Effects of image potential on electronic and impurity states in quantum wells

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(Received 21 January 1993)

The effects of an image potential on the electronic and hydrogenic impurity states in AlAs/GaAs/AlAs quantum wells are calculated by using variational solutions to the effective-mass equation. The results we have obtained show that when the image potential is added the variations of electronic state energy levels and impurity binding energies are significant, especially when the width of the quantum well becomes narrow. The results also show that the effects of the impurity-ion image potential on impurity binding energies are much larger than those of the electron image potential.

I. INTRODUCTION

With the recent advances in the epitaxial crystalgrowth techniques such as metal-organic chemical vapor deposition and molecular-beam epitaxy, studies of the electronic and impurity states in a quantum well consisting of alternate layers of GaAs and $Ga_{1-x}Al_xAs$ have in the past few years attracted considerable attention. 1^{-3} However, in these intensive investigations the image potential due to the dielectric mismatch inside and outside the quantum well is neglected. Recently, several researchers have considered the image potential in semiconductor interfaces and heterostructures, and found that the results are interesting and that the image potential is important.⁴⁻⁸ Gabovich and Rozenbaum⁴ have studied the potential energy of the image forces in metalinsulator-semiconductor (MIS) structures, and their results agree with experimental data on electron tunneling in MIS structures. Lee and Antoniewicz^{5,6} have included the image potential in their investigation of the electron bound states and surface polaron in the vicinity of two orthogonal surfaces. Cappellini and Delsole⁷ have calculated the effects of image-potential perturbation on the direct and inverse angle-resolved normal photoemission in Si and GaAs semiconductor surfaces, and the results have shown that the energy shifts due to image potential are of the order of tens of meV. In addition, in Ref. 9 the impurity-ion image potential is included in calculating the impurity binding energies in quantum-well structures, but how much change of binding energy the image potential results in is left unknown.

Very recently, Elabsy¹⁰ studied the effects of image potential on hydrogenic impurity binding energies in quantum wells. Unfortunately, the image-potential-energy operator he gave is incorrect, and only the electron image potential was considered. The question is whether the effects of image potential on electronic and impurity states are negligible. In this paper we discuss this problem by introducing the image potentials of electrons and impurity ions in the independent AlAs/GaAs/AlAs quantum wells correctly. In our calculation, the effective-mass approximation and variational approach are adopted. Only the lower electronic states whose energies (<250 meV) are much smaller than the conductionband offset between AlAs and GaAs (=1.07 eV) are considered. The potential barrier between AlAs and GaAs is assumed to be infinitely high.

The paper is organized as follows: In Sec. II we consider the effects of image potential on electronic states. In Sec. III the effects of image potential on impurity states are calculated. The results and a discussion are presented in Sec. IV.

II. ELECTRONIC STATES

Let us consider an independent AlAs/GaAs/AlAs quantum well, which is assumed to have an infinitely high potential barrier between GaAs and AlAs. In the effective-mass approximation, the Hamiltonian describing the motion of an electron in the quantum well can be written as

$$H^{(0)}(\mathbf{r}) = \frac{\mathbf{P}^2}{2m^*} + V_0 , \qquad (1)$$

where **P** and **r** are the electron momentum and coordinate, respectively, and m^* is the electron-band effective mass, which is $m^*=0.67m_0$ in the GaAs, with m_0 the free-electron mass. The electron-confining potential well V_0 is given by

$$V_0 = \begin{cases} 0, & |z| < d_z \\ \infty & \text{elsewhere }, \end{cases}$$
(2)

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where $2d_{z}$ is the width of the quantum well.

