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Binding energy and density of shallow impurity states in GaAs–(Ga, Al)As quantum wells: effects of an applied hydrostatic stress

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Abstract
The effects of hydrostatic stress on the binding energy and the density of shallow-donor and shallow-acceptor impurity states in a GaAs–(Ga, Al)As quantum well are calculated using a variational procedure within the effective-mass approximation. Results are for different well widths and hydrostatic stresses, as a function of the impurity position along the growth direction of the structure. We have found that in the low-pressure regime the binding energy changes linearly for both donor and acceptor impurities, independently of the sizes of the well. However, for high pressures (greater than 13.5 kbar) this is valid for acceptors but not for donors due to the Γ-X crossover. We have shown that there are two special structures in the density of impurity states, one associated with on-centre and the other with on-edge impurities. Also, we have observed that the density of impurity states depends strongly on the applied hydrostatic stress.

1. Introduction

Due to the impressive development and improvement of semiconductor growth techniques such as molecular beam epitaxy (MBE), there has been a lot of experimental and theoretical work to study electron, exciton and impurity related phenomena in low semiconductor heterostructures such as the absorption and photoluminescence spectra under the action of applied electric, magnetic and uniaxial stress [1–12]. Miller *et al* [13] have investigated the photoluminescence spectra from GaAs-$Al_xGa_{1-x}As$ quantum wells (QW) with nonuniform distribution of Be acceptors along the growth direction of the structure. They have found a significant temperature dependence in the electron–acceptor impurity photoluminescence spectra. Internal intra-acceptor-impurity transitions have been observed in GaAs-$Al_xGa_{1-x}As$ QW by Rune *et al* [14, 15] finding a good agreement with the theoretical calculations for on-centre acceptor impurities.

However, up to now as we know, the hydrostatic stress effects on the density of impurity states (DOIS) as well as on the shallow-donor (acceptor) related optical absorption (photoluminescence) spectra in GaAs–(Ga, Al)As QW have not been studied theoretically with conclusive results. The hydrostatic pressure affects various parameters of the QW, such as the width, effective mass, dielectric constant, and (for certain values) a crossing of conduction bands, changing the semiconductor from a direct band gap material to an indirect gap one [4, 5, 7].

The conduction-effective mass in the well and the barrier increases with pressure having the effect of decreasing the confinement due to the increasing of the curvature of the parabolic band. The dielectric constant decreases when one raises the pressure. This increases the impurity potential, leading to a more confined impurity carrier. The conduction-barrier height remains constant up to 13.5 kbar, in the direct bang gap regime, and then decreases monotonically to zero at 35 kbar. This effect dominates the decreasing of the confinement of the electron 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 [7, 12]. For acceptors the barrier potential does not change appreciably with the applied hydrostatic pressure [2, 3].

In the present work, we are devoted to studying the binding energy of donor and acceptor impurities in GaAs–(Ga, Al)As QWs. The binding energy is calculated as a function of the impurity position along the growth direction and for different values of the applied hydrostatic pressure. The DOIS is obtained as a function of the binding energy and from this it is possible to infer the optical response associated with donor and acceptor impurities.

2. Theoretical framework

In the effective-mass approximation, the Hamiltonian for a hydrogenic shallow-donor (or acceptor) impurity in a GaAs–$Ga_{1-x}Al_xAs$ QW under the effect of a uniaxial stress (P) in the z-direction is given by

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

Here r is the carrier-impurity distance and subscripts w and b stand for the QW and barrier layer (BL) materials, respectively. $m^*_{w,b}(P)$ are the conduction effective masses for both the QW and BL materials, as functions of P [16]. $\varepsilon_{w,b}(P)$ is the static dielectric constant in the QW and BL materials [17] and V_B (P, T, z) is the temperature (T) and pressure dependent barrier potential, which confines the electron (or the hole) in the QW [18].

In our calculations we use a variational procedure and assume an impurity trial wavefunction of the form

$$\Psi(r) = N\varphi(z)\exp(-\lambda r), \quad (2)$$

where $\varphi(z)$ is the eigenfunction of the Hamiltonian in equation (1) without the impurity term [11, 12], and N is the normalization constant.

