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Abstract

Theoretical calculations on the influence of both an external electric field and hydrostatic stress on the binding energy and impurity polarizability of shallow-donor impurities in an isolated GaAs–(Ga, Al)As quantum well are presented. A variational procedure within the effective-mass approximation is considered. The pressure-related Γ–X crossover is taken into account. As a general feature, we observe that the binding energy increases as the length of the well decreases. For the low-pressure regime we observe a linearly binding energy behaviour. For the high-pressure regime the simultaneous effects of the barrier height and the applied electric field bend the binding energy curves towards smaller values. For low hydrostatic pressures the impurity polarization remains constant in all cases with an increasing value as the field increases. This constant behaviour shows that the small variations in well width, effective mass, and dielectric constant with pressure do not appreciably affect polarizability. For high hydrostatic pressure, we see a non-linear increase in polarizability, mainly due to the decrease of barrier height as a result of the external pressure, which allows further deformation of the impurity.

1. Introduction

Carrier dynamics and recombination mechanisms in semiconductor single, double, and multiple quantum wells (QWs), especially those with staggered band alignment, have been the subject of much research [1]. High-quality heterostructures comprising alternating layers of GaAs and AlAs, fabricated by epitaxial techniques with monolayer precision, are of great interest. This is due to the possibility of producing by design many physical situations, which appear as a result of dimensional changes. Combining these with external perturbations, such as applied electric field and stress, one can tune the electronic states with respect to one another, thus revealing the nature and extent of various interactions [2].

Studies of the effect of hydrostatic stress have proven to be invaluable in the context of the optical properties of semiconductors and their heterostructures [3, 4]. For a given structure,

the difference in energy between the type-I and type-II transitions can be tuned with external hydrostatic pressure in a continuous and reversible manner. This makes possible an elucidation of the properties of various interband transitions. Further motivation for pressure studies is provided by the wish to gain insight into the intervalley scattering rate, which plays an important role in relaxation of photoexcited carriers and high-field transport.

Using photomodulated transmission spectroscopy, Dai *et al* [5] have investigated the transitions in GaAs/Al$_x$Ga$_{1-x}$As multiple QWs as a function of hydrostatic pressure up to 50 kbar. They observe a number of spectral structures associated with both direct and indirect transitions. Additionally, they have found that the pressure coefficients of the direct transitions, derived from the confined subbands in GaAs, fall between those of the GaAs and Ga$_{1-x}$Al$_x$As bulks. Smith *et al* [6] have obtained a value for the light effective X mass of $m^*_{X,T} = (0.25 \pm 0.03)m_0$ by fitting the model to the measured X$_t$(1)–X$_t$(2) resonance for transverse X states in GaAs/AlAs double-barrier structures under elevated hydrostatic pressure.

The effect of the Γ–X crossover on the lowest-energy states and on the binding energies of confined donors in single GaAs/Al$_x$Ga$_{1-x}$As QWs have been studied by Elabsy [7]. It was shown that the Γ–X crossing changes the donor energies dramatically, especially when the hydrostatic pressure reaches the Γ$_w$–X$_b$ crossover point. Oyoko *et al* [8] have calculated the uniaxial stress dependence of the binding energy of shallow-donor impurities in GaAs–(Ga, Al)As quantum dots (QDs). They found that the binding energy for various values of the donor position along the *z*-axis, for constant quantum-well box sizes, increases not only with stress but also with the proximity of the impurity to the centre of the structure.

The application of an electric field in the growth direction of the heterostructure gives rise to a polarization of the carrier distribution and to an energy shift of the quantum states. Such effects may introduce considerable changes in the energy spectrum of the carriers, which could be used to control and modulate the output of optoelectronic devices. López-Gondar *et al* [9] and Santiago *et al* [10] have reported on the electric field effects on shallow impurity states in GaAs–(Ga, Al)As QWs; they found, as a general feature, that the density of impurity states and impurity-related optical absorption for finite electric fields exhibit van Hove-like singularities.

