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Spatially dependent screening calculation of binding energies of hydrogenic impurity states in GaAs-$Ga_{1-x}Al_xAs$ quantum wells

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The effect of spatially dependent screening is taken into account with an r-dependent dielectric response to evaluate the binding energies of shallow hydrogenic impurity states in GaAs-$Ga_{1-x}Al_xAs$ quantum wells. A variational calculation, in the effective-mass approximation, was performed as a function of the position of the impurity in a quantum well of finite depth and for various well thicknesses. It is shown that spatially dependent screening effects can be quite important for acceptors in a GaAs-$Ga_{1-x}Al_xAs$ quantum well due to the relatively small effective Bohr radius (~ 22 Å) of the hole. The binding energies of on-edge impurities are shown to increase, for sufficiently large well thicknesses, when the barrier potential (or the Al concentration) decreases, a behavior which contrasts with results previously reported in the literature.

I. INTRODUCTION

In the past few years, a great deal of interest has been shown in the properties of hydrogenic impurities in quantum wells and superlattices. Bastard[1] was the first to treat this problem theoretically by considering a hydrogenic impurity in a quantum well with infinite-barrier height and assuming a parabolic conduction band: The binding energy of hydrogenic impurities was found to vary with the position of the impurity in the well and with the well thickness. The pioneering work by Bastard was followed by several other calculations. Mailhiot *et al.*[2] and Greene and Bajaj[3] independently calculated the energies of the ground state and a few excited states of a hydrogenic impurity in a GaAs-$Ga_{1-x}Al_xAs$ quantum well using a variational method and taking into consideration the finite size of the well barrier. Mailhiot *et al.*[2] further considered the problem of effective-mass and dielectric-constant mismatches at the well interfaces. The complex structure of the valence band in the case of acceptors was taken into account by Masselink *et al.*[4] and the effect of nonparabolicity of the conduction band for an on-center donor in a finite quantum well was considered by Chaudhuri and Bajaj.[5] The effect of spatially dependent screening in the case of an infinite-barrier height was studied by Csavinszky and Elabsy[6] for donors and by Oliveira and Falicov[7] for donors and acceptors. Experimentally, the first observation of impurity-related (acceptor) features in the optical spectra was reported by Miller *et al.*[8] in nonintentionally doped molecular-beam-epitaxy(MBE)-grown GaAs-(Ga,Al)As quantum wells. Recently, various experimental measurements of the properties of donors in GaAs-(Ga,Al)As quantum wells have been reported.[9–11] A detailed list of theoretical and experimental work on hydrogenic impurities in quantum wells can be found in recent reviews on the subject.[12–16]

In this paper we report a variational calculation in the effective-mass approximation of the binding energies of shallow donors and acceptors in GaAs-(Ga,Al)As quantum wells. Calculations are performed as functions of the position of the impurity in a GaAs quantum well of finite depth and for various slab thicknesses. Further, the effect of spatially dependent screening[7] is analyzed with an r-dependent dielectric response characteristic of bulk GaAs.

II. THEORY

The Hamiltonian of a shallow hydrogenic impurity in a GaAs quantum well sandwiched between two semi-infinite slabs of $Ga_{1-x}Al_xAs$ can be written, in the effective-mass approximation, as

$$H=-\frac{\hbar^2\nabla^2}{2m^*}-\frac{e^2}{\epsilon(r)[\rho^2+(z-z_i)^2]^{1/2}}+V(z)\ , \qquad (2.1)$$

where the barrier potential $V(z)$ is taken to be a square well of height V_b and width L,

$$V(z)=\begin{cases}0, & |z|<L/2\\ V_b, & |z|>L/2\ .\end{cases} \qquad (2.2)$$

We assume that the band-gap discontinuity[17,18] in the GaAs-$Ga_{1-x}Al_xAs$ heterostructure is distributed about 40% on the valence band and 60% on the conduction band with the total band-gap difference, ΔE_g, between GaAs and $Ga_{1-x}Al_xAs$, given as a function of the Al concentration $x<0.45$ as[19]

$$\Delta E_g(\text{eV})=1.247x\ . \qquad (2.3)$$

The position of the impurity is denoted by z_i with respect to the $z=0$ origin chosen at the center of the well, $r=[\rho^2+(z-z_i)^2]^{1/2}$ with $\rho=(x^2+y^2)^{1/2}$ is the distance from the carrier to the impurity site, and

$$\epsilon^{-1}(r)=\epsilon_0^{-1}+(1-\epsilon_0^{-1})\exp(-r/a) \qquad (2.4)$$

is the spatially dependent dielectric screening,[7,20–22]

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characteristic of bulk GaAs ($a \sim 1.1$ a.u.), used in the calculation.

