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1 Introduction

With the development of experimental techniques and different analysis methods, there has been an increasing amount of work devoted to the study of the states of hydrogenic impurities in low-dimensional semiconductor heterostructures such as quantum wells, quantum well wires (QWWs), and quantum dots. Due to the importance of these systems in the development of new semiconductor devices and applications, the effects of external perturbations, such as magnetic field, hydrostatic pressure, and electric field, on the electronic and optical properties constitute a subject of considerable interest from both the theoretical and technological point of view.

Some studies have been reported on the applied electric field and hydrostatic pressure dependencies of the shallow-donor–impurity and/or acceptor–impurity binding energies of the ground and first few excited states in QWW heterostructures [1–4]. The aim of the work reported in the present paper was to study the hydrostatic pressure and electric field effects on confined donor and acceptor impurities in transverse-rectangular section GaAs–(Ga,Al)As QWWs. Calculations are done using a variational procedure within the effective mass approximation. Image effects are not considered and the dielectric constant and effective masses are taken as the GaAs values throughout all regions of the structure. The paper is organized as follows. In Section 2 we give our theoretical framework, Section 3 is concerned with the results and discussion, and, finally, our conclusions are given in Section 4.

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2 Theoretical framework

Using the effective mass approximation, the Hamiltonian for a donor or acceptor impurity confined in a rectangular-transverse section GaAs–(Ga,Al)As QWW under the effects of transverse electric field, $\boldsymbol{F}$, and hydrostatic pressure, P, is given by

$$H = -\frac{\hbar^2}{2m^*(P)}\nabla^2 + |e|\,F[x\cos(\theta) + y\sin(\theta)] + V(P,x,y) - \frac{e^2}{\varepsilon(P)r}\,, \tag{1}$$

where r is the carrier–impurity distance, $\varepsilon(P)$ and $m^*(P)$ are the pressure-dependent static dielectric constant and electron (or hole) effective mass [5–7], θ is the electric field angle relative to the x-axis, and $V(P, x, y)$ is the potential barrier that confines the carrier in the wire region which is considered as zero within the wire region and $V_0(P)$ for $|x| \geq L_x(P)/2$ and $|y| \geq L_y(P)/2$, where $L_x(P)$ and $L_y(P)$ are the dimensions of the transverse section of the wire. For the Γ–X crossover, induced by hydrostatic pressure, we have followed the phenomenological model of Elabsy [6].

Because of the rectangular domain and the hydrogenic-like impurity, we write the solution of Eq. (1), using a variational procedure, in the form

$$\Psi(r) = Nf(x)\,f(y)\,\mathrm{e}^{-\lambda r}\,, \tag{2}$$

where N is the normalization constant, λ the variational parameter, and the functions $f(x)$ and $f(y)$ are given by

$$f(\Omega) = \begin{cases} \mathrm{e}^{+k_{1\Omega}\Omega}, & \Omega \leq -L(P)/2 \\ \alpha_{\Omega} A_i(\Omega) + \beta_{\Omega} B_i(\Omega), & |\Omega| \leq +L(P)/2\,, \\ \mathrm{e}^{-k_{2\Omega}\Omega}, & \Omega \geq +L(P)/2 \end{cases} \tag{3}$$

where Ω runs over x and y and the functions $A_i(\Omega)$and $B_i(\Omega)$ are the Airy functions. The impurity binding energy is calculated from the definition

$$E_{\mathrm{b}} = E_1 - E_{\min}(\lambda)\,, \tag{4}$$

where E_1 is the eigenvalue for the Hamiltonian without the impurity term in Eq. (1) and $E_{\min}$ is the expectation value for the complete Hamiltonian in Eq. (1), minimized with respect to the variational parameter λ. The transition energy is defined by

$$E_{\mathrm{T}} = E_{\mathrm{g}} + E_{1\mathrm{v}} + E_{1\mathrm{c}} - E_{\mathrm{b}}\,, \tag{5}$$

were E_{g} is the energy gap, $E_{1\mathrm{v}}$ is the energy of the first state for holes in their QW, $E_{1\mathrm{c}}$ is the corresponding one for electrons, and E_{b} refers to donor and/or acceptor impurities. The E_{b} term includes the carrier–impurity correlations effects, which are important due to the dimensions of the transverse section of the wire we consider here. The density of impurity states (DOIS) and the impurity polarizability are obtained, respectively, from the expressions [2, 8]

$$g[E_{\mathrm{b}}(P,T)] = \frac{1}{L_z(P)}\int_{S[E_{\mathrm{b}}=\mathrm{const}]}\frac{\mathrm{d}S}{\nabla E_{\mathrm{b}}(P,T)}\,, \tag{6}$$

and

$$\alpha = -\frac{e}{F}\left[\left(\langle\Psi|\,x\,|\Psi\rangle|_{F\neq 0} - \langle\Psi|\,x\,|\Psi\rangle|_{F=0}\right)^2 + \left(\langle\Psi|\,y\,|\Psi\rangle|_{F\neq 0} - \langle\Psi|\,y\,|\Psi\rangle|_{F=0}\right)^2\right]^{1/2}. \tag{7}$$