The polarizability measurements shed light on the dynamics of the carriers (through the wavefunction) in low-dimensional heterostructures. Using the Hasse variational method within the effective-mass approximation, Ilaiwi [11] has made a theoretical calculation which disclosed a relation between the effect of screening and the polarizabilities of shallow donors and acceptors in infinite-barrier QWs. As a result of this relation, the effect of spatially dependent screening is negligible for shallow donors and quite important for acceptors. Theoretical calculations of the effects of the electric field on energy levels in a Ga(In)As–GaAs surface quantum-well wire (QWW) and on the geometry-dependent polarizability of a shallow donor in a rectangular-cross-section QWW have been reported [12–14] as well. As a general feature, the polarizability increases with the size of the structure and on increasing the electric field.

As far as we know, no studies of the simultaneous electric and hydrostatic stress effects on the shallow-donor and shallow-acceptor binding energy and impurity polarizability in single GaAs–(Ga, Al)As QWs have been made. In the present paper we consider these effects on the binding energy and polarizability of shallow-donor impurities in single GaAs–(Ga, Al)As QWs. The calculations encompass the Γ–X crossing. In this paper we use a variational scheme within the effective-mass approximation. In section 2 we present the theory of the problem, and our results are presented and discussed in section 3. Our conclusions are given in section 4.

2. Theoretical framework

In the effective-mass approximation, the Hamiltonian for a hydrogenic shallow-donor impurity in a GaAs–Ga$_{1-x}$Al$_x$As QW, under the influence of a uniaxial stress (P) and electric field (F), in the z-direction is given by

$$H = -\frac{\hbar^2}{2m^*_{w,b}(P)}\nabla^2 - \frac{e^2}{\varepsilon_{w,b}(P)r} + V_B(z, P) + |e|Fz \tag{1}$$

where $r = \sqrt{x^2 + y^2 + (z - z_i)^2}$ is the carrier–impurity distance and subscripts w and b stand for the QW and barrier layer (BL) materials, respectively. In our case, $z_i = 0$. $m^*_{w,b}(P)$ are the conduction effective masses of both the QW and BL materials, as functions of P [7, 15, 16]. The static dielectric constants in the QW and BL materials are given by $\varepsilon_w(P)$ and $\varepsilon_b(P)$, respectively, as functions of P [16, 17].

$V_B(P, T, z)$ is the barrier potential which confines the donor electron in the QW. It is given by

$$V_B(P, T, z) = \begin{cases} 0 & \text{for } |z| \leqslant L(P)/2 \\ V_0(P, T) & \text{for } |z| \geqslant L(P)/2 \end{cases} \tag{2}$$

where

$$V_0(P, T) = \begin{cases} \Gamma_b(P, T) - \Gamma_w(P, T) & \text{for } P \leqslant P_1 \\ X_b(P, T) - \Gamma_w(P, T) + S_0 x(P - P_1)/P & P_1 < P \leqslant P_2 \end{cases} \tag{3}$$

with P_1 (=13.5 kbar) the crossover pressure between the X$_b$ conduction band and the Γ_b band, P_2 (=35 kbar) the crossover pressure between the X$_b$ conduction band and the Γ_w band, and T the temperature of the system. S_0 (=250 meV) [7] is an adjustable parameter used to match the predicted energy at P_1 with the experimental result; x (=0.3 in this work) is the aluminium molar fraction. The conduction and valence band parameters in this work are taken from photoluminescence measurements [18, 19].

In equation (2), $L(P)$ gives the pressure-dependent width of the QW:

$$L(P) = L(0)[1 - (S_{11} + 2S_{12})P] \tag{4}$$

where S_{11} (=1.16 × 10^{-3} kbar^{-1}) and S_{12} (= − 3.7 × 10^{-4} kbar^{-1}) [15, 16, 20] are the elastic constants of the GaAs and $L(0)$ is the zero-pressure width of the QW.