Although the effective mass, m^*, and the dielectric constant, ϵ, vary across the boundary between the two materials, GaAs and $Ga_{1-x}Al_xAs$, we follow Greene and Bajaj[3] and assume the values of m^* and ϵ in GaAs for all regions of the heterostructure. This is a reasonably good approximation since the carrier is to a large extent confined in the GaAs layer due to the large barrier heights. In the case of acceptors, we neglect the effect of coupling of the top four valence bands[4] of both semiconductors and consider a spherical carrier effective mass $m^* \sim 0.30 m_0$ (m_0 is the free-electron mass) which gives a bulk value[8,23] of 26 meV for the acceptor binding energy.

We follow the variational approach of Bastard[1] and assume a trial wave function of the form

$$\psi(\mathbf{r}) = \begin{cases} e^{k_1(z+L/2)}\Gamma(\rho,z,z_i,\lambda), & z \le -L/2 \\ \alpha\cos(k_2 z)\Gamma(\rho,z,z_i,\lambda), & -L/2 \le z \le L/2 \\ e^{-k_1(z-L/2)}\Gamma(\rho,z,z_i,\lambda), & z \ge L/2 \end{cases} \tag{2.5}$$

where λ is a variational parameter,

$$k_1 = [2m^*(V_b - E_0)]^{1/2}/\hbar \ , \tag{2.6a}$$

$$k_2 = (2m^* E_0)^{1/2}/\hbar \ , \tag{2.6b}$$

$$\alpha = 1/\cos(k_2 L/2) \ , \tag{2.6c}$$

$$\Gamma(\rho,z,z_i,\lambda) = \exp\{-[\rho^2 + (z - z_i)^2]^{1/2}/\lambda\} \ , \tag{2.6d}$$

and $E_0 = E_0(V_b, L)$ is the ground-state energy of the above Hamiltonian without the impurity potential term, which is determined by numerically solving the transcendental equation,

$$(V_b/E_0 - 1)^{1/2} = \tan[(2m^* E_0)^{1/2} L/2\hbar] \ . \tag{2.7}$$

Notice that the above trial wave function corresponds to the eigenfunction of the Hamiltonian in (1.1) without the impurity potential and a hydrogenic-type 1s function containing the variational parameter λ and is therefore expected to represent appropriately the actual shallow-impurity state in the $GaAs$-$Ga_{1-x}Al_xAs$ quantum well.

The trial impurity ground-state energy,

$$\epsilon(L,z_i) = \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle \tag{2.8}$$

is then minimized with respect to λ. All necessary integrals in (2.8) are performed analytically and only the minimization requires numerical handling. The impurity binding energy is then given by

$$E(L,z_i) = E_0 - \epsilon(L,z_i) \ , \tag{2.9}$$

where the first term corresponds to the energy of a free electron (hole) at the bottom (top) of the conduction (valence) band.

In the following section we sometimes use reduced atomic units which correspond to a length unit of one effective Bohr radius $a_0^* = \hbar^2\epsilon_0/m^*e^2$, and an energy unit of one effective Rydberg $R_0^* = m^*e^4/2\hbar^2\epsilon_0^2$. For GaAs, these units are $a_0^* \simeq 100$ Å and $R_0^* \simeq 5.72$ meV for donors (electrons), and $a_0^* \simeq 22$ Å and $R_0^* \simeq 26$ meV for acceptors (holes).

III. RESULTS AND DISCUSSION

In Fig. 1 we present the binding energies $E(L, z_i = 0)$ for shallow donors and acceptors at the center of a $GaAs$-$Ga_{1-x}Al_xAs$ quantum well as functions of the well thickness and for three Al concentrations ($x = 0.15$, 0.30, and 0.45). Figure 1 also shows, for comparison, the results corresponding to the infinite-potential-barrier height. In the case of on-center donors, for example, for $L = 100$ Å and $x = 0.30$ ($V_b = 224$ meV), the calculated binding energy is 11.7 meV to be compared with a value of 13.0 meV for an infinite barrier [cf. Fig. 1(a)]. For on-center acceptors, $L = 100$ Å and $x = 0.30$ ($V_b = 150$ meV), the corresponding binding energies are 34.6 meV and