The donor (acceptor) binding energy is calculated from the definition

$$E_b = E_0 - E_{\min}, \quad (3)$$

where E_0 is the eigenvalue related to $\varphi(z)$, and $E_{\min}$ is the energy expected value with the impurity potential term, minimized with respect to the variational parameter λ.

If the size (L) of the QW structure is not too small, one may treat the impurity position as a continuous random variable and, provided that there is no intentional doping, one can define a DOIS per unit energy as

$$g(E_i) = \frac{1}{L}\int_{S(E_i)} \frac{\mathrm{d}s}{|\nabla(E_i)|}, \quad (4)$$

where $S(E_i)$ is the surface of constant energy $E = E_i$ and ∇ means the gradient with respect to the impurity position.

In our calculations we have assumed a spherical effective mass for both donor and acceptors. Also, we have considered variations in the effective mass and dielectric constant in the well and barrier regions. We have not considered charge image effects.

In what follows, we present theoretical results for the impurity binding energy and the DOIS in a GaAs–(Ga, Al)As QW at $T = 4$ K. From our results one can infer about the origin of the peaks in the absorption and photoluminescence spectra related to impurity states.

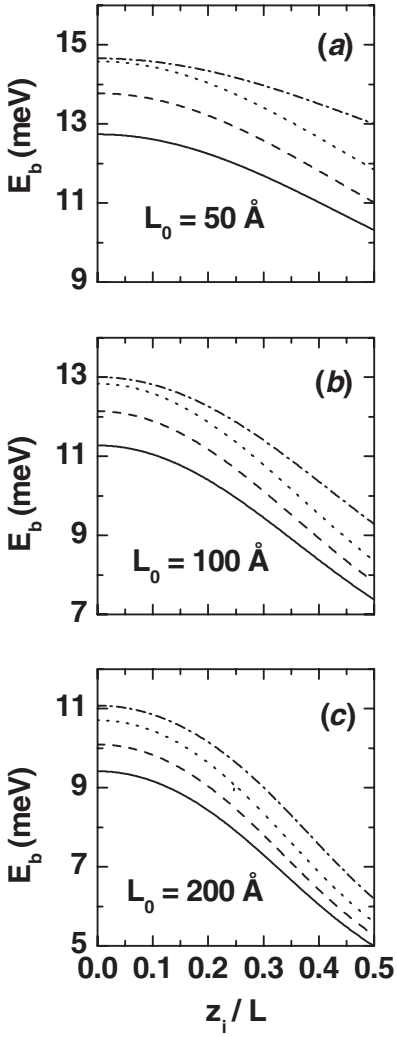

Figure 1. Binding energies of a donor impurity as a function of the impurity position along the growth direction of the GaAs–(Ga, AlAs) QWs, whose zero-pressure well sizes are 50, 100 and 200 Å. Different hydrostatic pressure values are considered: 0 kbar (solid lines), 10 kbar (dashed lines), 20 kbar (dotted lines) and 30 kbar (dashed/dotted lines).

3. Results and discussion

In figure 1 we present our results for the binding energy of a donor impurity as a function of the impurity position along the growth direction of a GaAs–(Ga, Al)As QW. Results are for different QW sizes and applied hydrostatic pressures. As is observed, the hydrostatic pressure raises the binding energy for all impurity positions inside the QW. However, for on-centre impurities the main changes are registered for low pressures (in the direct band gap regime), while for on-edge impurities the binding energy always increases with the hydrostatic pressure, with greater increments each time the well is less in width. From this behaviour of the binding energy, we can infer that the DOIS as well as the donor-related optical-absorption spectra will present peaks related to on-centre and on-edge impurities separated by 2.0–4.0 meV, approximately. As is well known, we can observe that the geometric confinement increases the binding energy. It is observed that the difference between the binding energy of on-centre and on-edge impurities increases