The trial wavefunction for the ground state is chosen as [9, 10]

$$\Psi(r) = N\varphi(z)\exp(-\lambda r) \tag{5}$$

with

$$\varphi(z) = \begin{cases} C_1 \exp(K_1(z + L(P)/2)) & \text{for } z \leqslant -L(P)/2 \\ \alpha A_i(\xi) + \beta B_i(\xi) & \text{for } |z| \leqslant L(P)/2 \\ C_2 \exp(-K_2(z - L(P)/2)) & \text{for } z \geqslant +L(P)/2. \end{cases} \tag{6}$$

N is the normalization constant. A_i and B_i are the usual Airy functions [9, 10].

The donor binding energy is calculated from the definition

$$E_b = E_0 - E_{\min} \tag{7}$$

where E_0 is the eigenvalue of the Hamiltonian, equation (1), without the impurity potential term on the right, and $E_{\min}$ is the eigenvalue with the impurity potential term, minimized with respect to the variational parameter λ:

$$E = E_0 + \frac{\hbar^2\lambda^2}{2m^*_w(P)} - e^2N^2 \int_V d^3r \frac{(\varphi(z)\exp(-\lambda r))^2}{\varepsilon_{w,b}(P)r} \tag{8}$$

with

$$N^{-2} = \int_V \mathrm{d}^3 r \, (\varphi(z) \exp(-\lambda r))^2. \tag{9}$$

It is clear that, due to the variational method, the E-value gives an upper bound to the exact eigenvalue of the Hamiltonian in equation (1).

The impurity polarizability is calculated by means of [13]

$$\alpha_P = -\frac{e}{F}[\langle\Psi|x|\Psi\rangle_{F\neq0} - \langle\Psi|x|\Psi\rangle_{F=0}]. \tag{10}$$

3. Results

As far as we know, no studies of the simultaneous electric and hydrostatic stress effects on the shallow-donor and shallow-acceptor binding energy and impurity polarizability in GaAs–(Ga, Al)As QWs have been made. In the present paper we consider those effects. The hydrostatic pressure affects various parameters of the QW such as the width, effective mass, dielectric constant, and (for certain values) a crossing of bands, changing the semiconductor from a direct-band-gap material to an indirect-gap one. As the pressure increases, the well's length decreases leading to more confinement of the impurity electron; we call this the pressure-related change in width.

The effective mass in the well and the barrier also increases with pressure, which has the effect of decreasing the confinement due to the larger curvature of the parabolic band. The dielectric constant decreases when one increases the pressure. This increases the impurity potential, leading to a more confined impurity electron (confinement of the impurity).

The barrier height remains constant up to a pressure value of 13.5 kbar, in the direct-band-gap regime, and then decreases monotonically to zero at a pressure of 35 kbar. This effect dominates the decreasing of the confinement of the impurity for pressures larger than 13.5 kbar, since the barrier height varies from 240 meV, at 13.5 kbar, to 40 meV at 33 kbar.

The application of an external electric field to the QW leads to larger or smaller confinement of the impurity electron, depending on the impurity position [21]. This is due to the distortion of the QW potential. The electric field either displaces or concentrates the electron cloud at the impurity site; the first case is the relevant part here, since our impurity is at the centre of the well. It is not possible to assess the individual effects of the different parameters (mass, width, dielectric constant, barrier height), because they enter the equations in a complicated way.

In what follows, we present theoretical results for the binding energy and the impurity polarizability at $T = 4$ K.

In figure 1 the results for the binding energy as a function of the applied pressure for shallow-donor impurities in GaAs–(Ga, Al)As QWs are presented. In figure 1(a) we show the results of the calculation for $L = 200$ Å, considering various values of the applied electric field. In figure 1(b) the results are given for a fixed electric field, $F = 100$ kV cm^{-1}, and various values of the QW size. In both cases, figures 1(a) and (b), the binding energy increases linearly with pressure up to 13.5 kbar. In this pressure regime the barrier height remains constant. For higher pressures the rate at which the binding energy increases is slower and finally the curves bend down to smaller values. This behaviour is due mainly to the linear decrease of the barrier height as discussed above; this bending is larger for higher electric fields since both effects, barrier decrease and increasing field, contribute to delocalization of the impurity.

