Eur. Phys. J. B **62**, 257–261 (2008)
DOI: 10.1140/epjb/e2008-00161-6

THE EUROPEAN PHYSICAL JOURNAL B

$\Gamma - X$ mixing in GaAs-$Ga_{1-x}Al_xAs$ quantum wells under hydrostatic pressure

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Received 12 October 2007
Published online 19 April 2008 –

Abstract. The mixing between the Γ and X conduction-band valleys in GaAs-$Ga_{1-x}Al_xAs$ quantum wells is investigated by using a phenomenological model which takes into account the effects of applied hydrostatic pressure. The dependencies of the variationally calculated photoluminescence peak-energy transitions on the applied hydrostatic pressure and quantum-well width are presented. A systematic study of the $\Gamma - X$ mixing parameter is also reported. In particular, it is shown that the inclusion of the $\Gamma - X$ mixing explains the non-linear behavior in the photoluminescence peak of confined exciton states that has been experimentally observed for pressures above 15 kbar in GaAs-$Ga_{1-x}Al_xAs$ quantum wells.

PACS. 71.55.Eq III-V semiconductors – 73.21.Fg Quantum wells

1 Introduction

The $\Gamma - X$ mixing phenomenon in GaAs-based systems has been studied by several authors [1–6]. Pulsford et al. [2] performed an experimental and theoretical work in strongly coupled GaAs/AlAs superlattices under applied magnetic fields and reported the anticrossing behavior between the Γ and X conduction band minima. Some studies, within the effective-mass approximation (EMA), take into account the elastic $\Gamma - X$ intervalley transfer by introducing an additional δ-function scattering potential at each well/barrier heterointerface of GaAs/AlAs/GaAs heterostructures [4–6].

The application of hydrostatic pressure is quite useful to experimentally investigate the electronic states in semiconductor heterostructures. When hydrostatic pressure is applied to a heterojunction, the band gap increases and the carrier density decreases. It is worthwhile to mention that several investigations on the effects of hydrostatic pressure in the optical and electronic properties in these systems have been reported [7–11]. There are studies on the pressure-dependent refractive index, $\Gamma - X$ hybridization of donor levels, variations of the exciton binding energy and band gaps, atmospheric-pressure band offsets in GaAs-$Al_xGa_{1-x}As$ heterostructures, and high-mobility and high conductance electron channels. The dependence with the hydrostatic pressure of the (i) electron-hole recombination peaks in the photoluminescence (PL) spectrum of single and double GaAs-$Ga_{1-x}Al_xAs$ quantum wells (QWs) [12,13] and (ii) negative-donor-ion singlet and singlet-like bound magnetosplasmon transitions in doped GaAs/AlGaAs QWs [14] may also be mentioned. In addition, the pressure-induced $\Gamma - X$ crossing has been studied from PL data in InAs/GaAs quantum dots [15], whereas a theoretical description of the experimentally observed anticrossing between the energy levels of donor states in GaAs under hydrostatic pressure has been reported by Bednarek and Adamowski [16]. The band anticrossing effects in the conduction band of GaNAs-based QW structures under hydrostatic pressure were considered by Tomić et al. [17].

There is no systematic study on the mixing-parameter which describes the coupling between the Γ and X conduction band minima in low dimensional heterostructures such as GaAs-(Ga,Al)As QWs. As the $\Gamma - X$ mixing may be induced by an applied hydrostatic pressure in such heterostructures, an appropriate understanding of the physics related to the mixing-parameter could be very useful in obtaining a realistic description of the excitonic-related optical properties of low-dimensional semiconductor systems. Therefore, here we are concerned with a theoretical study of the PL energy transitions associated with confined excitons in GaAs-$Ga_{1-x}Al_xAs$ QWs, with the combined effects of hydrostatic pressure and conduction band mixing discussed and compared with available experimental results [12,13]. A systematic study of the $\Gamma - X$ mixing-parameter is also reported. The paper is organized

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Table 1. Parameters used in the present calculations [20].