3 Results and discussion

Figure 1 shows the transition energy as function of the side length of a square-transverse section QWW, using different configurations of hydrostatic pressure, applied electric field, and its angle with respect to the *x*-axis. In both cases, i.e. donors and acceptors, the transition energy curves are rigidly shifted when the pressure varies (increases). For the zero electric field cases, and in the regime of large side length of the QWW, the transition energies go to the GaAs bandgap limit minus the acceptor and/or donor binding energy. In the regime of wires with low transverse section the strong variations in the transition energy are due to the strong dependence on the side length of the wire of the E_{1c} state. In the case of applied electric field, both the E_{1c} and E_{1v} states diminish with increasing electric field [1]. Due to the fact that the hydrostatic pressure is a constant for each set of solid or dashed curves, the transition energy follows the same observed decreasing behaviour with electric field as that of the first confined electron and hole states in the QWW.

Figure 2 shows the transition energy as a function of the hydrostatic pressure for a square-transverse section QWW considering donor and acceptor cases and using different configurations of the well width, applied electric field, and its direction with respect to the *x*-axis. Some experimental data are shown [9, 10]. Here we can observe that for donor and acceptor transitions all curves follow a linear behaviour with pressure, with a pressure coefficient (dE_T/dP) equal to 10.48 meV/kbar (Fig. 2a), 10.42 meV/kbar (Fig. 2b), 10.58 meV/kbar (Fig. 2c), and 10.52 meV/kbar (Fig. 2d). These values are slightly lower than the corresponding value for the GaAs bandgap (10.7 meV/kbar). When comparing Figs. 2a with 2c (or Figs. 2b with 2d), we note an increasing behaviour of the pressure coefficient with increasing transverse section of the wire [9, 11]. Symbols in Fig. 2c and d represent the pressure-dependent bulk GaAs bandgap [10], in very good agreement with our calculations for the GaAs bulk limit of the QWW system. The inset in Fig. 2d shows the very good agreement for the hydrostatic pressure dependence of the transition energy obtained for a rectangular-transverse section GaAs–$Ga_{0.75}Al_{0.25}As$ QWW with L_x = 150 Å and L_y = 2000 Å (in order to simulate an L = 150 Å QW) and the experimental findings for sample 3 of Venkateswaran et al. [9].

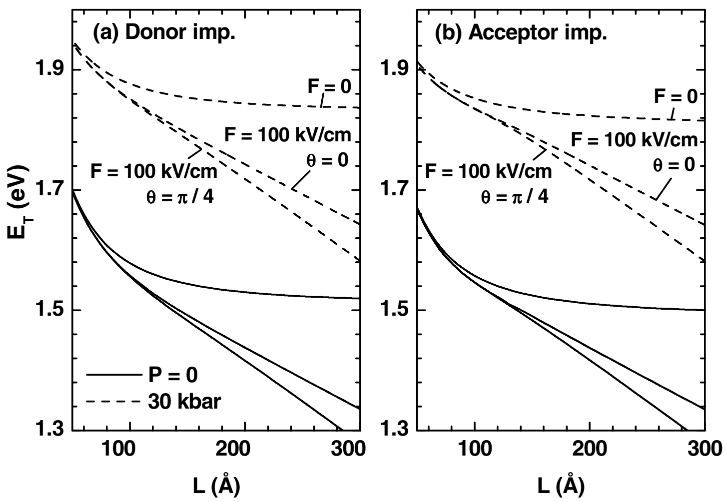

Fig. 1 Transition energy of a square QWW as function of the side length of size *L*, using two values of applied electric field, two directions of the field, and two values of hydrostatic pressure. a) Results for transitions from the donor impurity band to the first valence confined state in the wire. b) Transitions from the first conduction state of the wire to the acceptor–impurity band. The solid lines have the same sequence of values of electric field and angle shown for the dotted lines.

