bottom of an electron. The value and direction of this change depend on both the NF thickness and concentration of $Al_xGa_{1-x}As$ solution. In NF of the thickness more than 35-40 nm the shift value increases depending on the concentration by about 25-30 %.

In NF thinner than 10 nm with increasing temperature the shift value can increase, decrease or remain almost constant depending on the values of the thickness a and concentration x. The reason of non-monotonic behavior of the specified temperature changes is the features of the interaction between an electron and interface phonons – dispersion dependence of the coupling function provides the possibility of change of the contribution caused by the absorption processes to the value of the total shift Δ in NF of different thicknesses [6].

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