	$\Gamma-$GaAs	$X-$GaAs	$\Gamma-Ga_{1-x}Al_xAs$	$X-Ga_{1-x}Al_xAs$
E_1 (meV)	1519	1981	$1519+1155\,x+370\,x^2$	$1981+124\,x+144\,x^2$
α (meV/K)	-0.5405	-0.460	-0.5405	-0.460
β (meV/kbar)	10.7	-1.4	$10.8-3.2\,x+3.8\,x^2$	$-1.4+0.1\,x$
$A_{(\parallel/\perp)}$		1.3/0.26		1.25/0.19

as follows. In Section 2 we detail the present theoretical approach. Section 3 is concerned with the results and discussion, and finally, our conclusions are given in Section 4.

2 Theoretical framework

The calculation of the states in the conduction band of the GaAs-$Ga_{1-x}Al_xAs$ structures is carried out in the framework of the EMA. We limit ourselves to the ground state of the system, which is described by means of a model with two independent bands. The Hamiltonian of the problem is written as [3]

$$\begin{bmatrix} h^\Gamma & 0 \\ 0 & h^X \end{bmatrix} \begin{bmatrix} F^\Gamma \\ F^X \end{bmatrix} = \varepsilon \begin{bmatrix} F^\Gamma \\ F^X \end{bmatrix}, \qquad (1)$$

where

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

F^α are the $\Gamma-$ and $X-$related envelope-wave functions whereas ε_α refers to the conduction band edge at the point α in $\mathbf{k}$ space, in the spirit of the procedure followed by Wang et al. [3]. The mixing of bands is introduced according to the scheme in which the boundary conditions at the interfaces can be written in matrix form with the use of a matching matrix that involves an adjustable phenomenological γ-parameter [2]

$$\begin{bmatrix} F^\Gamma \\ F^X \\ m_\Gamma^{-1}\nabla F^\Gamma \\ m_X^{-1}\nabla F^X \end{bmatrix}_{\rm Well} = \mathbf{T} \begin{bmatrix} F^\Gamma \\ F^X \\ m_\Gamma^{-1}\nabla F^\Gamma \\ m_X^{-1}\nabla F^X \end{bmatrix}_{\rm Barrier}, \qquad (3)$$

where

$$\mathbf{T} = \begin{bmatrix} \xi & -\gamma & 0 & 0 \\ +\gamma & \xi & 0 & 0 \\ 0 & 0 & \xi & -\gamma \\ 0 & 0 & +\gamma & \xi \end{bmatrix}, \qquad (4)$$

with $\xi=\sqrt{1-\gamma^2}$.

The exciton binding energy [18,19] is calculated with the use of a separable trial wavefunction depending on two-variational parameters [3]. In the above procedure, hydrostatic-pressure effects are incorporated via the dependencies with pressure of the basic input parameters of the EMA [20]. For the pressure and temperature dependent band gap and static dielectric constant, respectively, we have used

$$E_{\rm GAP}(P) = E_1 + \beta\,P + \alpha\,T^2/(T+204) \qquad (5)$$

and

$$\epsilon = 12.74\; e^{[9.4\times10^{-5}\,(T-75.6)-1.67\times10^{-3}\,P]}. \qquad (6)$$

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

$$m_{\Gamma-{\rm GaAs}} = \left[1+\frac{2\times7510}{E_{\Gamma-{\rm GaAs}}(P)}+\frac{7510}{E_{\Gamma-{\rm GaAs}}(P)+341}\right]^{-1} m_0, \qquad (7)$$

$$m_{\Gamma-{\rm Ga}_{1-x}{\rm Al}_x{\rm As}} = (m_{\Gamma-{\rm GaAs}}+0.083\,x\,m_0)\,\Lambda, \qquad (8)$$

and

$$m_{X,(\parallel/\perp)} = (A_{(\parallel/\perp)}+6.15\times10^{-3}\,P-1.22\times10^{-5}\,P^2)\,m_0. \qquad (9)$$

Here P is the hydrostatic pressure in kbar, T the temperature in K, and m_0 the free electron mass. Equation (8) gives the Γ-point effective mass without ($\Lambda=1$) and with ($\Lambda=1-0.4\,x$) inclusion of renormalization effects due to the interaction with the valence band, respectively. The pressure dependence of the QW-width can be obtained by the fractional change in volume of the structure [20]. For the heavy-hole effective mass, for example at $T=70$ K, we have chosen [21] the constant value $m_{hh}=0.45\,m_0$. In Table 1 we present the parameters that we have used in the present calculations.

