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Hydrostatic pressure effects on the Γ–X conduction band mixing and the binding energy of a donor impurity in GaAs–$Ga_{1-x}Al_xAs$ quantum wells

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Mixing between Γ and X valleys of the conduction band in GaAs–$Ga_{1-x}Al_xAs$ quantum wells is investigated taken into account the effect of applied hydrostatic pressure. This effect is introduced via the pressure-dependent values of the corresponding energy gaps and the main band parameters. The mixing is considered along the lines of a phenomenological model. Variation of the confined ground state in the well as a function of the pressure is reported. The dependencies of the variationally calculated binding energy of a donor impurity with the hydrostatic pressure and well width are also presented. It is shown that the inclusion of the Γ–X mixing explains the non-linear behavior in the photoluminescence peak of confined exciton states that has been observed for pressures above 20 kbar.

1 Introduction

There have been several antecedents of the study of the Γ–X mixing phenomenon in GaAs-based systems [1–7]. In addition, a significant number of works that investigate the effects of the hydrostatic pressure on the optical and electronic properties in this kind of structures have also been put forward [8–11].

By the application of a magnetic field, Pulsford et al. [5], have demonstrated the anticrossing behavior between Γ and X in strongly coupled GaAs/AlAs superlattice. Their theoretical model was developed to deal with Γ–X mixing at the interfaces within the envelope-function approach.

The effective-mass approximation (EMA) can be extended to take into account mixing between Γ and X conduction-band valleys at heterointerfaces by including boundary conditions expressed in terms of an interface matrix providing a set of linear relations between the envelope functions and their derivatives at the interface [1, 5, 8]. Several works in the EMA have been reported taking into account the elastic Γ–X intervalley transfer by introducing an additional δ-function scattering potential at each well/barrier heterointerface of GaAs/AlAs/GaAs low dimensional heterostructures [2, 3, 7].

On the other hand, pressure-induced Γ–X crossing has been studied from photoluminescence data in InAs/GaAs quantum dots [4], while band anticrossing effects in the conduction band of GaNAs-based quantum well structures under hydrostatic pressure were considered in Ref. [6].

The influence of the Γ–X mixing on the donor impurity states in GaAs–AlAs quantum wells [8], as well as the dependence with the hydrostatic pressure of the electron–hole recombination peaks in the

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photoluminescence spectrum of single and double GaAs–$Ga_{1-x}Al_xAs$ quantum wells [9] can be mentioned as antecedents. However, up to our knowledge, the study of the combined action of the hydrostatic pressure and Γ–X mixing on the donor impurity states in quantum wells based on GaAs has not been yet reported.

In this work we are presenting results of the calculation of the binding energy of a shallow-donor impurity in a GaAs–$Ga_{1-x}Al_xAs$ quantum well. The effects of the hydrostatic pressure are included jointly with a description of the electronic states in the conduction band that takes into account the mixing between the Γ and X minima.

2 Theoretical framework

The calculation of the states in the conduction band of the GaAs–$Ga_{1-x}Al_xAs$ structures is carried out inside the effective mass approximation. A model with two independent bands is employed and we limit ourselves to consider only the ground state of the system. The Hamiltonian of the system is written as [8]:

$$\begin{bmatrix} h^{\Gamma} & 0 \\ 0 & h^{\mathrm{X}} \end{bmatrix} \begin{bmatrix} F^{\Gamma} \\ F^{\mathrm{X}} \end{bmatrix} = \varepsilon \begin{bmatrix} F^{\Gamma} \\ F^{\mathrm{X}} \end{bmatrix}, \tag{1}$$

with

$$h^{\alpha} = -\frac{\hbar^2}{2m_{\alpha\parallel}}\frac{\partial^2}{\partial z^2} - \frac{\hbar^2}{2m_{\alpha\perp}}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{\partial^2}{\partial\rho^2}\right) + U(\boldsymbol{r}) + \varepsilon_{\alpha}, \qquad \alpha = \Gamma, \mathrm{X}. \tag{2}$$