The energy levels of the unperturbed quantum well are given by

$$E_{mk_xk_y}^{(0)} = E_m^{(0)} + \frac{\hbar^2}{2m^*} (k_x^2 + k_y^2) , \qquad (3a)$$

$$E_m^{(0)} = \frac{\hbar^2 \pi^2}{8m^*} \frac{m^2}{d_z^2} , \qquad (3b)$$

corresponding to the envelope functions

$$\psi_{mk_xk_y}^{(0)}(\mathbf{r}) = \phi_m^{(0)}(z) \frac{1}{S^{1/2}} \exp[i(k_x x + k_y y)], \qquad (4a)$$

$$\phi_m^{(0)}(z) = \frac{1}{d_z^{1/2}} \sin \frac{m\pi}{2d_z} (z+d_z) , \qquad (4b)$$

where m = 1, 2, ... and S is the area of the interface of the quantum well.

Now we let the dielectric mismatch between GaAs and AlAs be expressed as

$$p = \frac{(\epsilon_{1\infty} - \epsilon_{2\infty})}{(\epsilon_{1\infty} + \epsilon_{2\infty})} , \qquad (5a)$$

$$p' = \frac{(\epsilon_1 - \epsilon_2)}{(\epsilon_1 + \epsilon_2)}$$
, (5b)

with $\epsilon_{1\infty} = 10.9$, $\epsilon_{2\infty} = 8.16$ and $\epsilon_1 = 13.1$, $\epsilon_2 = 10.1$ the optical and static dielectric constants for GaAs and AlAs, respectively. When the electron lies at point (x,y,z), the positions of the electron image charges in the z direction are obtained as follows:

$$z^{+}(k) = 2\left\{ \left[k - \left[\frac{k+1}{2} \right] \right] (d_z + z) + \left[\frac{k+1}{2} \right] (d_z - z) \right\} + z,$$

$$z^{-}(k) = -2\left\{ \left[\frac{k+1}{2} \right] (d_z + z) + \left[k - \left[\frac{k+1}{2} \right] \right] (d_z - z) \right\},$$
(6)

where $k = 1, 2, \ldots$ and

[x] = intx.

The electron image charge lies at point $[x,y,z^{i}(k)]$ (i = +, -); its corresponding charge value is $-ep^{k}$. The interaction force between the electron and its k-order image charge which lies at position $[x,y,z^{+}(k)]$ is

$$F = \frac{1}{\epsilon_{1\infty}} e^2 p^k \frac{1}{[z^+(k) - z]^2} .$$
 (7)

The interaction potential between the electron and its korder image charge mentioned above is equal to the work done by one that resists their electric-field force and moves the two interfaces of the quantum well simultaneously from infinity to the positions $-d_z$ and d_z , respectively, that is,

$$V_{k}^{+}(\mathbf{r}) = -\int_{\infty}^{d_{z}} Fd(d_{z}) = \frac{1}{2\epsilon_{1\infty}} e^{2} p^{k} \frac{1}{k|z^{+}(k)-z|} .$$
(8)

In the same way, the interaction potential between the electron and its other k-order image charge which lies at position $[x,y,z^{-}(k)]$ can be also obtained as

$$V_{k}^{-}(\mathbf{r}) = \frac{1}{2\epsilon_{1\infty}} e^{2} p^{k} \frac{1}{k|z^{-}(k) - z|} .$$
(9)

Thus, the electron image potential is written as

where $z_m = 0.85$ Å is the image-plane location which lies outside the AlAs barrier surface.¹⁰ Equation (10) is very different from the result obtained by Elabsy.¹⁰

The electronic Hamiltonian including the electron image potential reads

$$H(\mathbf{r}) = \frac{\mathbf{P}^2}{2m^*} + V_{\rm im}(\mathbf{r}) + V_0 \ . \tag{11}$$

