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Effects of hydrostatic stress on the density of impurity states and donor-related optical absorption spectra in GaAs–(Ga,Al)As quantum wells

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The effects of hydrostatic stress on the density of donor impurity states and donor-related optical absorption spectra in a GaAs–(Ga,Al)As quantum well are investigated. The shallow-donor binding energy for different well widths and different values of the hydrostatic stress has been calculated. It has been found that for wider well widths the binding energy increases slowly with hydrostatic stress contrary to the behavior of the binding energy for wells with smaller widths. In particular, it has been found that the binding energy does not change appreciably with the impurity position when the width of the well is small and for large values of hydrostatic stress. Two structures in both the density of states and the optical absorption spectra, associated with impurities located close to the center and to the edges of the structure, are obtained. Also, it has been observed that the density of states and the optical absorption spectra depend strongly on the applied hydrostatic stress.

1. Introduction Carrier dynamics and recombination mechanisms in semiconductor quantum wells (QWs) have been the subject of many studies. Combined with external perturbations, such as applied electric and magnetic fields as well as stress, one can tune the electronic states with respect to one another, thus revealing the nature and extent of various interactions.

Studies of the effect of hydrostatic stress have proved to be invaluable in the context of the optical properties of semiconductors and their heterostructures [1–4]. For a given structure, the difference in energy between type I and II transitions can be tuned with external hydrostatic pressure in a continuous and reversible manner.

To date, there has been a lot of theoretical work devoted to the study of the density of impurity states and of the donor-related optical absorption spectra in GaAs–(Ga,Al)As semiconductor heterostructures [5–8]. However, there are no studies in this regard that include the effects of hydrostatic pressure in the analysis of the density of impurity states and the donor-related optical absorption spectra. For this reason in the present work we present such a study. We use a variational scheme within the effective mass approximation.

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2. Theoretical framework In the effective mass approximation, the Hamiltonian for a hydrogenic shallow-donor impurity in a GaAs–$Ga_{1-x}Al_xAs$ QW (of size L_0 at zero pressure) under the effect of a hydrostatic stress (P) is given by [4]

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

where r is the carrier–impurity distance, subscripts w and b stand for the QW and barrier layer (BL) materials, respectively, $m^*_{\mathrm{w,b}}(P)$ is the conduction effective mass for both the QW and BL materials as a function of P [9], $\varepsilon_{\mathrm{w,b}}(P)$ is the static dielectric constant in the QW and BL materials [10] and $V_{\mathrm{B}}(P, T, z)$ is the temperature- (T) and pressure-dependent barrier potential, which confines the electron (or the hole) in the QW [11].

The pressure dependence of the parameters in Eq. (1) is as follows: (i) the conduction effective mass increases with pressure having the effect of decreasing the confinement; (ii) the dielectric constant decreases with increasing pressure, leading to a more confined impurity carrier; and (iii) the conduction barrier height remains constant up to 13.5 kbar, and then decreases monotonically to zero at 35 kbar. This last effect dominates the decreasing of the confinement of the electron for pressures greater than 13.5 kbar.

We use a variational procedure and assume an impurity trial wave function of the form

$$\Psi(r) = N\varphi(z)\exp(-\lambda r)\,, \tag{2}$$

where $\varphi(z)$ is the eigenfunction of the Hamiltonian in Eq. (1) without the impurity term at the right [4], and N is the normalization constant.

The donor binding energy is calculated from the definition

$$E_{\mathrm{b}} = E_0 - E_{\min}\,, \tag{3}$$

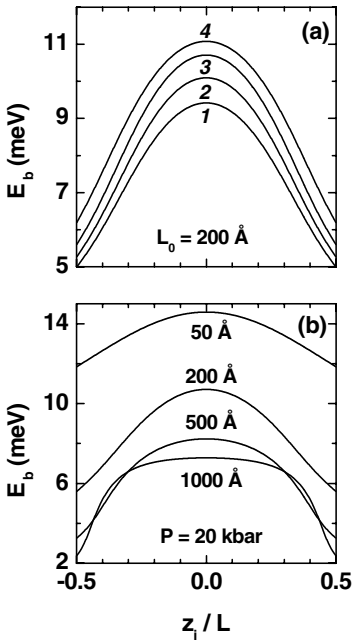
where E_0 is the eigenvalue related to the $\varphi(z)$ eigenfunction and $E_{\min}$ is the eigenvalue with the impurity potential term, minimized with respect to the variational parameter λ.

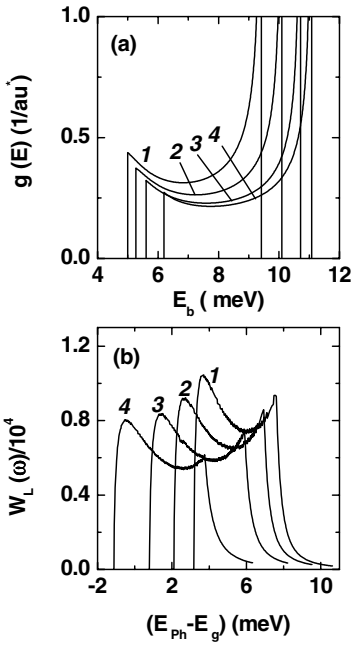
The transition probability per unit time for valence-to-donor transitions is given by [5]

$$W \approx \sum_i \left[\int_\Omega \mathrm{d}\boldsymbol{r}\; u^*_f(\boldsymbol{r})\, \boldsymbol{e}\cdot\boldsymbol{p}u_i(\boldsymbol{r}) \int \mathrm{d}\boldsymbol{r}\; F^*_f(\boldsymbol{r})\, F_i(\boldsymbol{r})\right]^2 \delta(E_f - E_i - \hbar\omega)\,. \tag{4}$$

In what follows, we present theoretical results for a GaAs–(Ga,Al)As QW at 4 K.