In our calculations the interfaces in the QWs are assumed perfect and abrupt. A more precise model could consider an effective width for the potential step between the regions of the well and the barrier. This effect could be modeled with a compositionally graded parabolic [22,23] or triangular QWs which can adjust the uncertainty in the measurement of the widths of the QWs (for example of ±5 Å) reported in the experiments [12].

3 Results and discussion

Here we consider that a pressure-induced $\Gamma-X$ band mixing effect may be present in layered heterostructures fabricated from GaAs and $Ga_{1-x}Al_xAs$ materials. Again, this mixing phenomenon is introduced through the phenomenological γ parameter associated to the boundary conditions for the wave functions at the interfaces.

In Figure 1 we present our theoretical findings for the hydrostatic pressure dependence of the PL-peak energy transition, for heavy-hole excitons, in a single GaAs-$Ga_{0.7}Al_{0.3}As$ QW. Results are for different values for the γ-parameter and QW-width. In the low pressure regime

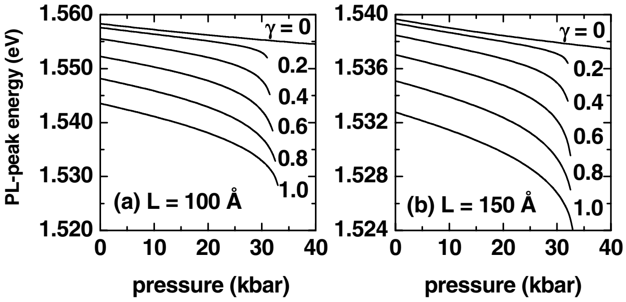

Fig. 1. Hydrostatic pressure dependence of the PL-peak energy transition for heavy-hole excitons in a single GaAs-Ga$_{0.7}$Al$_{0.3}$As QW. Results are for different values for the γ-parameter. In (a) results are for $L = 100$ Å, whereas in (b) are for $L = 150$ Å.

(approximately up to 15 kbar), the curves have a 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 ($P \sim 15$ kbar), 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 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 in the barrier material providing an increment in the expected value of the electron-hole distance. With increasing values of the γ-parameter, a decrease of the associate PL-peak energy transition is observed, mainly due to the decrease of the energy of the electronic confined state. This is also due to the reduction of the barriers heights which confine the electrons in the well region. This effect is larger for small well-widths since for them the confined electron state by the Γ-conduction profile is very close both to the top of the potential barriers and the X-band. For $\gamma = 0$ no mixing effects are observed and the electron wave function is essentially that one which is usually obtained with the Γ profile of the conduction bands. When the γ-parameter approaches unity, the wave function is essentially associated to the X profile. It is worth mentioning that we do not obtain the same behavior as Wang et al. [3]. In their work, they have shown an increasing behavior of the energy of the lowest unperturbed confined state in the well when the effects of the $\Gamma - X$ conduction band mixing are included (see Fig. 2 of Ref. [3]). Such a result clearly disagrees with the decrease in the confining potential barrier height, because of the presence of the perturbation from the X-band. We believe that the present result clarifies this point. Moreover, the validity of our calculation is further confirmed by the analysis of some experimental data that is presented below.