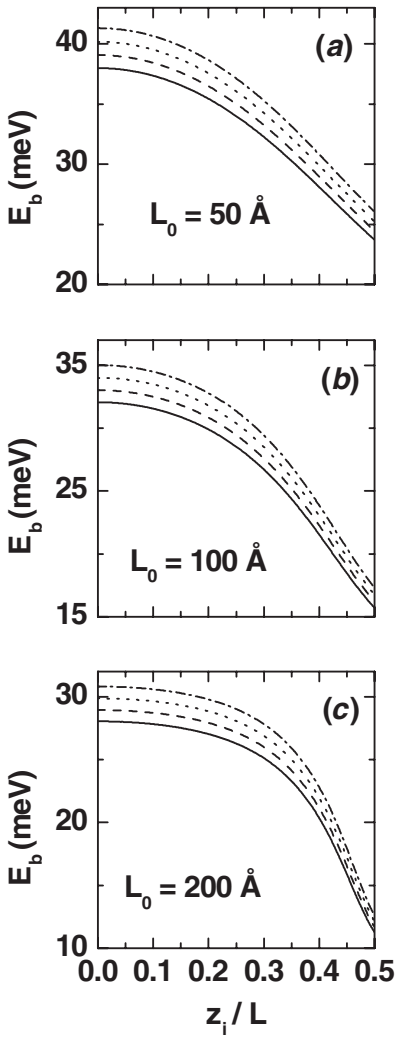

Figure 2. Binding energies of an acceptor impurity as a function of the impurity position along the growth direction of the GaAs–(Ga, AlAs) QWs. Well sizes and applied hydrostatic pressures are the same as in figure 1.

with the increment of the well width. This is due to the delocalization of the impurity wavefunction at the edge of the structure.

Analogous results for the same structures to those of figure 1, are presented in figure 2 for the binding energy of an acceptor impurity in a GaAs–(Ga, Al)As QW. As is observed, the hydrostatic pressure raises the binding energy for all impurity positions inside the QW. The main changes occur for on-centre than for on-edge impurities. This is related to the fact that the acceptor impurities have an effective Bohr radius shorter than that of the donor impurities, and for this reason they do not fill the presence of the barriers as the donors do. For any impurity position the binding energy increases linearly with the hydrostatic pressure due to the constant value of the barrier potential independently of the applied hydrostatic pressure. This result is similar to that for donor in the low-pressure regime (less than 13.5 kbar). We can expect from this behaviour of the binding energy that the DOIS as well as the acceptor-related photoluminescence spectra will present peaks related to on-centre and on-edge impurities separated by energies in the range from 14.0 to 17.0 meV,

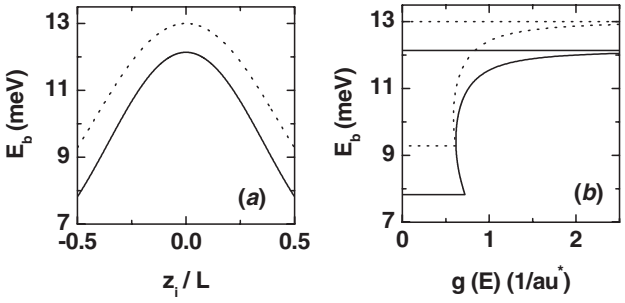

Figure 3. Binding energies of a donor impurity as a function of the impurity position along the growth direction of a GaAs–(Ga, AlAs) QW (*a*). The zero-pressure well size is 100 Å. Two values of the hydrostatic pressure are considered: 10 kbar (solid line) and 30 kbar (dotted line). In (*b*), the corresponding density of impurity states as a function of the binding energy for the two cases in (*a*).

