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EFFECT OF THE Γ-X CROSSOVER ON THE BINDING ENERGY OF SHALLOW-DONOR IMPURITIES IN RECTANGULAR GAAS-(GA,AL)AS QUANTUM DOTS

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ABSTRACT

Theoretical calculations related with the influence of the Γ-X crossover on the binding energy of shallow-donor impurities in GaAs-(Ga,Al)As quantum dots are presented. A variational procedure within the effective mass approximation is considered. As a general feature, we observe that the binding energy increases as the length of the well decreases. For the low-pressure range we observe a linearly binding energy behavior, whereas for the high pressure range the effects of the barrier height bend the binding energy curves toward smaller values.

INTRODUCTION

Studies under hydrostatic stress have proven to be invaluable in the context of the optical properties of semiconductors and their heterostructures [1, 2]. For a given structure, the difference in energy between the type-I and –II transitions can be tuned with external hydrostatic pressure in a continuos and reversible manner, thus enabling an elucidation of the properties of various interband transitions.

The effect of the Γ-X crossover on the lowest energy states and on the binding energies of confined donors in single $GaAs/Al_xGa_{1-x}As$ quantum wells have been reported by Elabsy [3]. He has obtained that the Γ-X crossing changes the energies of donor dramatically, especially when the hydrostatic pressure reaches the Γ_w-X_b crossover point. Oyoko et al. [4] have calculated the uniaxial stress dependence of the binding energy of shallow-donor impurities in GaAs-(Ga,Al)As quantum dots (QDs) finding 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 center of the structure.

In this work we are concerning with the theoretical calculations about the effects of an applied hydrostatic stress on the binding energy of shallow-donor impurities in GaAs-(Ga,Al)As QDs. Calculations are including the Γ-X crossing which induces the linear (below to 13.5 kbar) to non-linear (upper to 13.5 kbar) regimes on the binding energies. In our calculations we use a variational scheme within the effective mass approximation. In Sec. II we present the theory of the problem. Our results are presented and discussed in Sec. III, and our conclusions are given in Sec. IV.

THEORETICAL FRAMEWORK

In the effective-mass approximation, the Hamiltonian for a hydrogenic shallow-donor impurity in a $GaAs$-$Ga_{1-x}Al_xAs$ QD under the effect of a *z*-uniaxial stress (*P*) for low temperature (*T*) is given by

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

where r is the carrier-impurity distance and subscripts w and b stand for the QD and the barrier layer (BL) materials, respectively. $m^*_{w,b}(P,T)$ are the QD and BL materials conduction effective-masses as functions of P and T [3, 5, 6]. $\varepsilon_{w,b}(P,T)$ is the static dielectric constant in the QD and BL materials, respectively [6, 7], and $V_B(x, y, z, P, T)$ is the barrier potential which confines the donor electron in the QD, given by

$$V_B(x,y,z,P,T) = \begin{cases} 0 & \text{, for } |z| \le L_z(P)/2 \text{ with } |x| \le L_x/2 \text{ and } |y| \le L_y/2 \\ V_0(P,T) & \text{, for } |z| \ge L_z(P)/2 \text{ with } |x| \le L_x/2 \text{ and } |y| \le L_y/2 \\ \infty & \text{, for } |x| \ge L_x/2 \text{ with } |y| \ge L_y/2 \end{cases} \qquad [2]$$

Where

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

with P_1 the crossover pressure between the X_b conduction band and the Γ_b band, P_2 the crossover pressure between the X_b conduction band and the Γ_w band, S_0 (= 250 meV) [3] an adjustable parameter which is used to match the predicted energy at P_1 with the experimental result, and x (= 0.3 in this work) the aluminum molar fraction. The conduction- and valence-band parameters in this work are taken from photoluminiscence measurements [8]. In eq. (2), L_x, L_y, and $L_z(P)$ give the dimensions of the QD in the respective directions.