In Figure 2 we depicted the PL-peak energy transition for heavy-hole excitons in a single GaAs-Ga$_{0.7}$Al$_{0.3}$As QW as a function of the γ-parameter. Results are for different QW-width and hydrostatic pressure values. The de-

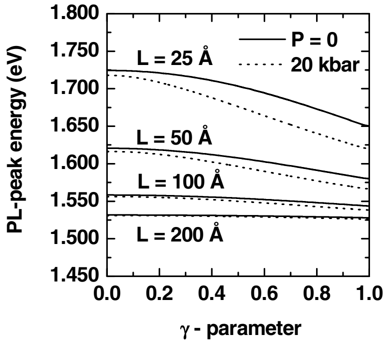

Fig. 2. PL-peak energy transition for heavy-hole excitons in a single GaAs-Ga$_{0.7}$Al$_{0.3}$As QW as a function of the γ-parameter. Results are for different values of the QW-width. Solid lines are for the zero-pressure case, whereas dotted lines are for $P = 20$ kbar.

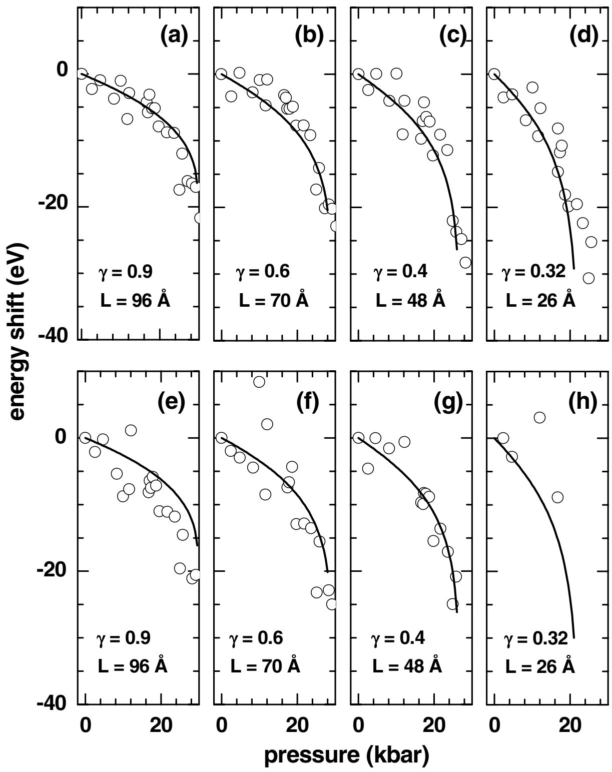

Fig. 3. Pressure dependent shift energy for the $e_1 - h_1$ transitions in GaAs-Ga$_{0.67}$Al$_{0.33}$As single QW. Results are for heavy-hole transitions (a–d) and light-hole transitions (e–h) and for different values of the QW width. Solid lines are our theoretical findings. The used γ-parameter and QW widths are shown. Open symbols are experimental data from Venkateswaran et al. [12]. Results are at 80 K.

crease of the PL-peak energy with increasing QW widths is a well-known result. Additionally, the decreasing behavior of the PL-peak energy transition with pressure and γ-parameter is in agreement with the calculated results in Figure 1. Figures 3 and 4 show the pressure dependence of the energy shift [24] of the $e_1 - h_1$ transitions in GaAs-Ga$_{0.67}$Al$_{0.33}$As and in GaAs-Ga$_{0.7}$Al$_{0.3}$As single QWs, respectively. Results are for heavy-hole transitions (a–d) and light-hole transitions (e–h) and different values