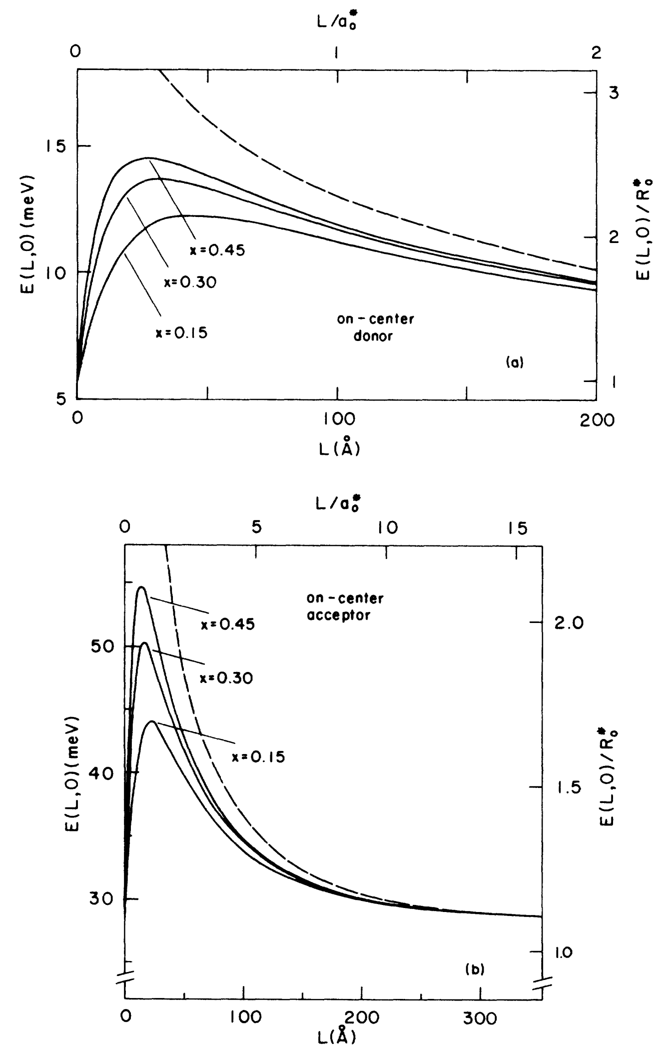

FIG. 1. Thickness dependence of the on-center donor (a) and acceptor (b) binding energies in a $GaAs$-$Ga_{1-x}Al_xAs$ quantum well for various Al concentrations. The dashed lines correspond to the GaAs quantum well of infinite depth. Results were obtained including the effect of a spatially dependent $\epsilon^{-1}(r)$ screening.

36.4 meV, respectively [cf. Fig. 1(b)]. At the zero-thickness limit ($L=0$) in the case of a finite barrier, the electron (hole) wave function is entirely in $Ga_{1-x}Al_xAs$ and one recovers the bulk value for the binding energy of a donor (acceptor) in this material.[2,3] Of course, for thick wells ($L \gg a_0^*$), all curves in Figs. 1(a) and 1(b) go to the same limit, i.e., the bulk binding energy of a donor or acceptor in GaAs. It should be mentioned that all results in Fig. 1 were obtained including the effect of a spatially dependent $\epsilon(r)$ dielectric function which, as opposed to a dielectric constant ϵ_0, leads to an increase of the binding energy of the impurity[7] [for $L=100$ Å and $x=0.30$, the increase in the binding energy is ~ 0.1 meV (2.0 meV) for the on-center donor (acceptor)]. It is clear, therefore, that spatially dependent screening effects can be quite important for acceptors due to the relatively small (hole) effective Bohr radius ($a_0^* \sim 22$ Å) while these effects are essentially negligible for shallow donors in a GaAs-$Ga_{1-x}Al_xAs$ quantum well because of the large (electron) effective Bohr radius ($a_0^* \sim 100$ Å).