The trial wave function is chosen as [9, 10]

$$\Psi(x,y,z) = N\, f(r)\, g(r) \qquad [4]$$

Where

$$g(r) = exp(-\lambda\, r) \qquad [5]$$

is the hydrogenic part and

$$f(r) = cos(\pi\, x / L_x)\, cos(\pi\, y / L_y)\, h(z) \qquad [6]$$

With

$$h(z) = \begin{cases} cos(\eta\, z) & \text{, for } |z| < L_z/2 \\ cos(\eta\, L_z/2)\, exp[\beta(L_z/2 - z)] & \text{, for } z \ge +L_z/2 \\ cos(\eta\, L_z/2)\, exp[\beta\,(L_z/2 + z)] & \text{, for } z \le -L_z/2 \end{cases} \qquad [7]$$

and N is the normalization constant.

The uniaxial stress dependence of the donor binding energy is calculated from the definition

$$E_b(P) = E_0(P) - E_{\min}(P)\text{ ,} \qquad [8]$$

where E_0 is the eigenvalue of Hamiltonian in eq. (1) without the impurity potential term at the right, and E_{min} is the eigenvalue with the impurity potential term, minimized with respect to the variational parameter λ.

RESULTS

In the present study we are considering the effects of uniaxial stress [7, 8] on the binding energy of shallow-donor impurities in GaAs-(Ga,Al)As QDs. The stress on its own affects various parameters of the QD like the $L_z(0)$ length, the effective mass, the 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, $L_z(0)$ decreases leading to more confinement of the impurity electron. The effective mass in the well and in the barrier also increases with pressure having the effect of decreasing the confinement due to the larger curvature of the parabolic band. The dielectric constant decreases with increasing pressure producing an increase in the impurity potential leading to a more bound impurity electron (confinement of the impurity). The barrier height remains constant up to a pressure value of 13.5 kbar, in the direct bang gap regime, and then decreases monotonically to zero at a pressure of 35 kbar. This effect dominates the decrease in the confinement of the impurity for pressures larger than 13.5 kbar since the barrier height decreases from 240 meV, at 13.5 kbar, to 40 meV at 33 kbar. 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.

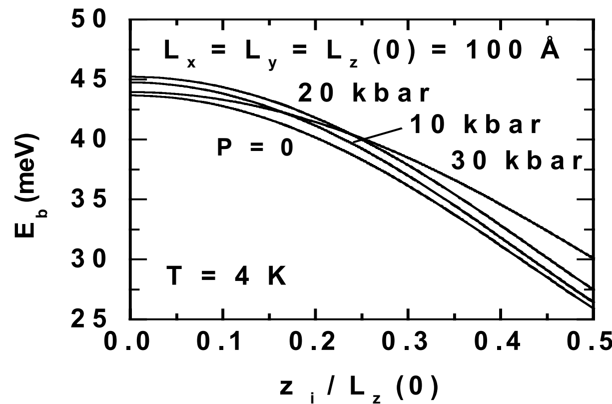

Figure 1. Binding energy for a shallow-donor impurity in a cubic-shaped GaAs-(Ga,Al)As QD as a function of the impurity position along the z-direction. The zero limit and three different values of the applied stress are presented.

In fig. 1 we present our results for the binding energy of a shallow-donor impurity in a rectangular-shaped GaAs-(Ga,Al)As QD as a function of the impurity position along the z-direction of the structure. Results are for the zero limit and for three different values of the z-direction applied stress. In each case, the binding energy for on-edge impurity is lower than for the on-center impurity. This effect is due to the repulsion of the wave

function by the potential barrier. For increasing stress up to 20 kbar, we observe an increasing in the binding energy due to the diminishing in L_z-dimension of the structure. Additionally, when the impurity is located close to the center of the structure the binding energy starts to decrease as the stress is increased upper to 20 kbar

CONCLUSIONS

Theoretical calculations related with the influence of an applied stress on the binding energy of shallow-donor impurities in rectangular-shaped GaAs-(Ga,Al)As QDs are presented. A variational procedure within the effective mass approximation is considered. The pressure related Γ-X crossover is taken in account.

The results of this work show that the binding energy of a donor impurity in a QD depends on the applied stress, on the size of the dot, and on the donor position along the *z*-axis inside the dot. It is important, therefore, that in experimental studies on GaAs-(Ga,Al)As heterostructures such as density of impurity states and impurity-related optical absorption spectra, considerations should be given to the effect of the applied stress and the impurity positions on the donor binding energy.

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