As the pressure increases the binding energy also increases until a pressure value is reached where the binding energy starts to decrease. In this pressure range the impurity confinement gradually increases and the effects of the pressure-related decrease in length and the application
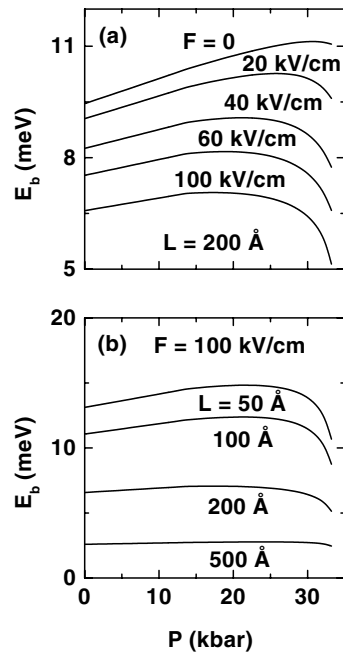
Figure 1. Binding energy as a function of applied pressure for shallow-donor impurities in GaAs–(Ga, Al)As QWs. In (a) the results are for $L = 200$ Å and various values of the applied electric field. In (b) the results are for a fixed electric field, $F = 100$ kV cm^{-1}, and various values of the QW size.

of an external electric field dominate over other effects that tend to free the impurity. After reaching a maximum binding energy it starts to decrease due to the fact that the barrier height moves quickly to lower values making the impurity less confined in the well. This barrier effect dominates, in this range of high pressures, over other effects mentioned above. In figure 1(b), the binding energy is shown to increase as the length of the well decreases, reaching it highest value for $L = 50$ Å. For the high-pressure range the simultaneous effects of the barrier height and applied electric field bend the curves towards smaller binding energies; this effect becomes larger as the well width decreases. In figure 1(a), the case for zero electric field reproduces Elabsy's results for the binding energy as a function of pressure [7].

In figure 2 we show the results for the binding energy as a function of the applied electric field for shallow-donor impurities in GaAs–(Ga, Al)As QWs. In figure 2(a) the results are given for $L = 200$ Å and various values of the applied pressure. In figure 2(b) we take three values for the QW size and consider two values for the applied pressure: 5 and 33 kbar (dotted and solid curves, respectively). In this case the binding energy decreases steadily as the external electric field increases, producing a bell-shaped curve. For zero pressure (see figure 2(a)) we reproduce the effect of the electric field alone [9, 10]: a decrease in the binding energy as the field increases due to the displacement of the impurity electron away from the impurity site.

For pressures up to 13.5 kbar the curves show similar shapes, indicating that the effect of the external electric field dominates the behaviour at each pressure. The curves, at fixed pressure, keep steadily increasing and remain fairly parallel to each other over the whole range of the electric field. The increasing binding energy, when we maintain a fixed value for the external electric field, is dominated by the pressure-related decrease of the well width as the pressure increases, showing a stronger confinement of the impurity. When the pressure
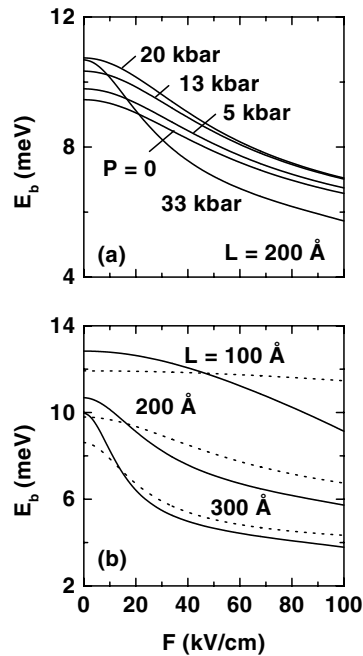
Figure 2. Binding energy as a function of applied electric field for shallow-donor impurities in GaAs–(Ga, Al)As QWs. In (a) the results are for $L = 200$ Å and various values of the applied pressure. In (b) we take three values for the QW size and consider two values for the applied pressure: 5 and 33 kbar (dotted and solid curves, respectively).