The thickness dependence of the on-edge ($z_i=L/2$) donor and acceptor binding energies in a GaAs-$Ga_{1-x}Al_xAs$ quantum well is shown in Fig. 2 for Al concentrations of $x=0.15$, 0.30, and 0.45. It is clearly seen that, for a given well width L, the binding energies of on-edge donors and acceptors in a GaAs-$Ga_{1-x}Al_xAs$ quan-

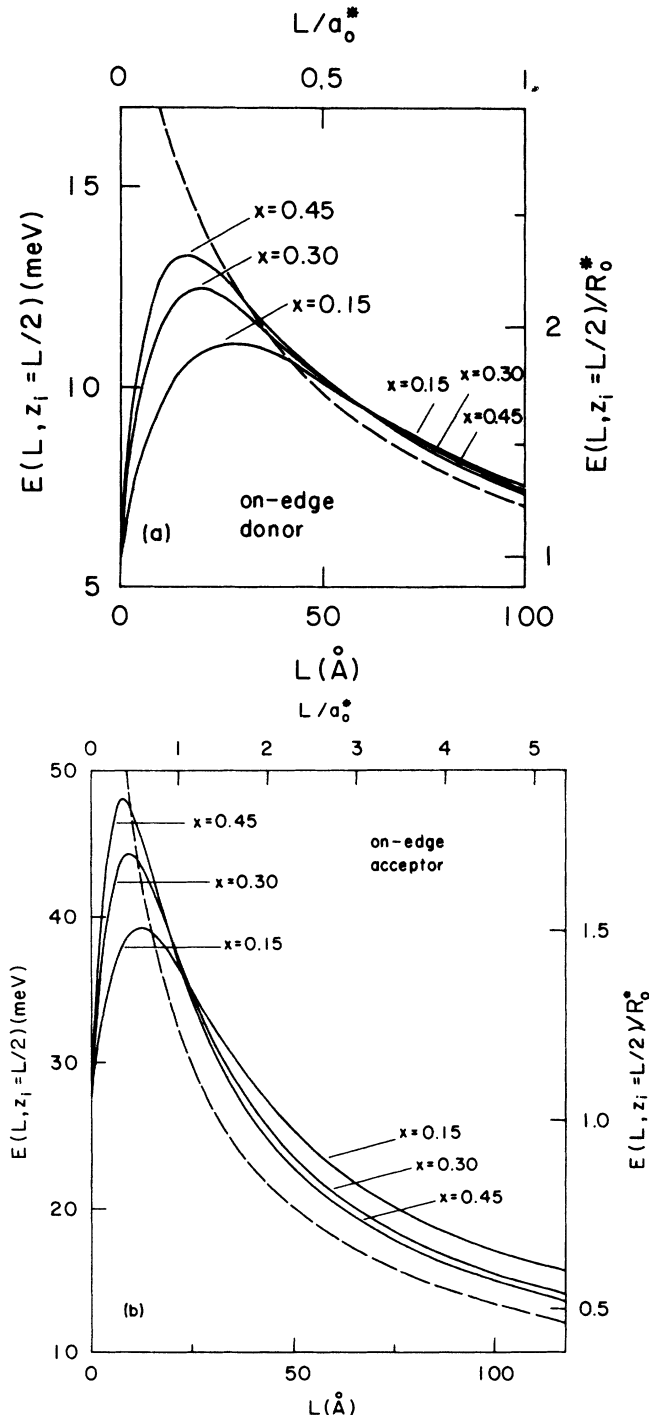

FIG. 2. Thickness dependence of the on-edge donor (a) and acceptor (b) binding energies in a GaAs-$Ga_{1-x}Al_xAs$ quantum well for various Al concentrations. The dashed lines correspond to the GaAs quantum well of infinite depth. Results were obtained including the effect of a spatially dependent $\epsilon^{-1}(r)$ screening.