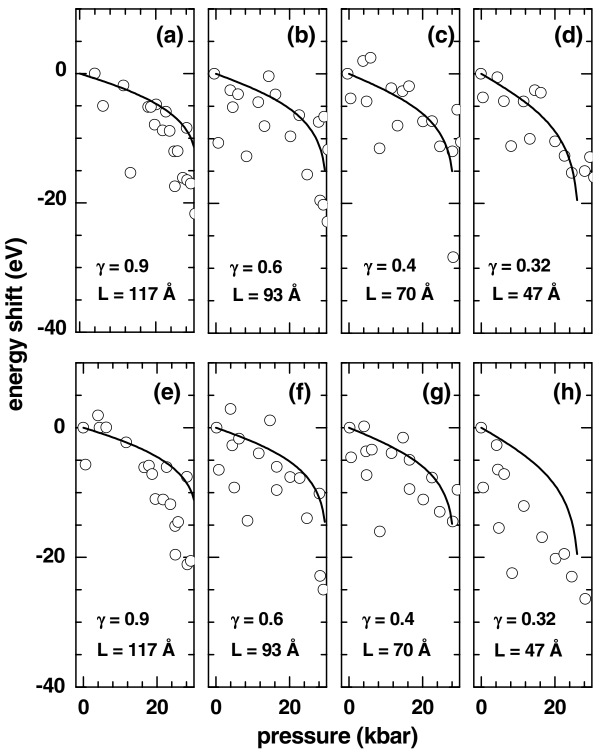

Fig. 4. The same as in Figure 3, but for a GaAs-$Ga_{0.7}Al_{0.3}As$ single QW.

of the QW width. Solid lines are the present theoretical findings by using appropriate values of the γ-parameter that fit the experimental findings, shown as open symbols, from Venkateswaran et al. [12]. Figures 3 and 4 show that the $\Gamma - X$ conduction band mixing accounts for the experimentally detected nonlinear behavior of the PL peak energy for pressures over which the X band in the barrier region is below in energy to the corresponding Γ profile. In the low pressure regime (approximately up to 15 kbar), the curves have a linear behavior associated with the fact that the minimum in X for the barrier material is essentially above the energy value corresponding to the minimum in Γ. In the pressure regime close to the transition from type I to type II X-potential profile of the combined structure ($P \sim 15$ kbar), the X-perturbative effect leads to an appreciable decrease 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 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 in the barrier material providing an increment in the expected value of the electron-hole distance.

In Figure 5 we depict the γ-parameter as a function of the QW width. Symbols are taken from Figures 3 and 4 and the lines are the corresponding quadratic fittings. Calculated results show that the appropriate γ-parameter must increase with increasing QW widths. In the pressure range in which the energy shift is not linear, the system is closer to the $\Gamma - X$ crossover and indirect transitions,

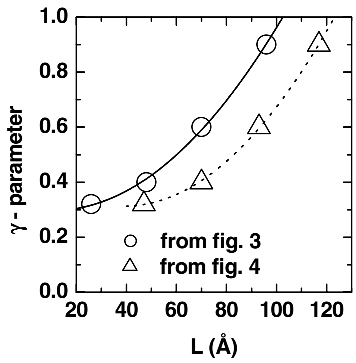

Fig. 5. The γ-parameter as a function of the width of a single GaAs-$Ga_{1-x}Al_xAs$ QW. The symbols are taken from Figure 3 and 4 and the lines are the corresponding quadratic fittings. For the solid line $\gamma = 0.31 - 1.9 \times 10^{-3} L + 8.4 \times 10^{-5} L^2$, whereas for the dotted line $\gamma = 0.46 - 7.5 \times 10^{-3} L + 9.7 \times 10^{-5} L^2$.

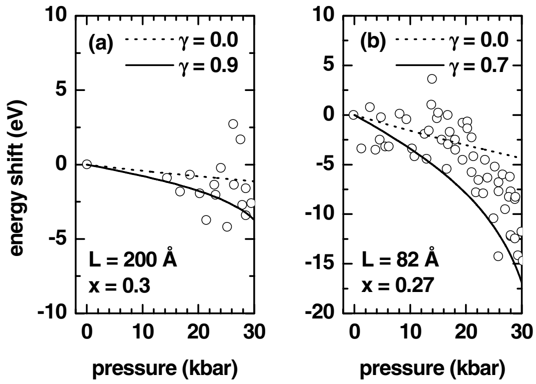

Fig. 6. Pressure dependent shift energy for the $e_1 - h_1$ transitions in a GaAs-$Ga_{1-x}Al_xAs$ single QW. Open symbols are experimental data from Burnett et al. [13] for heavy-hole transitions at $T = 4$ K in a single QW ($L = 200$ Å) (a) and in a strongly coupled symmetrical double QW (72 Å for each well region and 18 Å for the central barrier) (b). Solid lines are our theoretical findings by using the γ-parameter in according with the fitting equations from Figure 5. The dotted lines are for $\gamma = 0$. In (b) the dimension of the single QW, used in the calculation – 82 Å, has been chosen in order to fit the sum $e_1(P = 0) + h_1(P = 0)$ of the coupled double QW from Burnett et al. [13].

