Effect of image forces on the binding energies of impurity atoms in $Ga_{1-x}Al_xAs/GaAs/Ga_{1-x}Al_xAs$ quantum wells

A. M. Elabsy*
Department of Physics, Faculty of Science, Mansoura University, Mansoura, Egypt
(Received 5 February 1991; revised manuscript received 24 March 1992)

The present work investigates the effect of image forces due to the dielectric mismatch in $Ga_{1-x}Al_xAs/GaAs/Ga_{1-x}Al_xAs$ superlattices on the binding energies of hydrogenic impurity atoms placed at the center of a $Ga_{1-x}Al_xAs/GaAs/Ga_{1-x}Al_xAs$ quantum well. The theory of images of classical electrodynamics is used to derive the potential energy of an impurity carrier (electron or hole) in a GaAs quantum well. Since the image-potential energy diverges as the charge approaches the interfaces, one can use the Lang-Kohn theory to study this system. It is pointed out that the image forces are important factors in studies of the binding energies of impurity atoms in GaAs quantum wells of narrow widths. Furthermore an accurate determination of image-plane locations in superlattice structures requires further investigations.

I. INTRODUCTION

Modern materials growth techniques, such as molecular-beam epitaxy (MBE) (Ref. 1) and metal organic chemical vapor deposition (MOCVD),[2] made it possible to fabricate systems consisting of alternate layers of two different semiconductors with controlled thickness and sharp interfaces. These new periodic structures are called superlattices. The most studied semiconductor superlattice consists of GaAs sandwiched between two $Ga_{1-x}Al_xAs$ slabs (x is the aluminum mole fraction). Depending on the Al concentration, the band gap in $Ga_{1-x}Al_xAs$ can be made considerably larger than that of GaAs. This leads to discontinuities of the conduction- and valence-band edges at the interface Γ point.[3,4] Until recently, there was little debate concerning the energy-band alignment in GaAs/(Al,Ga)As heterojunctions. Recently, Batey and Wright[5] have reported that about 60% of the band-gap difference between the two semiconductors is associated with the conduction-band discontinuity at the interface. Thus, electrons and holes in the GaAs matrix find themselves in potential wells whose depths depend on the Al concentration in the surrounding $Ga_{1-x}Al_xAs$ layers. Such a GaAs layer, sandwiched between two $Ga_{1-x}Al_xAs$ layers, is called a quantum well (QW).

Potential device applications, such as photodetectors, phototransistor, and solar cells,[6-8] as well as purely scientific interest, provide the motivation for studying the nature of the impurity states in QW's. The hydrogenic impurity states in a GaAs QW have been studied by Bastard,[9] who assumed an infinite well depth, and carried out variational calculations to determine the binding energy of a donor atom both as a function of the GaAs layer thickness and the position of the donor atom in the GaAs QW.

Bastard's work[9] was followed by papers by Mailhiot, Yia-Chung, and McGil,[10] Greene and Bajaj,[11] and Liu and Quinn.[12] A common feature of these papers is the hydrogenic approximation; in the main, the Coulomb energy interaction between the donor ion and the donor electron is scaled by the static dielectric constant of GaAs. In all of these calculations,[9-12] the conduction band of GaAs has been assumed to be parabolic. The effect of nonparapolicity of the conduction band of GaAs on the binding energy of a donor, placed at the center of a GaAs QW, has been assessed by Chaudhuri and Bajaj.[13] Csavinszky and Elabsy[14,15] went beyond the hydrogenic approximation by considering the dielectric response of a GaAs QW to the presence of a donor ion placed at on-center and off-center positions in a GaAs QW. Recently, Csavinszky and Elabsy[16] have also carried out numerical calculations of the binding energy of a hydrogenic donor placed at the center of a GaAs QW by using a model effective-mass Hamiltonian and the associated wave-function-matching condition for abrupt heterojunctions.

Considerably less attention has been paid to the subject of acceptor states in GaAs QW.[17] Masselink, Chang, and Morkoc[17] have adopted a hydrogenic approximation based on the Luttinger[18] formalism, and have correctly considered the valence-band structure of GaAs. Csavinszky and Elabsy[19] have considered the dielectric response of a GaAs QW of finite depth to the presence of an acceptor ion placed at its center. They calculated the binding energy of heavy-hole and light-hole acceptor atoms as a function of the width of the well.