F^{α} are the Γ and X related envelope-wave functions whereas ε_{α} refers to the conduction band edge at the point α in $\boldsymbol{k}$ space. The mixing of bands is introduced according to the scheme proposed by Pulsford et al. [5], in the same spirit of Ref. [8]. The boundary conditions at the interfaces are introduced via an unitary matrix that involves an adjustable phenomenological parameter γ [5]

$$\begin{bmatrix} F^{\Gamma} \\ F^{\mathrm{X}} \\ m_{\Gamma}^{-1}\nabla F^{\Gamma} \\ m_{\mathrm{X}}^{-1}\nabla F^{\mathrm{X}} \end{bmatrix}_{\mathrm{Well}} = \boldsymbol{T} \begin{bmatrix} F^{\Gamma} \\ F^{\mathrm{X}} \\ m_{\Gamma}^{-1}\nabla F^{\Gamma} \\ m_{\mathrm{X}}^{-1}\nabla F^{\mathrm{X}} \end{bmatrix}_{\mathrm{Barrier}}, \tag{3}$$

where

$$\boldsymbol{T} = \begin{bmatrix} \xi & -\gamma & 0 & 0 \\ +\gamma & \xi & 0 & 0 \\ 0 & 0 & \xi & -\gamma \\ 0 & 0 & +\gamma & \xi \end{bmatrix}, \tag{4}$$

with $\xi = \sqrt{1-\gamma^2}$. The hydrostatic pressure effects are included from the dependencies with pressure of the basic input parameters of the EMA [12–15]. For the pressure and temperature dependent band gap and static dielectric constant, respectively, we have used

$$E_{\mathrm{GAP}}(P) = E_1 + \beta P + \alpha T^2/(T + T_1) \tag{5}$$

and

$$\varepsilon = \varepsilon_0\, \mathrm{e}^{C_1 (T - T_2) + C_2 P}. \tag{6}$$

Table 1 Parameters used in the present calculations for Eqs. (5)–(11) [12–15].

	Γ-GaAs	X-GaAs	Γ-$Ga_{1-x}Al_xAs$	X-$Ga_{1-x}Al_xAs$
E_1 (eV)	1.519	1.981	$1.519+1.155x+0.37x^2$	$1.981+0.124x+0.144x^2$
α (eV/K)	-5.405×10^{-4}	-4.60×10^{-4}	-5.405×10^{-4}	-4.60×10^{-4}
T_1 (K)	204	204	204	204
β (eV/kbar)	10.7×10^{-3}	-1.4×10^{-3}	$(10.8-3.2x+3.8x^2)\times10^{-3}$	$-(1.4-0.1\,x)\times10^{-3}$
$A_{(\|/\perp)}$		1.3/0.26		1.25/0.19

$\varepsilon_0 = 12.74$, $T_2 = 75.6$ K, $C_1 = 9.4\times10^{-5}$ K^{-1}, $C_2 = -1.67\times10^{-3}$ $kbar^{-1}$, $E_p = 7.51$ eV, $\Delta = 0.341$ eV.

The masses for the Γ and X conduction bands, both in the well and barrier regions, are given by

$$m_{\Gamma-\mathrm{GaAs}} = \left[1+\frac{2E_p}{E(P)_{\Gamma-\mathrm{GaAs}}}+\frac{E_p}{E(P)_{\Gamma-\mathrm{GaAs}}+\Delta}\right]^{-1} m_0\,, \tag{7}$$

$$m_{\Gamma-\mathrm{Ga_{1-x}Al_xAs}} = m_{\Gamma-\mathrm{GaAs}} + 0.083x m_0\,, \tag{8}$$

$$m_{\Gamma-\mathrm{Ga_{1-x}Al_xAs}} = (m_{\Gamma-\mathrm{GaAs}} + 0.083x m_0)\,(1-0.4x)\,, \tag{9}$$

and

$$m_{\mathrm{X},(\|/\perp)-\mathrm{GaAs}} = (A_{(\|/\perp)} + 6.15\times10^{-3}\,P - 1.22\times10^{-5}\,P^2)\,m_0\,. \tag{10}$$

Equations (8) and (9) are without and with inclusion of renormalization effects due to the interaction with the valence band. For the heavy-hole effective mass we have used the constant value $m_{hh} = 0.30242 m_0$. In Table 1 we present the parameters we have used in our calculations.