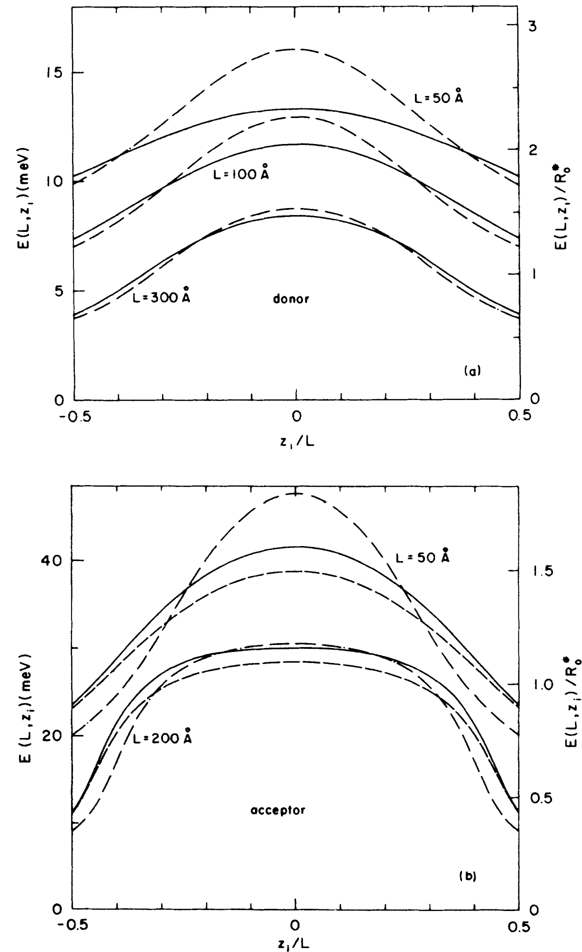

FIG. 3. Binding energies for the ground state of a donor (a) or acceptor (b) as functions of the impurity position z_i within the GaAs-$Ga_{1-x}Al_xAs$ quantum well, for various quantum-well thicknesses. The Al concentration x is 0.30. The solid curves are for spatially dependent $\epsilon=\epsilon(r)$ and finite-barrier potentials; the dash-dotted curves are for spatially dependent screening and infinite depth barriers; the dashed curves in (b) are for constant screening $\epsilon=\epsilon_0$ and finite-barrier potentials.

tum well *increase* as the concentration of Al (or the barrier potential) *decreases,* provided that the quantum-well width is not too small. Also, the results associated to the *infinite* potential barrier (dashed lines in Fig. 2) correspond, for L not too small, to *smaller* on-edge binding energies than for *finite* barriers. As is well known,[1,24] in the case of an infinite potential barrier, the large-L limit of the binding energies of on-edge impurities is $R_0^*/4$. Moreover, for $L \rightarrow \infty$ and vanishingly small ($x \rightarrow 0$) Al concentrations (or barrier potentials) one should obtain the limiting value of R_0^* for the binding energy of on-edge impurities.[3] Therefore, the binding energies of *on-edge* impurities should, for sufficiently large L, *increase* when the barrier potential (or the Al concentration) *decreases* (cf. Fig. 2). This behavior for the binding energies of on-edge impurities is *not* in agreement with the results displayed in Fig. 7 of Mailhiot *et al.*[2] (or Fig. 5 of the review by Shanabrook[15]) and also contrasts with the results shown in Fig. 1 of Bastard's review[13] (or Fig. 2 of the review by Delalande[14]). On the other hand, Greene and Bajaj[12] obtained, in the case of on-edge donors and $V_b = 323$ meV, values for the binding energies of about $1.95R_0^*$ (for $L = 50$ Å) and about $1.40R_0^*$ (for $L = 100$ Å) which are larger than the values obtained by Bastard[1] with an infinite barrier ($\sim 1.73R_0^*$ for $L = 50$ Å and $\sim 1.23R_0^*$ for $L = 100$ Å), and in agreement with the behavior in Fig. 2(a). Also, Tanaka *et al.*[25] have obtained the binding energies of on-edge donors for finite barriers higher than for the infinite-barrier case (see Fig. 3 of their work), which agrees with our results in Fig. 2(a).

The donor or acceptor binding energies as functions of the impurity position in a GaAs-$Ga_{1-x}Al_xAs$ quantum well are shown as solid curves in Fig. 3 for various slab thicknesses and for a concentration $x = 0.30$ (corresponding to $V_b = 224$ meV for donors and $V_b = 150$ meV for acceptors) of Al. For comparison we also display, as dash-dotted curves, the corresponding results for the infinite-potential-barrier limit.[7] Our results in Fig. 3(a) are in good agreement with the ones obtained by Greene and Bajaj[12] for $V_b = 323$ meV. The acceptor binding energies for constant screening $\epsilon = \epsilon_0$ and finite barrier potential are shown as dashed curves in Fig. 3(b) and a comparison with the spatially dependent $\epsilon = \epsilon(r)$ results [solid curves in Fig. 3(b)] indicates that spatially dependent screening effects can be quite important for acceptors in GaAs-(Ga,Al)As quantum wells over a large range of slab thickness.

Summing up, our results unequivocally demonstrate that a realistic calculation of the binding energies of acceptors in GaAs-$Ga_{1-x}Al_xAs$ requires an adequate description of spatially dependent screening (together, of course, with inclusion of the coupling[4] of the top four valence bands of both the well and barrier materials). Also, we have shown that the binding energies of on-edge impurities should, for sufficiently large well thicknesses, increase when the barrier potential (or the Al concentration) decreases, a behavior that contrasts with results obtained by other authors.

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