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SHALLOW DONOR IMPURITIES IN GAAS-(GA,AL)AS QUANTUM DOTS: THE UNIAXIAL STRESS AND TEMPERATURE DEPENDENCIES

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ABSTRACT

Using a variational procedure and considering the effective mass approximation, we have make a theoretical study about the effects of an uniaxial stress and the temperature on the binding energy of a shallow donor impurity in a parallelepiped-shaped GaAs-(Ga,Al)As quantum dot. Our results show that the donor binding energy increases with increasing stress and for decreasing sizes of the quantum dot. Also, we have found that the binding energy for various values of the donor position along the z-axis for constant quantum well box size increases with the proximity of the impurity to the center of the structure. Moreover, we obtain the shallow-donor binding energies as functions of uniaxial stress not only in the limit of low stress, but in the situations in which the quantum dot turns into either in a quantum well or in a quantum-well wire.

INTRODUCTION

Using the masked implantation enhanced intermixing technique (MIEI), and the dry etching technique with subsequent overgrowth, Schweizer et al [1] have realized rectangular transversal section GaAs-(Ga,Al)As quantum-well wires (QWWs) and quantum dots (QDs). With the MIEI technique, wire structures down to 40 nm and dot structures down to a radius of 100 nm could be achieved, and several effects, like stress on low dimensional heterostructures, could be experimentally studied.

The man-made diamond anvil cell (DAC) [2] and the use of low-temperature photoluminescence measurements made it possible to study the electronic and optical properties of microstructure semiconductors such as GaAs/$Al_xGa_{1-x}As$ quantum wells (QWs) under high hydrostatic pressure. These structures have had a considerable number of studies made on their optical and electronic properties under atmospheric pressure [3] and high hydrostatic pressure [4].

In the present work we report on theoretical calculations of the binding energy of shallow donor impurities in parallelepiped-shaped QDs, when under the effect of uniaxial stress. Calculations are performed using the effective-mass approximation within a variational scheme. The QD structures we consider are of interest for experimentalist groups due to the realistic dimensions and shape [1]. This work is organized as follows. In section II the model calculation is presented. Section III is devoted to results and discussion, and in section IV we present our conclusions.

THEORETICAL FRAMEWORK

In the effective-mass approximation, the Hamiltonian for a hydrogenic shallow-donor impurity in a cubic-shaped GaAs-Ga$_{1-x}$Al$_x$As QD under the effect of a uniaxial stress (*P*) in the z-direction and for low temperature (*T*), is given by

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

where *r* is the carrier-impurity distance and subscripts *w* and *b* stand for the QW 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* [5]. $\varepsilon_{w,b}(P,T)$ is the static dielectric constant in the QD and BL materials, respectively [5, 6] and V_B is the barrier potential which confines the donor electron in the QD [7].

The trial wave function for the ground state is chosen as [8, 9]

$$\Psi(x,y,z) = N\, f(r)\, g(r) \tag{2}$$

Where

$$g(r) = exp(-\lambda\, r) \tag{3}$$

is the hydrogenic part and

$$f(r) = cos(\pi x / L_x)\, cos(\pi y / L_y)\, h(z) \tag{4}$$

With

$$h(z) = \begin{cases} cos(\eta\, z) & \text{, for } |z| < L_z/2 \\ cos(\eta\, L_z/2)\, exp[\beta(L_z/2 - z)], & \text{for } z \geq +L_z/2 \\ cos(\eta\, L_z/2)\, exp[\beta\,(L_z/2 + z)], & \text{for } z \leq -L_z/2 \end{cases} \tag{5}$$

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

$$E_b(P) = E_0(P) - E_{\min}(P) \tag{6}$$

Where $E_0(P)$ is the eigenvalue of Hamiltonian in eq. (1) without the impurity potential term at the right, and $E_{\min}(P)$ is the eigenvalue with the impurity potential term, minimized with respect to the variational parameter λ. For details of the calculation we refer to ref. 7.
As follow, we present our theoretical results for the binding energy for shallow donor impurities in GaAs-(Ga,Al)As QDs at T = 4 K