Finally, the impurity binding energy [16–18] is calculated with the use of a separable trial wavefunction depending on two-variational parameters [8].

3 Results and discussion

In Fig. 1, the binding energy of a shallow-donor impurity located at the center of type I GaAs/AlAs single quantum well is presented as a function of the well width. Three different values are used for the valley mixing parameter. As in the work by Wang et al. [8], the results are shown for both, the band edge AlAs effective mass (Fig. 1a), and the renormalized one due to the interaction with the valence band (Fig. 1b). It can be observed that the mixing effect reflects in a decrease of the binding energy for all GaAs/AlAs quantum well widths. The reason for this is that the well depth in Γ, diminishes due to the interaction with the AlAs X minimum. For a larger band mixing, the greater will be the decrease of the barrier height at Γ. At this point it is worth mentioning that we do not obtain the same behavior of the above cited work. In that work Wang et al. show an increasing behavior of the energy of the lowest unperturbed confined state in the well when the effects of the Γ–X conduction band mixing are included (see Fig. 2, Ref. [8]). This result clearly disagrees with the diminishing effect in the confining potential barrier height resulting from the perturbation induced by the presence of the X-band.

For $\gamma \neq 0$ it is not possible to extend the curve to very small values of the well width without taking into account the transition of the system to a type II structure, in whose case, the value of the E_0 level (the first conduction-confined uncorrelated state) would lie above the X minimum of the AlAs. E_0 is precisely the value for which the well width arrives to the minimum value that keeps the type I structure. As can be seen, on that point the curve of the binding energy suffers an abrupt fall, due to the loss of confinement in the electronic wave function, which significantly penetrates into the AlAs region.

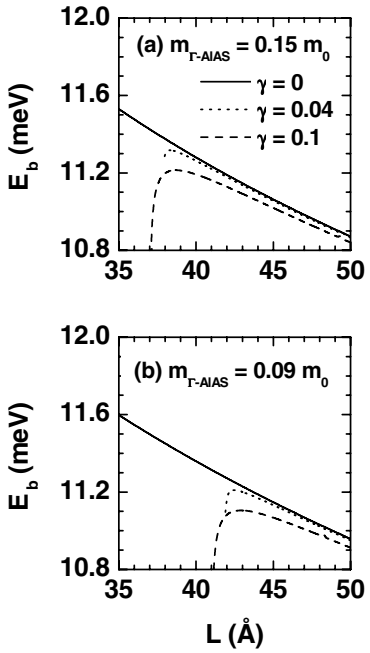

Fig. 1 Binding energy of a shallow-donor impurity located at the center of type I GaAs/AlAs single quantum well as a function of the well width. Three different values are used for the valley mixing parameter. Results are shown for both, the band edge AlAs Γ effective mass of $0.15m_e$ (where m_e is the free-electron mass) (a) and the renormalized one due to the interaction with the valence band [8] (b).

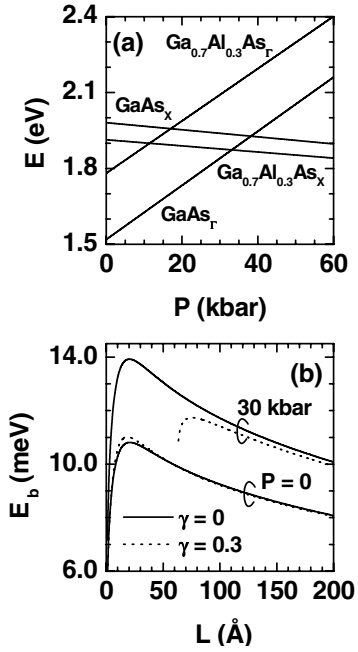

Fig. 2 (a) Variations of the Γ and X band edges as functions of the hydrostatic pressure for both GaAs and $Ga_{0.7}Al_{0.3}As$ [9]. The energy values are taken with respect to the top of the GaAs valence band. (b) The binding energy of on-center shallow-donor impurity in type I GaAs–$Ga_{0.7}Al_{0.3}As$ single quantum well as a function of the well width. Different values are used for the valley mixing parameter and hydrostatic pressure.