increases beyond 13.5 kbar the binding energy increases, for a fixed value of the electric field, at a lower rate. For example, we observe that for high values of the electric field the curves for $P = 13$ and 20 kbar merge, showing a decrease in the amount of confinement due to the decrease of the barrier height at 20 kbar. In this case the effect of the barrier dominates over the effect of the pressure-related decrease in the well width. The curve for $P = 33$ kbar presents the steepest change in the binding energy, crossing the others on its way down and lying well down the curve for $P = 0$ kbar, indicating a strong delocalization of the impurity electron. This curve has the same bell shape as the others. Notice also that at zero electric field the binding energy at 33 kbar is already smaller than that at 20 kbar. This behaviour can be attributed to the barrier height value being the smallest at this pressure, close to 40 meV.

In figure 2(b) the curves show the same behaviour as in the previous case for different values of L, but with the crossing occurring at different values of the electric field. The crossing point occurs at higher values of the external electric field as the well width decreases. As discussed above, this behaviour can be explained by the difference in barrier height: for $P = 5$ kbar it is 240 meV and for $P = 33$ kbar it is 40 meV. The decrease in binding energy ranges from $L = 100$ to 300 Å, due to the increase of the well width. Looking at each pair of curves, with L fixed, we notice that the one corresponding to higher pressure produces more confinement, up to the crossing point, of the impurity electron, due mainly to the pressure-related decrease of the well width. Beyond the crossing point the effect of the external electric field takes over, leading to a less confined impurity electron.

In figure 3 we present our results for the impurity polarization as a function of the applied pressure for shallow-donor impurities in GaAs–(Ga, Al)As QWs. The dimensions of the
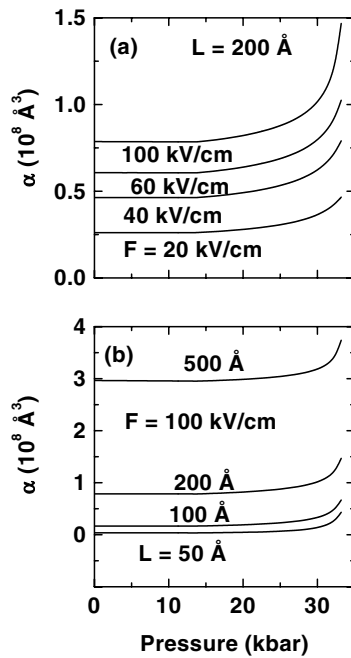
Figure 3. Impurity polarization as a function of applied pressure for shallow-donor impurities in GaAs–(Ga, Al)As QWs. The dimensions of the structure and applied electric field are the same as those for figure 1.

structure and applied electric field are the same as those for figure 1. In figure 3(a), for pressures up to 13.5 kbar, the polarization remains constant in all cases but with an increasing value as the field increases. This constant behaviour shows that the small variations in well width, effective mass, and dielectric constant with pressure do not appreciably affect the polarizability. For pressures larger than 13.5 kbar, we see a non-linear increase of polarizability, mainly due to the decrease of the barrier height, which allows further deformation of the impurity. This increase becomes more pronounced as the electric field increases. In figure 3(b) we see that the polarizability increases as the well width increases from 50 to 500 Å; this is due to the fact that the impurity is less confined for larger widths, having more space in which to be deformed.