RESULTS AND DISCUSSIONS

In fig. 1, we present our theoretical results for the binding energy of a shallow-donor impurity in a parallelepiped-shaped GaAs-(Ga,Al)As quantum dot as a function of the $L_z(0)$-side of the structure considering different values of the stress along the z-direction. In (a) results are for the on-center interface-impurity, whereas those in (b) are for the on-center impurity. In both cases, (a) and (b), we note that the binding energy diminishes as $L_z(0)$ increases. This is due to the fact that the wave function is more spread along the z-direction because the potential barriers are far away. Additionally, the higher effect due to the external stress is observed when the impurity is on-center located [see fig. 1(b)]. In fact, when the impurity is close to one of the potential barriers (interfaces), the effect of the opposite barrier on the impurity is lower. However, when the impurity is on-center located, the effect of both opposite barriers is enhanced, i.e., the effect of the compression due to the applied stress will be stronger at the on-center impurity.

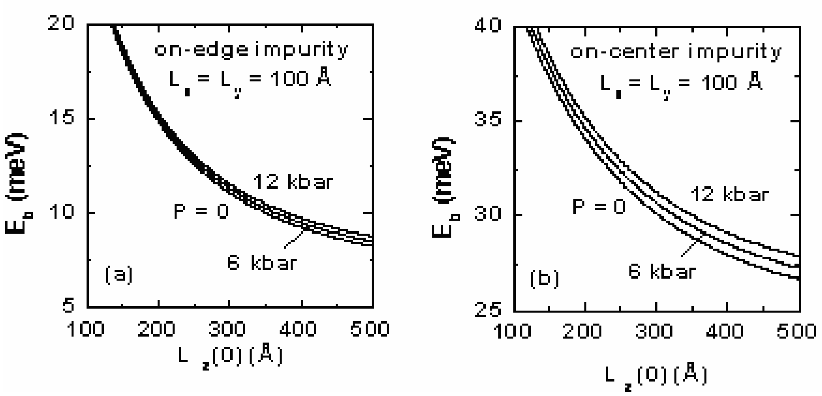

Figure 1. Binding energy for a shallow-donor impurity in a parallelepiped-shaped GaAs-(Ga,Al)As quantum dot as a function of the $L_z(0)$ - thickness of the structure.

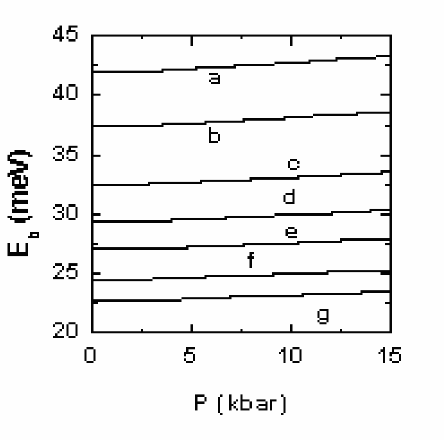

Figure 2. Binding energy of shallow-donor impurity in a parallelepiped–shape GaAs-(Ga,Al)As quantum dot as a function of the stress applied in the z-direction for different values of the box size (L_x, L_y, L_z): (100, 100, 100) Å (curve a), (150, 150, 100) Å (curve b), (100, 100, 150) Å (curve c), (150, 150, 150) Å (curve d), (200, 200, 150) Å (curve e), (150, 150, 200) Å (curve f), and (200, 200, 200) Å (curve g).

In Fig. 2 we present the binding energy of a shallow-donor impurity in a parallelepiped-shape GaAs-(Ga,Al)As QD as a function of the stress applied in the z-direction and considering different values of the box size (L_x, L_y, L_z). The binding energy shows a nearly linear increase with applied stress. Additionally, it is clear that as the size of the structure increases the slope of the curve goes to zero. This is because the wave function does not feel the small compression in the structure when the size of the structure is very large.

CONCLUSIONS

The results of this work show that the binding energy of a donor impurity in a quantum dot increases almost linearly with applied stress and diminishes with the size of the structure. Also, we have 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 center of the structure. It is important, therefore, that in experimental studies on GaAs-(Ga,Al)As heterostructures such as the 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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