Let us now discuss the details of the Γ–X mixing in quantum wells under hydrostatic pressure effects. In Fig. 2a the hydrostatic pressure dependence of the energies associated to the conduction Γ and X minima in bulk GaAs and $Ga_{0.7}Al_{0.3}As$ is shown. In accordance, we consider that a pressure-induced band mixing effect can be present in heterostructures fabricated from both materials. Such a phenomenon is studied in the present work with the use of the model previously described. That is to say, the band mixing is introduced through the phenomenological γ parameter.

Figure 2b shows our results for the binding energy of on-center shallow-donor impurity in type I GaAs–$Ga_{0.7}Al_{0.3}As$ single quantum well as a function of the well width. In the case in which no mixing is presented (solid lines), our results go to the exact limits of the bulk in the GaAs and $Ga_{0.7}Al_{0.3}As$ when L tends to infinite and to zero, respectively. In this case, the increment of the binding energy with the pressure is mainly owed to the increment of the Coulombic interaction due mainly to the increasing in the electron effective mass, which is proportional to the gap increase with pressure, and a little bit due to the decreasing behavior in the dielectric constant with pressure. In the zero-pressure regime we see that the Γ–X mixing effect (dotted lines) generates only small changes. They correspond to well widths associated with the maximum in the binding energy curve. In this situation, and for the critical matter of well width tending to zero, the minimal energy separation between the fundamental state E_0 – without correlation – and the energy minimum in X for the barrier is of the order of 200 meV. This justifies the very light perturbative effect mentioned above.

On the other hand for pressure equals to 30 kbar, the limit of the bulk in the barrier cannot be obtained under the type I structure energy profile. To the extent that the energy E_0 approaches the limit value of

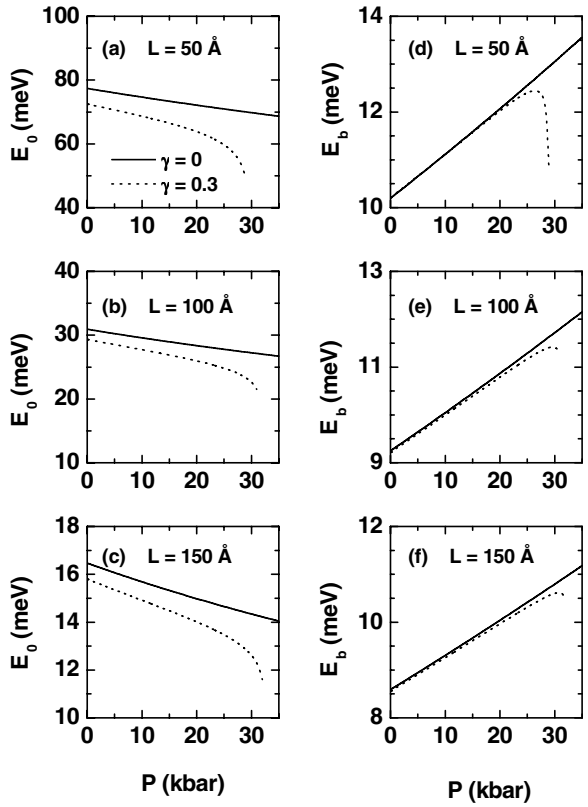

Fig. 3 Uncorrelated ground state electron energy (a–c) and the binding energy of on-center shallow-donor impurity (d–f) in type I $Ga_{0.7}Al_{0.3}As$ single quantum well as a function of the hydrostatic pressure. Different values are used for the valley mixing parameter and the well width.

the energy corresponding to the minimum in the X valley of the $Ga_{0.7}Al_{0.3}As$, the perturbative effects become more important resulting in an effective decrease of the confining potential barrier height and, because of it, in a decrease in the binding energy.

In Fig. 3, the uncorrelated ground state electron energy and the binding energy of on-center shallow-donor impurity in type I GaAs–$Ga_{0.7}Al_{0.3}As$ single quantum well as a function of the hydrostatic pressure is displayed. In the case of E_0 we note that the mixing effect, in the entire pressure range, results in a decrease of this energy. In the low pressure regime (approximately up to 15 kbar), the curves have a strong linear behavior associated with the fact that the minimum in X for the barrier material is essentially above of the energy value corresponding to the minimum in Γ.