Since the dielectric mismatch p is about 15%, the contribution of first-order image charge terms to the electron image potential is important, and the contributions of second- and higher-order image charge terms to the electron image potential could be viewed as a perturbation. Now we consider the electronic Hamiltonian including the electron image potential only up to first-order terms, that is, we set

$$H_1(\mathbf{r}) = \frac{\mathbf{P}^2}{2m^*} + V_1(\mathbf{r}) , \qquad (12)$$

with

$$V_1(\mathbf{r}) = \frac{C}{d_z^2 - z^2}$$
(13)

the contribution of first-order image charge terms to the electron image potential, where

$$C = \frac{1}{\epsilon_{1\infty}} \frac{1}{2} d_z p e^2 . \tag{14}$$

The eigenvalue equation for the Hamiltonian $H_1(\mathbf{r})$ reads

$$H_1(\mathbf{r})\psi^{(1)}(\mathbf{r}) = E\psi^{(1)}(\mathbf{r}) , \qquad (15)$$

with $\psi^{(1)}(\mathbf{r})$ the eigenfunction. If we assume that the eigenfunction for $H_1(\mathbf{r})$ can be written as

$$\psi^{(1)}(\mathbf{r}) = \phi^{(1)}_{xy}(x, y)\phi^{(1)}_{z}(z) , \qquad (16)$$

then Eq. (15) can be divided into two independent equations which could be solved easily, that is,

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$$-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}\phi_z^{(1)}(z) + \frac{C}{d_z^2 - z^2}\phi_z^{(1)}(z) = E_z\phi_z^{(1)}(z) , \qquad (17a)$$

$$-\frac{\hbar^2}{2m^*} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right] \phi_{xy}^{(1)}(x,y) = E_{xy} \phi_{xy}^{(1)}(x,y) , \qquad (17b)$$

with eigenenergy

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$$E = E_z + E_{xy} av{18}$$

From Eq. (17b) we can easily see that the motion of the electron parallel to the interfaces of the quantum well is a plane wave, and its corresponding eigenvalue and wave function are the same as those described in Eqs. (3a) and (4a). By the coordinate transformation

$$z' = z / d_z \tag{19}$$

and with the condition of

$$|z'| < 1 \tag{20}$$

in the quantum well, we can make the series expansion in the vicinity of z'=0:

$$(1-z'^2)^{-1} = 1 + z'^2 + z'^4 + \cdots$$
 (21)

When we neglect the high-order terms of the series (21), Eq. (17a) can be transformed further into

$$-\frac{\hbar^2}{2m^*}\frac{d^2}{dz'^2}\phi_z^{(1)}(z') + [Cz'^2 + (C - d_z^2 E_z)]\phi_z^{(1)}(z') = 0.$$
(22)

It is apparent that Eq. (22) is the eigenvalue equation of a harmonic oscillator when the constant C is positive, and its corresponding eigenfunctions and eigenvalues are expressed as follows:

$$\phi_{zn}^{(1)}(z) = N_{zn} e^{(1/2)\alpha^2 z^2} H_n(\alpha z) , \qquad (23a)$$

$$E_{zn} = \frac{1}{d_z^2} \left[C + \hbar \omega (n + \frac{1}{2}) \right], \qquad (23b)$$

where $n = 0, 1, 2, ...; \alpha$ is the characteristic coefficient; N_{zn} is the normalization constant; ω is the oscillator eigenfrequency; and $H_n(\alpha z)$ is the Hermitian polynomial.

According to the analysis above, the variational envelope function $\psi(\mathbf{r})$ for the Hamiltonian $H(\mathbf{r})$ can be expanded in terms of the products of the basis eigenfunctions of $H^{(0)}(\mathbf{r})$ and $H_1(\mathbf{r})$:

$$\psi(\mathbf{r}) = \sum_{mn} C(mn)\phi_m^{(0)}(z)\phi_{zn}^{(1)}(z) , \qquad (24)$$

where C(mn) is the expansion coefficient. Here, the characteristic coefficient α is viewed as the variational parameter, and the electron kinetic energy moving parallel to the interfaces of the quantum well is assumed to be zero. The wave function $\psi(\mathbf{r})$ satisfies the boundary conditions.