3. Results and discussion Figure 1 shows the results for the binding energy of a donor impurity as a function of the impurity position along the growth direction. Figure 1a shows the results for L_0 = 200 Å and for different values of the hydrostatic pressure. As it is observed, the hydrostatic pressure increases the binding energy mainly for on-center impurities rather than for on-edge ones. From this behavior of the binding energy we can infer that the density of impurity states as well as the donor-related optical absorption spectra will show peaks related to on-center and on-edge impurities separated by approximately 4.5 meV. Figure 1b shows the results for a hydrostatic pressure of 20 kbar and different well widths. It is observed that for this pressure the geometric confinement increases the binding energy. We note that the difference between the binding energy of on-center and on-edge impurities increases with increasing well width. This is because as the well width increases the impurity wave function is less localized at the edge of the structure. Also, with the increase of the well width there is an increase in the separation in the structures of the density of impurity states and in the absorption spectra.





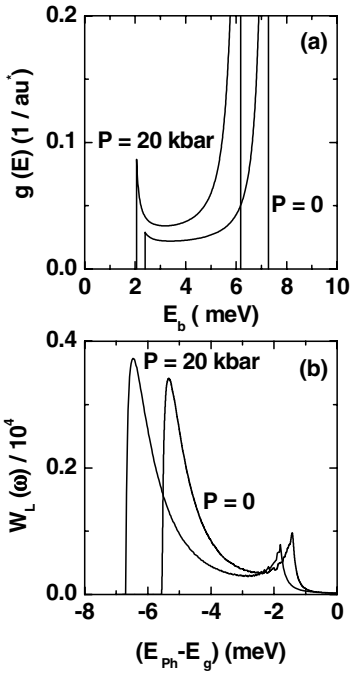


Fig. 1 **Fig. 2** **Fig. 3**

Fig. 1 Binding energies of a donor impurity as a function of the impurity position along the growth direction of the well: a) L_0 = 200 Å, hydrostatic pressure = 0, 10, 20, and 30 kbar, denoted by 1, 2, 3, and 4, respectively; b) hydrostatic pressure = 20 kbar at various well widths.

Fig. 2 a) Density of impurity states as a function of the binding energy and b) donor-related optical absorption spectra as a function of the difference between the photon energy and the gap energy for a donor impurity in a GaAs–$Ga_{1-x}Al_xAs$ QW for four values of the applied hydrostatic pressure: 0, 10, 20, and 30 kbar, denoted by 1, 2, 3 and 4, respectively (L_0 = 200 Å).

Fig. 3 a) Density of impurity states as a function of the binding energy and b) donor-related optical absorption spectra as a function of the difference between the photon energy and the gap energy for a donor impurity in a GaAs–$Ga_{1-x}Al_xAs$ QW for two values of the applied hydrostatic pressure: 0 and 20 kbar, respectively (L_0 = 1000 Å).

Figure 2 shows the density of impurity states as a function of the binding energy (Fig. 2a) and optical absorption spectra as a function of the difference between the photon energy and the gap energy (Fig. 2b) for a donor impurity in a GaAs–$Ga_{1-x}Al_xAs$ QW (L_0 = 200 Å) for different values of the applied hydrostatic pressure. For this well width, as expected, it is observed that the center of gravity of the density of states is closed to energies corresponding to on-center impurities, while the structure at the lowest energy values is related to on-edge impurities. A similar situation is observed for the absorption spectra. That is, for each pressure the peak at the left-hand side is the one related to on-center impurity transitions and the one at the right-hand side corresponds to on-edge impurities. It can be seen that the dependence of the band-gap energy with the pressure is reflected in the shifting of the spectra to lower energies.

In order to illustrate the behavior in the bulk limit, Fig. 3 shows similar results to those of Fig. 2 but for a GaAs–$Ga_{1-x}Al_xAs$ QW with L_0 = 1000 Å, for two values of the applied hydrostatic pressure. As expected, the structure associated with on-center impurities is dominant over that related to on-edge impurities. One of the roles of the hydrostatic pressure is to increase the intensity of the structure related to on-center impurities and to shift the entire spectrum to lower energy values. It is well to mention that for P = 20 kbar the spectra correspond to indirect transitions.

4. Conclusions Theoretical calculations related to the influence of hydrostatic pressure on the donor binding energy, density of impurity states, and donor-related optical absorption spectra in GaAs–(Ga,Al)As QWs are presented. As a general feature, we observe that the binding energy increases with the pressure and with decreasing well width. We have shown that there are two special structures in the density of impurity states and in the donor-related optical absorption spectra: an edge associated with transitions involving impurities at the center of the well and a peak associated with transitions related to impurities at the edges of the well. We have observed a shift to higher energies of the density of impurity states as a function of the binding energy and a change in the intensity with a red shift of the absorption spectra with hydrostatic pressure.

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