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Donor impurity-related optical absorption spectra in GaAs-$Ga_{1-x}Al_xAs$ quantum wells: hydrostatic pressure and $\Gamma - X$ conduction band mixing effects

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Using a variational procedure within the effective mass approximation, the mixing between the Γ and X conduction band valleys in GaAs-$Ga_{1-x}Al_xAs$ quantum wells is investigated by taking into account the effect of applied hydrostatic pressure. Some optical properties such as donor and/or acceptor binding energy and impurity-related transition energies are calculated and comparisons with available experimental data are presented.

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1 Introduction The effective-mass approximation (EMA) can be extended to take into account the mixing between the Γ and X conduction-band valleys at heterointerfaces, such as GaAs-$Ga_{1-x}Al_xAs$. This is done 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 [1,2]. The $\Gamma - X$ mixing and hydrostatic pressure effects in single GaAs-AlAs and double GaAs-$Ga_{1-x}Al_xAs$ quantum wells (QW) can be mentioned as antecedents [2,3]. However, up to our knowledge, the study of the combined action of the hydrostatic pressure and $\Gamma - X$ mixing on the donor and/or acceptor impurity-related transition energies in GaAs-$Ga_{1-x}Al_xAs$ QWs has not been yet reported.

In this work we are presenting results of the calculation of the donor and/or acceptor binding energy and impurity-related transition energies in a GaAs-$Ga_{1-x}Al_xAs$ QW. Calculations are performed using a variational procedure within the effective mass approximation.

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 [2]:

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

with

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

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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 **k** space. The mixing of bands is introduced according to the scheme proposed by Pulsford et al. [1], in the same spirit of Ref. [2]. The boundary conditions at the interfaces are introduced via an unitary matrix that involves an adjustable phenomenological parameter γ [1]

$$\begin{bmatrix} F^{\Gamma} \\ F^{X} \\ \nabla F^{\Gamma}/m_{\Gamma\,\|} \\ \nabla F^{X}/m_{X\,\|} \end{bmatrix}_{\text{Well}} = \begin{bmatrix} \xi & -\gamma & 0 & 0 \\ +\gamma & \xi & 0 & 0 \\ 0 & 0 & \xi & -\gamma \\ 0 & 0 & +\gamma & \xi \end{bmatrix} \begin{bmatrix} F^{\Gamma} \\ F^{X} \\ \nabla F^{\Gamma}/m_{\Gamma\,\|} \\ \nabla F^{X}/m_{X\,\|} \end{bmatrix}_{\text{Barrier}} , \tag{3}$$

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 [5]. Finally, the impurity binding energy [4] is calculated with the use of a separable trial wavefunction depending on two-variational parameters [2].