coming from the X-band, become more important. So, as for large QW widths the energy separation between the first confined electron state in the QW and the Γ-band is large, a higher value of the γ-parameter is necessary in order to include the perturbation of the first non-confined X-related state.

Burnett et al. [13] performed an experimental study of the PL excitation spectra (PLE) in isolated and strongly coupled double GaAs-$Ga_{1-x}Al_xAs$ QWs. A model including the same boundary conditions given in equations (3) and (4) was used by them to theoretically fit their results. A strong non-linear behavior of the PLE peaks with pressure was detected in the case of the strongly coupled double QWs, and it was explained through the effect of the $\Gamma - X$ mixing in the system. In Figure 6 we present the comparison between the present theoretical findings and the experimental data from Burnett et al. [13] for the pressure-dependent energy shift, for the $e_1 - h_1$ transitions, in a GaAs-$Ga_{1-x}Al_xAs$ single and strongly coupled QW. For Figure 6b the γ parameter was taken as 0.7 (see Fig. 5) whereas for Figure 6a we have used $\gamma = 0.9$, which is the limiting calculated value in Figure 5. By comparing the results represented by solid and dotted lines ($\gamma = 0$), one clearly sees the importance of taking into account the $\Gamma - X$ mixing in order to appropriately describe the experimental findings. Finally, one should mention that in the work by Venkateswaran et al. [12] they have reported the pressure coefficient for the electron-hole PL-peak transitions in single QWs, and fit their experimental data to pressure-dependent linear functions, without considering the non-linear behavior for pressure values larger than ~15 kbar. From Figure 6b one sees that, for example, at 30 kbar the deviations from the linear behavior are larger than the value of the exciton binding energy, which indicates that results in Figure 6 from Venkateswaran et al. [12] should be viewed with caution.

4 Conclusions

The effects of hydrostatic pressure and $\Gamma - X$ mixing on the exciton states in a single GaAs-$Ga_{1-x}Al_xAs$ QW have been investigated. Results suggest that the inclusion of the $\Gamma - X$ mixing can explain the observed non-linear behavior in the energy shift (for pressure values larger than 15 kbar) of confined exciton states in QWs, just as it has been shown in experimental reports [12,13]. Calculated results indicate that the γ parameter must increase with increasing QW widths. For example, for GaAs-$Ga_{0.67}Al_{0.33}As$ QW we have obtained $\gamma = 0.31 - 1.9 \times 10^{-3}L + 8.4 \times 10^{-5}L^2$, whereas for GaAs-$Ga_{0.7}Al_{0.3}As$ QW we obtained $\gamma = 0.46 - 7.5 \times 10^{-3}L + 9.7 \times 10^{-5}L^2$, where L corresponds to the QW-width in Å (see Fig. 5). In addition, results suggest that increasing values of the γ parameter lead to a decrease of the associate PL-peak energy transition, due to an effective reduction of the potential barriers which confines the electron in the well region.

The authors acknowledge support from CONACYT (México) and COLCIENCIAS (Colombia) through bilateral agreement J110.334/2005. This work has been partially supported by CODI-Universidad de Antioquia and by the Excellence Center for Novel Materials ECNM, under Colciencias contract No. 043-2005. CAD wishes to acknowledge the hospitality of the Instituto de Física at Unicamp, where part of this work was performed, and is grateful to Brazilian Agencies CNPq and FAPESP for partial financial support. C.A.D. is grateful to Barbara Chylewska for useful discussions.

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