The problem of solving the effective-mass equation

$$H(\mathbf{r})|\psi(\mathbf{r})\rangle = E|\psi(\mathbf{r})\rangle$$
(25)

can be reduced to that of solving the generalized eigen-

value problem

$$\sum_{m'n'} \left[\langle mn | H(\mathbf{r}) | m'n' \rangle - E \langle mn | m'n' \rangle \right] C(m'n') = 0 ,$$
(26)

with the eigenenergy E and the expansion coefficients C(mn) appearing in the expansion equation (24).

The energies are minimized by adjusting the variational parameter that describes the basis functions and by increasing the number of functions used. In our practical calculation, the first ten basis functions, which correspond to the lower eigenenergies for $H^{(0)}(\mathbf{r})$ and $H_1(\mathbf{r})$, are included in the variational wave function (24), and the variational parameter α is determined by minimizing the energy expectation value in the ground state. In addition, because the dielectric mismatch p is much smaller than 1, we only consider the electron image potential up to the second-order terms. In this paper only the energies of the ground and first excited electronic states including image potential are given.

III. IMPURITY STATES

When a hydrogenic donor impurity is placed in the quantum well, the electronic Hamiltonian reads

$$H^{(1)}(\mathbf{r}) = \frac{\mathbf{P}^2}{2m^*} - \frac{e^2}{\epsilon_1 [x^2 + y^2 + (z - z_0)^2]^{1/2}} + V_0 , \qquad (27)$$

where $(0,0,z_0)$ is the position of the impurity in the quantum well. Here, according to the geometric symmetry of the quantum well, we only consider the impurity along the z axis.

As in Eq. (6), the positions of the impurity-ion image charges in the z direction are obtained as follows:

$$z_{0}^{+}(l) = 2 \left\{ \left[l - \left[\frac{l+1}{2} \right] \right] (d_{z} + z_{0}) + \left[\frac{l+1}{2} \right] (d_{z} - z_{0}) \right\} + z_{0} ,$$

$$z_{0}^{-}(l) = -2 \left\{ \left[\frac{l+1}{2} \right] (d_{z} + z_{0}) + \left[l - \left[\frac{l+1}{2} \right] \right] (d_{z} - z_{0}) \right\} + z_{0} ,$$
(28)

where l = 1, 2, ... and

[x] = intx.

The image charge of the impurity ion lies at point $[0,0,z_0^i(l)]$ (j=+,-); its corresponding charge value is ep'^l . The electronic Hamiltonian for impurity states including the impurity-ion image potential can be written as

$$H^{(2)}(\mathbf{r}) = \frac{\mathbf{P}^2}{2m^*} + V_{io}(\mathbf{r}) + V_0 , \qquad (29)$$

with

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$$V_{io}(\mathbf{r}) = -\frac{e^2}{\epsilon} \sum_{l=0}^{\infty} \sum_{j} p^{\prime l} \{x^2 + y^2 + [z - z_0^j(l)]^2\}^{-1/2}$$
(30)

the sum of the impurity ion and its image potentials.

When we consider the image potentials of an impurity ion and an electron simultaneously, the electronic Hamiltonian for impurity states can be written as

$$H^{(3)}(\mathbf{r}) = \frac{\mathbf{P}^2}{2m^*} + V_{\rm io}(\mathbf{r}) + V_{\rm im}(\mathbf{r}) + V_0 . \qquad (31)$$

As in Sec. II, we only consider the image potentials of impurity ions and electrons up to second-order terms in our practical numerical calculation.

Because the image potentials of the impurity ion and the electron are small compared with the impurity-ion potential, the trial wave function of $H^{(j)}(\mathbf{r})$ (j = 1, 2, 3) we take is analogous, therefore, to that used in Refs. 1 and 2 and is written for the ground impurity state as

$$\phi(\mathbf{r}) = N \cos \frac{\pi}{2d_z} z \exp\{-[x^2 + y^2 + (z - z_0)^2]^{1/2} / \lambda\},$$
(32)

where N is the normalization constant and λ is the variational parameter. The trial wave function (32) satisfies the boundary conditions.