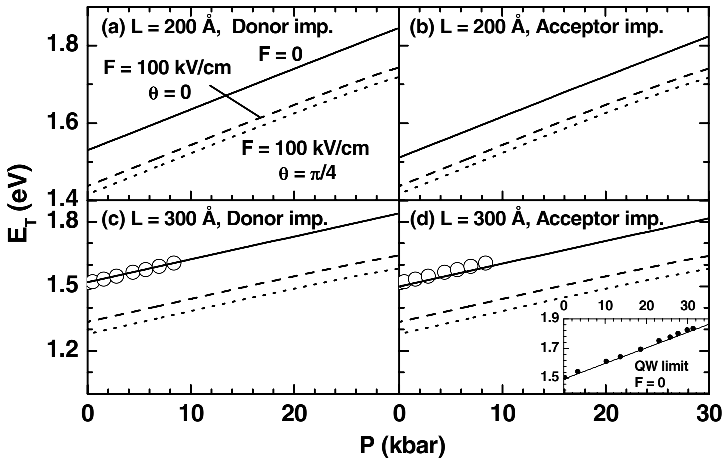

Fig. 2 Shallow impurity-related transition energy as a function of the hydrostatic pressure for a square-transverse section QWW. Different configurations of the well width and applied electric field have been considered. Open circles in c) and d) correspond to the GaAs band gap [10]. The inset in d) shows the comparison between our theoretical results (solid line) for $L_x = 150$ Å and $L_y = 2000$ Å, without including electric field effects, and the corresponding measured results for a $GaAs-Ga_{0.75}Al_{0.25}As$ superlattice (solid symbols) [9].

Figure 3 shows the DOIS for donor (A) and acceptor (B) impurities in a square-transverse section $GaAs-Ga_{0.7}Al_{0.3}As$ QWW considering different configurations of the direction of the applied electric field and values of the hydrostatic pressure. The results are for $L = 200$ Å, $F = 200$ kV/cm. For the donor case, three well-defined structures are observed: one structure, with infinite weight, corresponds to the maximum in the binding energy and is associated with impurities close to the axis of the wire; the other two structures, with finite weight, arise from on-edge impurities. For the acceptor case, three structures

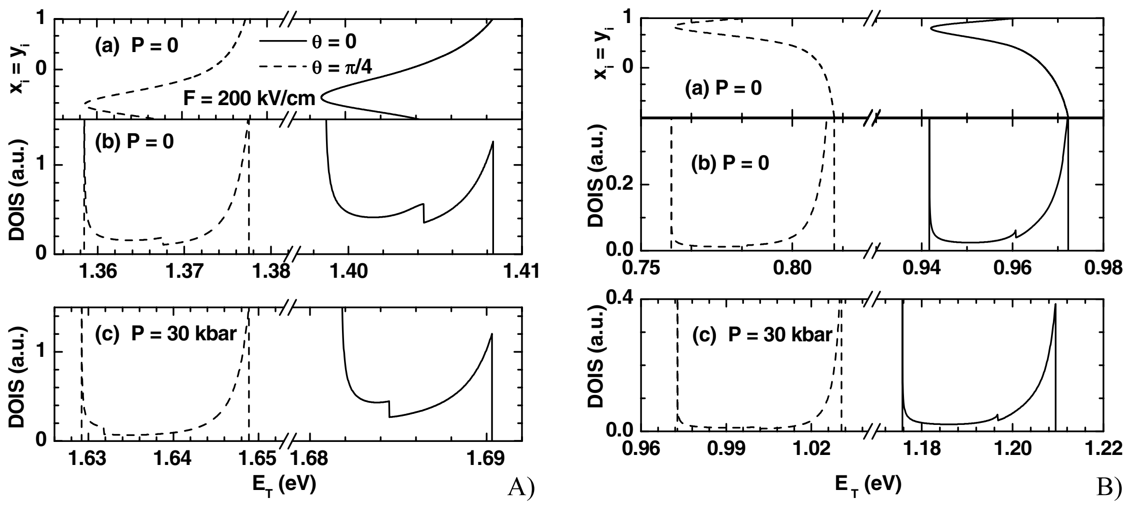

Fig. 3 (b), (c) Density of impurity states for a shallow impurity in a square-transverse section $GaAs-Ga_{0.7}Al_{0.3}As$ QWW. (a) Results show the impurity position dependence of the transition energy. The impurity moves along the diagonal direction of the transverse section of the wire. A) Results for a donor impurity and B) results for an acceptor impurity. The results are for $L = 200$ Å, $F = 200$ kV/cm, two directions of the applied electric field, and two hydrostatic pressure values.