In the pressure regime close to the transition from the type I to type II X-potential profile of the combined structure, the X-perturbative effect leads to an appreciable decreasing of the Γ-related confining potential barrier in the GaAs region in such a way that the curves move away quickly from their linear behavior with the pressure. This effect has been clearly detected in the high pressure regime for the e–h recombination lines in the photoluminiscence spectra of GaAs–$Ga_{1-x}Al_xAs$ single quantum wells [19] GaAs–$Ga_{1-x}Al_xAs$ single and double quantum wells [9], strained GaAs–$In_{0.2}Ga_{0.8}As$ multiple quantum wells [10], and strained GaAs–$In_{1-x}Ga_xAs$ multiple quantum wells under hydrostatic pressure [11]. This mixing-induced decay of the Γ potential barrier is also responsible for a reduction in the strength of the Coulomb interaction due to the fact that the electron wave function has a greater penetration to the $Ga_{0.7}Al_{0.3}As$ material providing an increment in the expected value of the electron-impurity distance.

From the binding energy curves of Fig. 3 it is clearly observed that the effects of the mixing are essentially important for values of the hydrostatic pressure larger than 20 kbar in which case the binding energy decays, strongly for small quantum well widths, and lightly for large quantum well width, by effect of the decrease of the Γ-related potential barrier. Here, the two confinement effects on the carriers, that

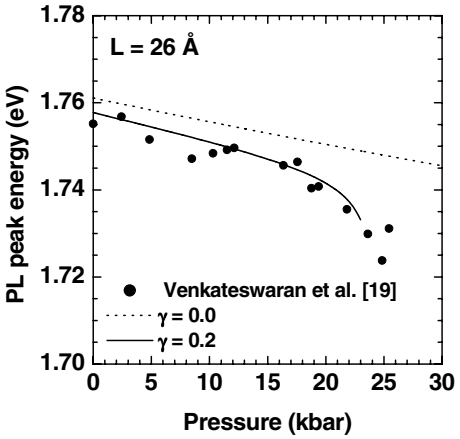

Fig. 4 Photoluminescence peak energy as a function of hydrostatic pressure in a single GaAs–$Ga_{0.67}Al_{0.33}As$ QW of width $L = 26$ Å. Two values of the γ parameter have been considered. The symbols are the experimental findings by Venkateswaran et al. [19].

of the potential barriers and that of Coulombic interaction clearly compete. In the low hydrostatic pressure regime the Coulomb effect is the dominant one and as a consequence non appreciable changes are observed associates to the band mixing.

In Fig. 4 we present the hydrostatic pressure dependence of the photoluminescence peak energy [20] in a single GaAs–$Ga_{0.67}Al_{0.33}As$ QW of width $L = 26$ Å. The dotted line corresponds to the calculation without including band mixing effects, whereas the solid line corresponds to the situation where the value of the γ parameter is equal to 0.2. One can notice that the inclusion of the Γ–X conduction band mixing really gives a good account of the non-linear behavior of the photoluminescence peak energy showed by the experiments for pressures over which the X band in the barrier region is below in energy to the correspondent Γ profile.

4 Conclusions

The effects of hydrostatic pressure and Γ–X mixing on the well ground state as well as on the shallow donor impurity binding energy in a single GaAs–$Ga_{1-x}Al_xAs$ quantum well have been investigated. The results that we have found suggest that the inclusion of the Γ–X mixing can give account of the observed non-linear behavior in the photoluminescence peak (for pressure values larger than 20 kbar) of confined exciton states in low dimensional heterostructures, such as single and double quantum wells, with dimensions in the order of 100 Å, just as it has been shown in experimental reports [9, 19]. Additionally, our work shows that to properly describe the fine structure of the impurity-related photoluminescence spectra in stressed systems (with hydrostatic components of the stress) and low dimensional systems under hydrostatic pressure it is important to consider the effects of the Γ–X mixing.

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