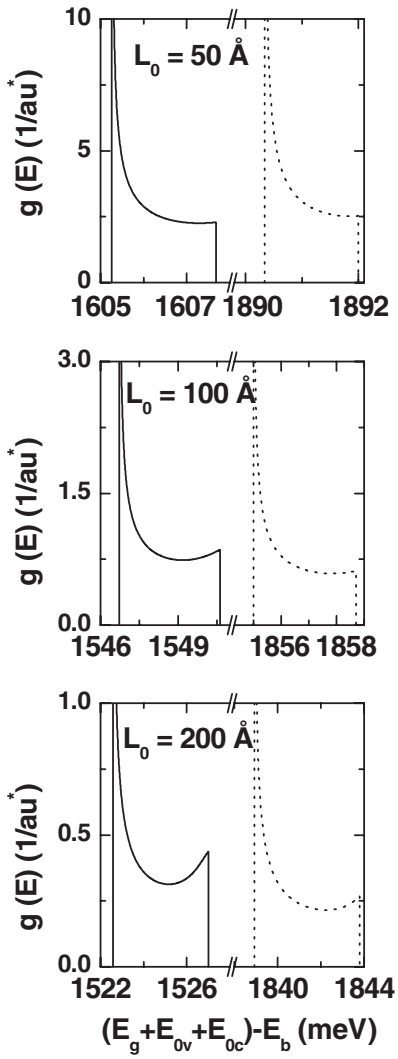

Figure 4. Density of donor impurity states as a function of the difference between the effective GaAs–(Ga, Al)As QW gap and the impurity binding energy. The well sizes are the same as in figure 1. Two values of the hydrostatic pressure are considered: 10 kbar (solid line) and 30 kbar (dotted line).

approximately. Despite the simplicity of our model in which we do not consider the coupling of the top four valence bands,

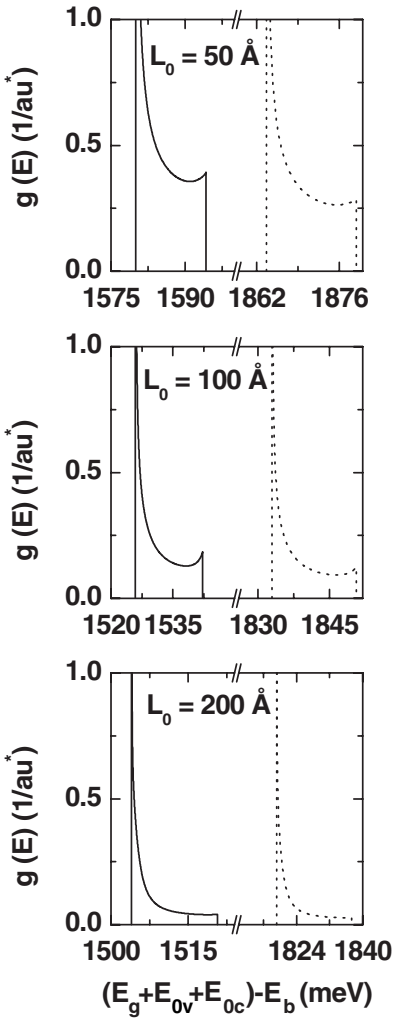

Figure 5. Density of acceptor impurity states as a function of the difference between the effective GaAs–(Ga, Al)As QW gap and the impurity binding energy. Well sizes and applied hydrostatic pressures are the same as in figure 4.

but only one spherical effective mass for both donor and acceptors, our results coincide well with the theoretical results of Masselink *et al* [2] and with the experimental results from Rune *et al* [14, 15].

The binding energy of a donor impurity as a function of the impurity position along the growth direction of a GaAs–(Ga, AlAs) QW, with zero-pressure well size of 100 Å, and the corresponding DOIS for 0 and 10 kbar are presented in figure 3. As was mentioned, in figures 1 and 2, we observe two structures in the DOIS related to on-centre and on-edge impurities. From these results we can infer a direct correspondence between the impurity position binding energy and the DOIS.

In figures 4 and 5 we display the density of donor and acceptor impurity states, respectively, as a function of the difference between the effective GaAs–(Ga, Al)As QW gap and the impurity binding energy for different well sizes and for two values of the hydrostatic pressure. We stress on the fact that the DOIS are similar for both donor and acceptor impurities, presenting two structures associated with on-centre (the main peak) and on-edge impurities. The shift in energy of the DOIS is due basically to the pressure dependence of the GaAs–(Ga, Al)As band gap.