In all of the calculations mentioned so far, with the exception of Mailhiot, Yia-Chung, and McGil,[10] the image forces arising from the dielectric mismatch between GaAs and $Ga_{1-x}Al_xAs$ have been neglected. Mailhiot, Yia-Chung, and McGil[10] have reported the contribution of the image forces to the binding energy of donors in a GaAs QW, but they have made the assumption that the conduction-band offset is 85% which is no longer accurate, and they have also neglected problems arising from the divergence of the image-potential energy as the charge approaches the interfaces. The present work goes beyond them by considering the most recently advocated assumption by Batey and Wright[5] that 60% of the band-gap discontinuity is contained in the conduction band,

and correctly deals with the complications arising from the divergence of the potential energy of a classical image charge when it approaches the interfaces. The present calculations are based on the Lang-Kohn[20] theory of metal surfaces, to calculate the effective position of the metal surface. Recently, Jennings and Jones[21] have reviewed the theoretical and experimental attempts considering moving charges near surfaces with dielectric overlayers.

The purpose of the present work is to determine the enhancement of the binding energies of both donor and acceptor atoms placed at the center of GaAs QW's of finite depths. This is accomplished by carrying out model calculations based on the effect of image forces arising from the dielectric mismatch between the well and barrier materials on the donor electron and the acceptor heavy hole located in GaAs QW's. Since our goal is the assessment of the magnitude of this effect, the dielectric response of a GaAs QW and the effective-mass mismatch are neglected, and parabolic conduction and valence bands of a GaAs QW are assumed.

This paper is organized as follows. Section II outlines the theoretical framework, and Sec. III presents the results of the calculations based on the image-potential-energy model and compares them with those obtained for the hydrogenic model.

All quantities appearing in the present work are expressed in atomic units.[22]

II. THEORY

The effective-mass Hamiltonian, in circular cylindrical coordinates, for a hydrogenic impurity atom placed at the center of a GaAs QW is given by

$$\hat{H}=\hat{T}+\hat{V}(r)+\hat{V}_B(z)+\hat{V}_{\rm im}(z)\ , \tag{1}$$

where $\hat{T}$ is the kinetic-energy operator, which in circular cylindrical coordinates ρ and z is given[22] by

$$\hat{T}=-\frac{1}{2m^*}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}+\frac{\partial^2}{\partial z^2}\right]\ . \tag{2}$$

In Eq. (2), m^* is either the conductivity effective mass m_e^* associated with a donor electron, or the valence-band effective mass m_h^* associated with an acceptor heavy hole. The subscripts e and h refer to electron and heavy hole, respectively. Their values[23] are listed in Table I. The z origin is chosen at the center of the well, whereas $\rho=(x^2+y^2)^{1/2}$ is the distance measured in a GaAs layer parallel to the $Ga_{1-x}Al_xAs$ interfaces (the impurity ion site is the x and y origin).

TABLE I. Values of various parameters used in the present work.

m_e^*	0.07
m_h^*	0.6
ϵ_1	13.18
ϵ_2	12.244
r_s	2.08
z_m	1.6
x	0.3
V_{0e}	227.88 meV
V_{0h}	151.92 meV

$\hat{V}(r)$ is the potential-energy operator, and is given by

$$\hat{V}(r)=-[\epsilon_1(\rho^2+z^2)]^{-1}\ . \tag{3}$$

In Eq. (3), ϵ_1 denotes the static dielectric constant of a GaAs QW. $\hat{V}_B(z)$ is the potential-energy barrier operator that confines the charge carriers in a QW of thickness L, and is given by

$$\hat{V}_B(z)=\begin{cases}0 & \text{for } |z|\le L/2\\ V_0 & \text{for } |z|\ge L/2\ ,\end{cases} \tag{4}$$

where V_0 is the conduction- or valence-band discontinuity between the well material and the barrier material, which is taken[5] to be

$$V_{0e}=0.6\Delta E_g^{\Gamma}(x) \tag{5}$$

for the conduction band, and

$$V_{0h}=0.4\Delta E_g^{\Gamma}(x) \tag{6}$$

for the valence band, whereas $\Delta E_g^{\Gamma}(x)$ is the difference between the $Ga_{1-x}Al_xAs$ and GaAs band gaps at the Γ point. For this quantity, Lee, Juravel, and Wolley[4] gave the expression

$$\Delta E_g^{\Gamma}(x)=1.155x+0.37x^2\ eV\ . \tag{7}$$

The values of x, V_{0e}, and V_{0h} used in the present work are listed in Table I.