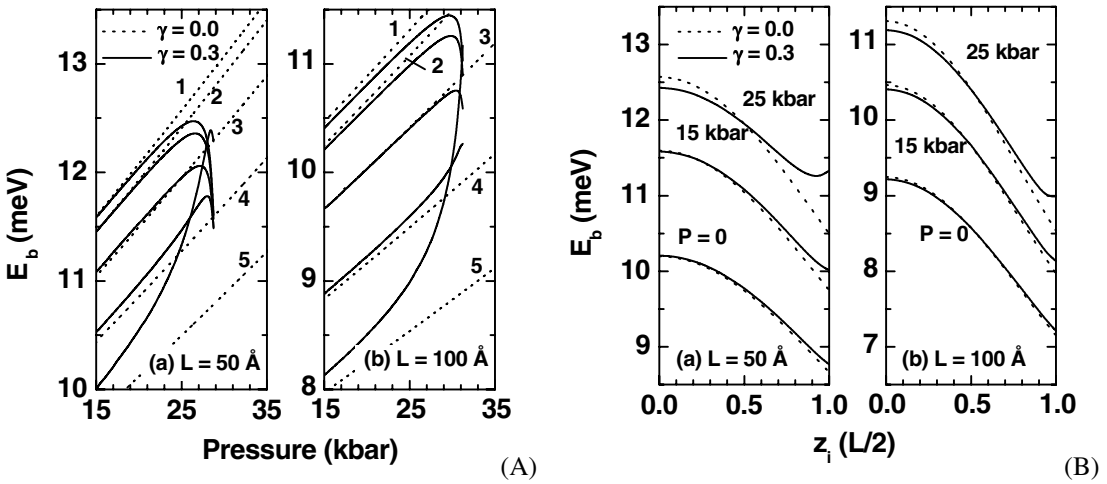

Fig. 1 **(A)** Hydrostatic pressure dependent binding energy for a donor impurity in GaAs-$Ga_{0.7}Al_{0.3}As$ QWs for two values of the QW width. Dashed lines are for zero value of the γ-mixing parameter whereas solid lines are for $\gamma = 0.3$. Different impurity positions are indicated by the labels: $z_i = 0$ (1), $z_i = L/8$ (2), $z_i = L/4$ (3), $z_i = 3L/8$ (4), and $z_i = L/2$ (5). Labels for solid lines follow the same shown sequence for the dotted cases. **(B)** In growth direction impurity position dependent binding energy for a donor impurity in GaAs-$Ga_{0.7}Al_{0.3}As$ QWs for several values of the well width. Different values of the hydrostatic pressure are presented. In **(A)** and **(B)** dotted and solid lines are for zero value of the γ-mixing parameter and $\gamma = 0.3$, respectively.

3 Results and discussion In Fig. 1 we present our results for a donor binding energy as a function of hydrostatic pressure (A) and the impurity position (B) in GaAs-$Ga_{0.7}Al_{0.3}As$ QWs and considering different configurations of the well width and the $\Gamma - X$ mixing parameter. The linear and increasing behavior with the pressure, for the $\gamma = 0$ case, is mainly due to the diminishing of the static dielectric constant with the pressure. For the $\gamma = 0.3$ case the binding energy grows with pressure up to a maximum (which depends of the impurity position) and then decreases due to the fact that the mixing effect induces a decreasing of the potential barrier confining the carriers. Because of this, in the high pressure regime, the different binding energy curves tend to the bulk hydrogenic limit for the $Ga_{0.7}Al_{0.3}As$ material.

In Fig. 2 we present our results for the pressure dependent impurity related transition energy in GaAs-$Ga_{1-x}Al_xAs$ QWs. In both cases (donor and acceptor transitions energies) we observe a quasi-linear behavior for the low pressure. In the donor case we obtained the $\Gamma - X$ crossing where the transitions are from the X-GaAs minimum to the first valence confined state of the QW. Our theoretical results are

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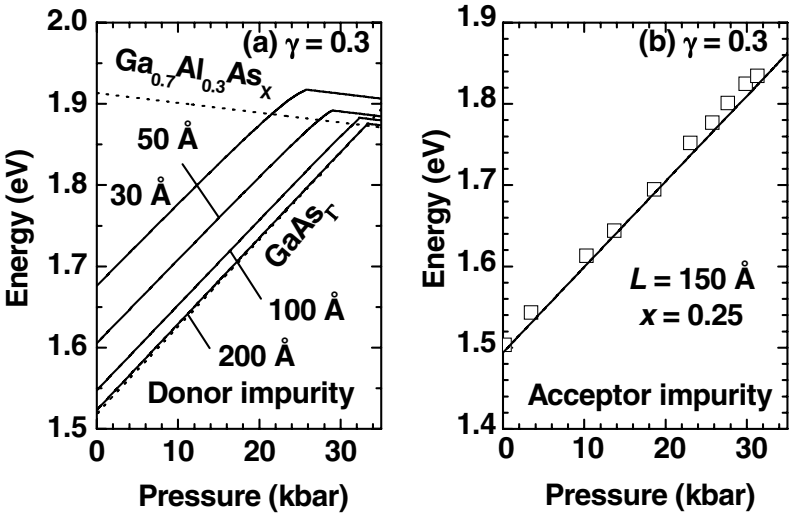

Fig. 2 Dependence of the transition energy upon the hydrostatic pressure in GaAs-$Ga_{1-x}Al_xAs$ QWs. In (a) the transitions are from the donor impurity band to the first confined valence state of the GaAs-$Ga_{0.7}Al_{0.3}As$ QW. In (b) the transitions are from the first confined conduction state of the GaAs-$Ga_{0.75}Al_{0.25}As$ QW to the acceptor impurity band. The open symbols in (b) are experimental data from Venkateswaran et al. [6].

in good agreement with available experimental findings showed in Fig. 2(b). Results can be improved by including, for example, image effects associated with the mismatch of the static dielectric constant.

4 Conclusions By using a variational procedure within the effective mass approximation, we have investigated the $\Gamma - X$ conduction band mixing and hydrostatic pressure effects on the donor and/or acceptor binding energy and impurity-related transition energies in GaAs-$Ga_{1-x}Al_xAs$ QWs. We have found that the mixing modifies in a substantial way these optical properties. Comparisons with available experimental findings shows good agreement.

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