From results in figures 4 and 5 it is expected that the impurity-related absorption and photoluminescence spectra must present two peaks associated with the on-centre and on-edge impurities corresponding to the structures of the DOIS for donors and acceptors, respectively. As the pressure increases, these spectra must be red shifted [19].

For $P = 0$ our results are in good agreement with those for an equal GaAs–$Ga_{1-x}Al_xAs$ QW reported by Santiago *et al* [20] and Oliveira and Pérez-Alvarez [21].

4. Conclusions

Summing up, using a variational procedure within the effective mass approximation, we have performed theoretical calculations related to the influence of a hydrostatic pressure on the donor and acceptor binding energy and DOIS in GaAs–(Ga, Al)As QWs. As a general feature, we observe that the binding energy increases with the pressure and with the diminishing of the well width. We have shown that there are two special structures in the DOIS, one associated with on-centre and the other with on-edge impurities. We have observed a shift to higher energies of the DOIS with the hydrostatic pressure. From these results we can infer a *redshift* for both the impurity related optical-absorption and the photoluminescence spectra due to the hydrostatic pressure. We hope that these results may be of importance in the future understanding of experimental results related to optical phenomena associated with shallow-impurities in QWs under applied pressures.

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References

[1] Bastard G 1981 *Phys. Rev.* B **24** 4714
[2] Masselink W T, Chang Yia-Chung and Morkoç H 1985 *Phys. Rev.* B **32** 5190
[3] Lefebvre P, Gil B, Mathieu H and Planel R 1989 *Phys. Rev.* B **39** 5550
[4] Burnett J H, Cheong H M, Paul W, Koteles E S and Elman B 1993 *Phys. Rev.* B **47** 1991
[5] Elabsy A M 1993 *Phys. Scr.* **48** 376
Elabsy A M 1993 *Superlatt. Microstruct.* **14** 65
Elabsy A M 1994 *J. Phys.: Condens. Matter* **6** 10025
[6] Latgé A, Porras-Montenegro N, de Dios-Leyva M and Oliveira L E 1996 *Phys. Rev.* B **53** 10160
[7] Duque C A, Morales A L, Montes A and Porras-Montenegro N 1997 *Phys. Rev.* B **55** 10721
[8] Smith J M, Klipstein P C, Grey R and Hill G 1998 *Phys. Rev.* B **57** 1740
Smith J M, Klipstein P C, Grey R and Hill G 1998 *Phys. Rev.* B **57** 1746
[9] Dai N, Huang D, Liu X Q, Mu Y M, Lu W and Shen S C 1998 *Phys. Rev.* B **57** 6566

[10] Latgé A, Porras-Montenegro N and Oliveira L E 1995 *Phys. Rev.* B **51** 13344
[11] Oyoko H O, Duque C A and Porras-Montenegro N 2001 *J. Appl. Phys.* **90** 819
[12] Morales A L, Montes A, López S Y and Duque C A 2002 *J. Phys.: Condens. Matter* **14** 987
[13] Miller R C 1984 *J. Appl. Phys.* **56** 1136
[14] Rune G C, Holtz P O, Sundaram M, Merz J L, Gossard A C and Monemar B 1991 *Phys. Rev.* B **44** 4010
[15] Rune G C, Holtz P O, Monemar B, Sundaram M, Merz J L and Gossard A C 1990 *Superlatt. Microstruct.* **7** 81
[16] Aspnes D E 1976 *Phys. Rev.* B **14** 5331
Adachi S 1985 *J. Appl. Phys* **58** R1
[17] Samara G A 1983 *Phys. Rev.* B **27** 3494
[18] Wolford D J and Bradley J A 1985 *Solid State Commun.* **53** 1069
Ehrenreich H J 1961 *J. Appl. Phys.* **32** 2155
[19] López S Y, Porras-Montenegro N and Duque C A 2003 *Phys. Status Solidi* c **0** 648
[20] Santiago R B, Oliveira L E and d'Albuquerque e Castro J 1992 *Phys. Rev.* B **46** 4041
[21] Oliveira L E and Pérez-Alvarez R 1989 *Phys. Rev.* B **40** 10460