As usual, we define the impurity binding energy as the energy difference between the bottom of the electronic conduction band without the impurity and the ground energy level of the impurity states in the quantum well, that is, we take

$$E_i^{(j)} = \frac{\hbar^2 \pi^2}{8m^*} \frac{1}{d_z^2} - \min_{\lambda} \langle \phi(\mathbf{r}) | H^{(j)}(\mathbf{r}) | \phi(\mathbf{r}) \rangle \quad (j = 1, 2) ,$$
(33)

for the Hamiltonians $H^{(1)}(\mathbf{r})$ and $H^{(2)}(\mathbf{r})$, and

$$E_i^{(3)} = E_1 - \min_{\lambda} \langle \phi(\mathbf{r}) | H^{(3)}(\mathbf{r}) | \phi(\mathbf{r}) \rangle , \qquad (34)$$

for the Hamiltonian $H^{(3)}(\mathbf{r})$, which included the electron image potential. Here, E_1 is the ground energy level of the electronic states including the image potential which has been obtained in Sec. II. The above integrals were calculated numerically.

IV. RESULTS AND DISCUSSION

From Fig. 1 we can easily see that when the electron image potential is added, the energies of ground and first excited electronic states change significantly, and the energies of electronic states including the image potential are larger than those that do not include the image potential. In Fig. 1 we can also see that the effects of an image potential on electronic states are more notable when the width of the quantum well becomes narrow, and the effects of an image potential on excited electronic states are larger than those on ground electronic states. When the width of a quantum well $2d_z = 500$ Å, the values $E_1 - E_1^{(0)}$ and $E_2 - E_2^{(0)}$ are 0.55 and 0.80 meV, and when

the width of a quantum well decreases to $2d_z = 100$ Å, the corresponding values $E_1 - E_1^{(0)}$ and $E_2 - E_2^{(0)}$ reach 2.48 and 3.01 meV, respectively.

From Fig. 2 it is apparent that when the impurity-ion image potential is added, the impurity binding energies change remarkably, and when the image potentials of the impurity ion and electron are added simultaneously, the variations of the impurity binding energy are almost the same as those including only the impurity-ion image potential. From Fig. 2(b), we can also see that the variations of the impurity binding energy in the center are smaller than those near the boundary of the quantum well when the image potential is included in the electronic Hamiltonian. When the impurity lies at the center of the quantum well, the values $(E_i^{(2)} - E_i^{(1)})$ and $(E_i^{(3)} - E_i^{(1)})$ are 2.43 and 2.31 meV, and when the impu-



FIG. 1. (a) The variations of the energies of ground and first excited electronic states with the width of the quantum well, where the dashed and solid lines represent the energies of electronic states including and not including the image potential, respectively. (b) The variations of the energy differences $(E_j - E_j^{(0)})$ (j = 1,2) for the ground and first excited electronic states between the two cases including and not including the image potential with the width of the quantum well.

rity is at the boundary of the quantum well, the corresponding values $(E_i^{(2)}-E_i^{(1)})$ and $(E_i^{(3)}-E_i^{(1)})$ reach 2.82 and 2.67 meV, respectively.

Figure 3(a) shows the dependence of the impurity binding energy on the width of the quantum well, where the impurity lies at the center of the quantum well. It can be easily seen that when the width of the quantum well becomes narrow, the binding energies increase rapidly, and the effects of the image potential on impurity states be-

I (a) 1 E, (meV) 10 20 30 40 50 0 Z₀(Å) (b) $\mathbf{E}_{i}^{(2,3)} - \mathbf{E}_{i}^{(1)}$ (meV) 5. $E_{1}^{(2)} - E_{1}^{(1)}$ 2 $E_{i}^{(3)} - E_{i}^{(1)}$ 0 50 Z_o(Å)