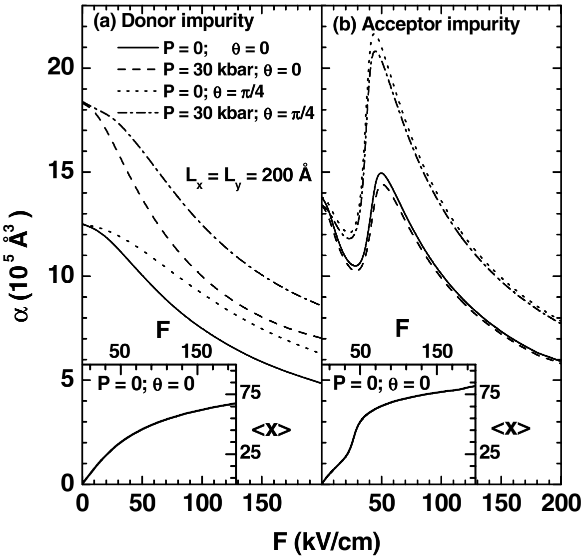

Fig. 4 Polarizability of a shallow impurity in a square-transverse section GaAs–$Ga_{0.7}Al_{0.3}As$ QWW as a function of the applied electric field. Results are for a) on-axis donor and b) acceptor impurity. Different values of the hydrostatic pressure and the direction of the applied electric field have been considered. The insets show the applied electric field dependence of the expectation value of x for the $P = 0$ and $\theta = 0$ cases.

also appear, but are not so well defined. This aspect reflects the difficulty of polarizing the acceptor system with applied electric field. The blue-shift behaviour with pressure and the red-shift with the direction of the applied electric field can be used to engineer optoelectronic devices.

Figure 4 shows our results for the impurity polarizability in a square-transverse section GaAs–$Ga_{0.7}Al_{0.3}As$ QWW as a function of the applied electric field. The insets show the applied electric field dependence of the expectation value of x, $\langle \Psi | x | \Psi \rangle$, for the $P = 0$ and $\theta = 0$ case. From the insets we observe that the impurity wave function tends to be strongly localized at the edges of the wire transverse section when the electric field is present. On the other hand, the polarizability decreases to zero in the high electric field regime, caused by the presence of the electric field in the denominator of its definition. A very interesting and unknown behaviour appears for the acceptor case in the intermediate range of electric fields. For these kinds of impurities, the expectation value of the impurity–hole distance in the 1s-like state is close to 30 Å, and due to this large value of the wire side length, the impurity does not feel the changes in the potential barrier with pressure. This is the reason that, at zero electric field, all the polarizability curves tend to the same value. We can see that at low fields the behaviour of the polarizability of acceptor impurities is similar to that of the donors case, for which the system responds softly when the field increases due to the high binding energy (close to 26 meV). In the intermediate range a very different behaviour is observed. The field modifies strongly the binding energy, and the hole wave function is localized at the edge of the wire. This unusual change in the slope of the expectation value of the hole–impurity x-distance versus field is responsible for the observed minimum in the polarizability curves. In contrast, when the hole–impurity system is strongly polarized, the acceptor-related polarizability behaviour is quite similar to that observed for the donor case.

4 Conclusions

In the framework of the effective mass approximation and using a variational procedure, we have calculated the influence of external electric field and hydrostatic pressure on the shallow-impurity optical properties in a rectangular-transverse section GaAs–$Ga_{1-x}Al_xAs$ QWW. The electric field is applied in the plane of the transverse section of the wire, and different angular directions have been considered. We have observed a red-shift behaviour of the transition energy with increasing electric field and with its in-plane direction in the transverse section of the wire. With increasing pressure a linear blue-shift behaviour is additionally observed. For the donor impurity-related density of states three well-defined structures are observed in the presence of the applied electric field. For the acceptor case only two well-defined structures appear. For the polarizability a very singular and unknown behaviour has been observed for the acceptor case. When we consider the quantum well and bulk limits, our theoretical findings are in good agreement with experimental data reported in the literature. In this sense, we expect our results to stimulate future experimental work related to combined electric field and hydrostatic pressure effects in QWWs. The model we have presented here could be used, for example, in calculations of electronic and optical properties in InAs/GaAs self-assembled QWWs, by including appropriately the stress effects in the bandgaps and in the carrier effective masses.

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