The last additional term $\hat{V}_{\rm im}(z)$ in the Hamiltonian [Eq. (1)] represents the image-potential-energy operator. It is related to the image forces acting on the donor electron or the acceptor hole in the vicinity of the $Ga_{1-x}Al_xAs$ surface, which is given as follows.

The hydrogenic charge carrier e attracted by the impurity ion and located at a point of coordinates ρ and z in the GaAs QW will produce an image charge e' in the barrier material at a distance $L/2-z$ from the interface, which is given[24] by

$$e'=\left[\frac{\epsilon_1-\epsilon_2}{\epsilon_1+\epsilon_2}\right]e\ . \tag{8}$$

This image charge will exert a force on the original charge, e, in the QW region as

$$F(z)=\frac{ee'}{4\pi\epsilon_1[2(L/2-z)]^2}\ . \tag{9}$$

Then, the charge e acquires a potential energy given by

$$V_{\rm im}(z)=-\int F(z)dz=-\left[\frac{\epsilon_1-\epsilon_2}{\epsilon_1+\epsilon_2}\right]\frac{e^2}{16\pi\epsilon_1(L/2-z)}\ . \tag{10}$$

Finally, in atomic units,[22] the image-potential-energy operator $\hat{V}_{\rm im}(z)$ due to a single image charge comes out as

$$\hat{V}_{\rm im}(z)=\begin{cases}-\left[\dfrac{\epsilon_1-\epsilon_2}{\epsilon_1+\epsilon_2}\right]\dfrac{1}{4\epsilon_1(L/2-z)}, & |z|\le L/2-z_m \\ 0, & |z|\ge L/2-z_m\ .\end{cases} \tag{11}$$

In Eq. (11), one assumes that the charge carrier (electron or heavy hole) in a GaAs QW is at a distance $L/2-z$ from the $Ga_{1-x}Al_xAs$ interface. ϵ_2 is the static dielectric constant of $Ga_{1-x}Al_xAs$ which is a function of the Al concentration.[23] The value of ϵ_2 is listed in Table I. z_m is the image-plane location, which lies outside the barrier ($Ga_{1-x}Al_xAs$) surface.[20]

Lang and Kohn[20] have shown a reversible relationship between the screening radius r_s (the radius of a sphere containing one electron) and z_m. To determine r_s for the barrier material $Ga_{1-x}Al_xAs$, one uses the expression[25]

$$r_s=(3/4\pi n)^{1/3}\ , \tag{12}$$

where n is the electronic density of $Ga_{1-x}Al_xAs$.

The principal structure type for $Ga_{1-x}Al_xAs$ is cubic zinc blende with a linear variational lattice constant a expressed[23] as $a=5.6533+0.0078x$ Å. To obtain n, consider that $Ga_{1-x}Al_xAs$ unit cube has a cube of side a and contains four Ga atoms (with one or more Al atoms substituting Ga atoms, depending on the Al concentration in $Ga_{1-x}Al_xAs$) and four As atoms,[26] with a Ga (or Al) atom contributing three electrons and an As atom contributing five electrons.

Since the magnitude of an effect is concerned, one can take as a good approximation the value of z_m corresponding to r_s equals 2 a.u., as determined by Lang and Kohn.[20] The values of r_s and z_m are listed in Table I.

The present calculations use the same ground-state trial wave function as previously used by Csavinszky and Elabsy,[18,25] namely

$$\Psi(\rho,z)=Nf(z)g(\rho,z)\ , \tag{13}$$

where N denotes a normalization constant, and the functions f and g are defined as

$$f(z)=\begin{cases}\cos(\eta z) & \text{for } |z|\le L/2 \\ B\ \exp(-K|z|) & \text{for } |z|\ge L/2\end{cases} \tag{14}$$

and

$$q(\rho,z)=\exp[-\alpha(\rho^2+z^2)^{1/2}]\ . \tag{15}$$

In Eq. (14), the quantities η and K are related to the first subband energy E_0 by

$$\eta=(2m^*E_0)^{1/2} \tag{16}$$

and

$$K=[2m^*(V_0-E_0)]^{1/2}\ , \tag{17}$$

whereas the quantity B can be defined from the boundary condition that f and df/dz be continuous at $z=\pm L/2$. Imposition of these requirements leads to

$$B=\exp(KL/2)\cos(\eta L/2) \tag{18}$$

and

TABLE II. Values of the binding energy (in meV) relative to the well width (in a.u.) for a donor atom located at the center of a GaAs QW of depth $V_{0e}=227.88$ meV, for $E_B^{\rm H}$ (hydrogenic theory) and E_B [present work, Eq. (23)].