For pressures below 13.5 kbar, for every well width, the polarizability remains almost constant, so the effect of the pressure-related changes in the parameters of the well is small, as discussed before. For pressures beyond 13.5 kbar where the barrier height starts to decrease, and for every width value, we have a similar behaviour to that shown in figure 3(a). For the smaller width of 50 Å we notice also that the rate of increase in the polarizability is smaller due to the larger confinement, which makes the system more difficult to deform.

In figure 4 we present the results for the polarization as a function of the applied electric field for shallow-donor impurities in GaAs–(Ga, Al)As QWs. The dimensions of the structure and applied pressure are the same as those for figure 2. In figure 4(a) we see that, for $L = 200$ Å, the polarizability increases as a function of the applied electric field for all pressures plotted. In the case of pressures 0, 5, and 13 kbar the curves fall closely together, as can also be deduced from figure 3(a). The rate of the polarizability increase for the 20 kbar curve is similar to the rates of increase for smaller pressures and the curve lies very close to the curves for smaller pressures. The rate at which the polarizability increases for 33 kbar is the largest, due to
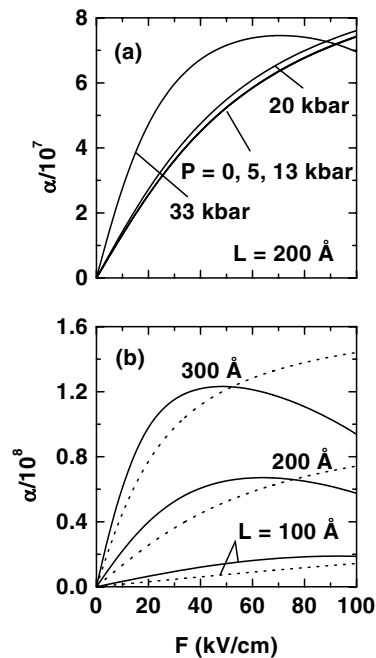
Figure 4. Impurity polarization as a function of applied electric field for shallow-donor impurities in GaAs–(Ga, Al)As QWs. The dimensions of the structure and applied pressure are the same as those for figure 2 and the same units as in figure 3.

the strong decrease in the barrier height. This leads to more delocalization of the impurity. In figure 4(b) we see that for the larger well width of 300 Å, the curves, for 5 and 33 kbar, have the same shape, with concave curvature and the largest rate of increase of the impurity polarizability. The curve for 200 Å, the same as that in figure 4(a), shows a similar behaviour with a larger polarizability for the 33 kbar curve due to the smaller barrier height, 40 meV. For the more confined case of 100 Å, we notice that the 5 kbar curve is almost linear due to the poor impurity deformability at this confinement. Finally, the 33 kbar curve shows a softer curvature which we believe is also due to the strong confinement, recalling that the effective Bohr impurity radius is of the order of 100 Å.

4. Conclusions

Theoretical calculations related to the influence of an external applied electric field and hydrostatic stress on the binding energy and impurity polarizability of shallow-donor impurities in GaAs–(Ga, Al)As QWs are presented. A variational procedure within the effective-mass approximation is considered. The pressure-related Γ–X crossover is taken into account. As a general feature, we observe that the binding energy increases as the length of the well decreases. For the low-pressure regime we observe a linear binding energy behaviour, whereas for high pressure the simultaneous effects of the barrier height and applied electric field bend the binding energy curves towards smaller values. For the range of low hydrostatic pressures (up to 13.5 kbar in GaAs–(Ga, Al)As) the impurity polarization remains constant in all cases but at a higher value as the field increases. This constant behaviour shows that the small variations in well width, effective mass, and dielectric constant with pressure do not appreciably affect

the polarizability. For the high-hydrostatic-pressure range (larger than 13.5 kbar), we see a non-linear increase of the polarizability mainly due to the decrease of the barrier height as a result of the external pressure, which allows further deformation of the impurity. Theoretical data related to the line shape for the valence-to-shallow-donor transition absorption spectra will be published elsewhere.

Acknowledgments

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