FIG. 2. (a) The variations of impurity binding energy with the impurity position along the z axis, where the width of the quantum well is $2d_z = 100$ Å. The solid line represents the impurity binding energies that do not include the image potential; the dashed and dot-dashed lines represent the corresponding impurity binding energies, including the impurity-ion image potential and including the image potentials of the impurity ion and the electron simultaneously, respectively. (b) The variations of the differences $(E_i^{(j)} - E_i^{(l)})$ (j = 2, 3) of the impurity binding energies between the cases including and not including the image potential with the impurity position along the z axis, where the width of the quantum well is $2d_z = 100$ Å. The dashed and dot-dashed lines represent the corresponding values including the impurity-ion image potential and including the image potentials of the impurity ion and the electron simultaneously, respectively.

come more notable. When the width of the quantum well $2d_z = 500$ Å, the values $E_i^{(2)} - E_i^{(1)}$ and $E_i^{(3)} - E_i^{(1)}$ are 0.61 and 0.68 meV, and when the width of the quantum well decreases to $2d_z = 100$ Å, the corresponding values $E_i^{(2)} - E_i^{(1)}$ and $E_i^{(3)} - E_i^{(1)}$ reach 2.43 and 2.31 meV, respectively.

The results obtained above are interesting, and their physical interpretation and discussion are given as follows: From Eq. (5), it is apparent that the dielectric mismatch p,p' between GaAs and AlAs is larger than



FIG. 3. (a) The dependence of impurity binding energy on the width of the quantum well, where the impurity lies at the center of the quantum well. The solid line represents the impurity binding energies without including the image potential, the dashed and dot-dashed lines represent the corresponding impurity binding energies including the impurity-ion image potential and including the image potentials of the impurity ion and the electron simultaneously, respectively. (b) The dependence of the differences $(E_i^{(j)} - E_i^{(1)})$ (j = 2, 3) of the impurity binding energies between the cases including and not including the image potential on the width of the quantum well, where the impurity lies at the center of the quantum well. The dashed and dotdashed lines represent the corresponding values including the impurity-ion image potential and including the image potentials of the impurity ion and the electron simultaneously, respectivelv.

zero; therefore, the electron image potential in Eq. (10) is positive. This results in an increase of the energies of ground and excited electronic states when the electronic Hamiltonian includes the image potential. At the same time, we can also see that the impurity-ion image potential in Eq. (30) is negative, and the impurity binding energies will increase when the electronic Hamiltonian for the impurity states includes the impurity-ion image potential. On the other hand, since the electron image potential is positive, it will enhance the ground energy level of the electronic states in the first term of Eq. (34) and the ground energy level of the impurity states in the second term of Eq. (34) simultaneously, and the sum of the effects of the electron image potential on impurity binding energies is not too large. So when the image potentials of the impurity ion and the electron are added simultaneously, the variations of the impurity binding energy are almost the same as those including only the impurity-ion image potential. These demonstrate that the effects of the impurity-ion image potential on impurity binding energy are much more important than those of the electron image potential which is very different from the conclusion obtained in Ref. 10 where the impurityion image potential is found to be of little importance. In addition, when the width of the quantum well decreases, the quantum confinement of the electron in the quantum well is strengthened, and the interaction potential be-

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tween the electron and the image charges increases. This causes the increase of the differences of the energies for the electronic and impurity states between the two cases including and not including the image potential when the width of the quantum well becomes narrow. The results obtained above also remind us that the image potential in the quantum well is important. Strictly speaking, the image potential in the quantum well cannot be neglected in considering electronic and impurity states, especially when the width of the quantum well is narrow.

In conclusion, we have studied the effects of an image potential on electronic and impurity states in the independent AlAs/GaAs/AlAs quantum wells. The results we have obtained show that when the electron image potential is added, the energy levels of electronic states change significantly, but the variations of impurity binding energies are not very apparent. The results also show that the impurity-ion image potential is important in calculating impurity binding energies, especially when the width of the quantum well becomes narrow.

ACKNOWLEDGMENTS

This work was supported by the National Committee of Education and by NSF Grant No. 69188006.

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