L (a.u.)	$E_B^{\rm H}$ (meV)	E_B (meV) [Eq. (23)]
9.84	8.96	9.18
29.51	11.75	12.41
39.34	12.27	13.01
59.01	12.59	13.33
98.36	12.23	12.79
196.72	10.73	11.01
295.07	9.61	9.78
393.43	8.80	8.92
491.79	8.19	8.29
590.15	7.72	7.80
688.51	7.35	7.41
786.87	7.05	7.11

$$K=\eta\tan(\eta L/2)\ . \tag{19}$$

From Eqs. (16), (17), and (19) it follows that the first subband energy E_0 is determined from

$$(E_0/V_0)^{1/2}=\cos[(2m^*E_0)^{1/2}(L/2)]\ . \tag{20}$$

In Eq. (15), α is a variational parameter.

The ground-state energy $E(L,\alpha)$ is determined from

$$E(L,\alpha)=\int\Psi^*\hat{H}\Psi\,d\tau \tag{21}$$

subject to the requirement

$$\frac{\partial E(L,\alpha)}{\partial\alpha}=0\ . \tag{22}$$

The binding energy $E_B(L,\alpha)$ of an impurity atom is calculated from

$$E_B(L,\alpha)=E_0-E(L,\alpha)\ . \tag{23}$$

The results of the present work are summarized in Tables II and III.

TABLE III. Values of the binding energy (in meV) relative to the well width (in a.u.) for a heavy-hole acceptor atom located at the center of a GaAs QW of depth $V_{0h}=151.92$ meV, for $E_B^{\rm H}$ (hydrogenic theory) and E_B [present work, Eq. (23)].

L (a.u.)	$E_B^{\rm H}$ (meV)	E_B (meV) [Eq. (23)]
4.25	61.37	61.70
8.50	69.63	70.76
10.63	72.29	73.67
21.26	76.55	78.25
63.77	65.74	66.49
106.29	58.61	59.02
148.81	54.91	55.19
191.32	52.86	53.07
212.58	52.18	52.37

III. DISCUSSION

Table I lists the values of the parameters (in atomic units[22] used in the present work. In the present calculations of the binding energies for both donor and acceptor atoms, the well width L must be greater than twice the value of z_m, the effective image-plane location. In Tables II and III, the abbreviation E_B^{H} stands for the binding energy due to the hydrogenic theory[12] [it is expressed by the Hamiltonian, Eq. (1), in which the last term, $\hat{V}_{\mathrm{im}}(z)$, is removed].

Table II shows the variation of the magnitude of the binding energy of a donor atom placed at the center of the GaAs QW as a function of the width of QW when the height of the barrier is $V_{0e}=277.88$ meV. The present calculations are compared with those obtained for the hydrogenic theory. It is seen from Table II that the value of the binding energy exhibits a maximum at a certain QW width of about 59 a.u. It is also seen that inclusion of the image-potential-energy due to image forces enhances the binding energy with respect to that of the hydrogenic theory. The reason that the magnitude of the binding energies converges with increasing the width of the QW is due to the fact that the location of the donor electron with respect to the effective image plane will be increased, which leads to a reduction of the image-potential energy [Eq. (11)]. This reduction will in turn lower the magnitude of the binding energy due to image forces until it approaches that obtained by the hydrogenic model.

Table III shows how the binding energy of a heavy-hole acceptor atom, located at the center of a GaAs QW of finite depth ($V_{0h}=151.92$ meV), depends on the width of the QW. It is seen from Table III that, at a given value of L, consideration of the image forces acting on a heavy hole in a GaAs QW leads to an increase in the magnitude of the binding energy, E_B [Eq. (23)], relative to the corresponding hydrogenic value, E_B^{H}. It is also noticed from Tables II and III that the values of the binding energies for both donor and acceptor impurity atoms increase until they approach maximum values and then decrease. This is in good agreement with previous findings.[12,15,19]

For the case of an on-center $z=0$ hydrogenic impurity atom in a GaAs QW, the effect of image charge due to the impurity ion will be smaller in magnitude than that attributed to the charge carrier (electron or hole). In the present work this effect is neglected not only for its small contribution but also for simplifying the calculations. We believe that this contribution will be more effective for studying an off-center impurity, which is not our present case.

It is also seen from Tables II and III that the correction of the present model considering the effect of a single image force to the binding energy is more pronounced for studying donor binding energy (about 5.9% for a QW of width 59.01 a.u.), than for studying acceptor heavy-hole binding energy (about 2.2% for a QW of thickness 21.26 a.u.).

Since the aim of the present work is to emphasize the effect of image forces on studying the binding energies of impurity atoms in superlattices and the complications that arise when the charge carriers approach the interfaces, a simple model is used to ease the problem. The present work also raises a question about the accurate effective crystal surface location in $GaAs/Al_xGa_{1-x}As$ superlattices and other similar structures.

Finally, one concludes that the effect of the image forces arising from the dielectric mismatch in $Ga_{1-x}Al_xAs/GaAs/Ga_{1-x}Al_xAs$ superlattice is a main factor in studies of the binding energies of impurity atoms in GaAs QW's.

*Present address: Department of Physics, Teachers Training College, Mecca, Saudi Arabia.

[1]A. Y. Cho, J. Appl. Phys. **42**, 2074 (1971).
[2]H. M. Manasevit, J. Electrochem. Soc. **118**, 647 (1971).
[3]H. C. Casey and M. B. Panish, *Heterostructure Lasers* (Academic, New York, 1978), Pt. A.
[4]H. J. Lee, L. Y. Juravel, and J. C. Wooley, Phys. Rev. B **21**, 659 (1980).
[5]J. Batey and S. L. Wright, J. Appl. Phys. **59**, 200 (1986).
[6]R. A. Milano, T. H. Windhorn, E. R. Anderson, G. E. Stillman, R. D. Dupuis, and P. D. Dapkus, Appl. Phys. Lett. **34**, 562 (1978).
[7]R. Dingle, H. L. Störmer, A. C. Gossard, and W. Wiegmann, Appl. Phys. Lett. **33**, 665 (1978).
[8]J. P. Van der Ziel, R. Dingle, R. C. Miller, W. Wiegmann, and W. A. Nordland, Jr., Appl. Phys. Lett. **26**, 463 (1975).
[9]G. Bastard, Phys. Rev. B **24**, 4714 (1981).
[10]C. Mailhiot, Yia-Chung, and T. C. McGil, Phys. Rev. B **26**, 4449 (1982).
[11]R. L. Greene and K. K. Bajaj, Solid State Commun. **45**, 825 (1983).
[12]W. Liu and J. J. Quinn, Phys. Rev. B **31**, 2348 (1985).
[13]S. Chaudhuri and K. K. Bajaj, Phys. Rev. B **29**, 1803 (1984).
[14]P. Csavinszky and A. M. Elabsy, Phys. Rev. B **32**, 6498 (1985).
[15]P. Csavinszky and A. M. Elabsy, Int. J. Quantum Chem., Quantum Chem. Symp. **20**, 325 (1986).
[16]P. Csavinszky and A. M. Elabsy, Semicond. Sci. Technol. **3**, 1010 (1988).
[17]W. T. Masselink, Y. C. Chang, and H. Morkoc, Phys. Rev. B **32**, 5190 (1985).
[18]J. M. Luttinger, Phys. Rev. **102**, 1030 (1956).
[19]P. Csavinszky and A. M. Elabsy, Int. J. Quantum Chem., Quantum Chem. Symp. **21**, 79 (1987).
[20]N. D. Lang and W. Kohn, Phys. Rev. B **7**, 3541 (1973).
[21]P. J. Jennings and R. O. Jones, Adv. Phys. **37**, 341 (1988).
[22]$m=e^2=\hbar=1$: the unit of length a_0 is the Bohr radius and the unit of energy e^2/a_0 is the hartree.
[23]S. Adachi, J. Appl. Phys. **58**, R1 (1985).
[24]J. D. Jackson, *Classical Electrodynamics,* 2nd ed. (Wiley, New York, 1975), p. 147.
[25]N. D. Lang and W. Kohn, Phys. Rev. B **3**, 1215 (1971).
[26]C. Kittel, *Introduction to Solid State Physics,* 6th ed. (Wiley, New York, 1986), p. 20.