Bound impurity in GaAs-$Ga_{1-x}Al_xAs$ quantum-well wires

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The binding energies of a hydrogenic impurity located in quantum-well wires of GaAs surrounded by $Ga_{1-x}Al_xAs$ are calculated as a function of the size of the wire for several values of the heights of the potential barriers and different positions of the impurity inside the wire. The calculations are also performed for the case of an asymmetric potential barrier with different heights in the two directions perpendicular to the wire. The results we have obtained show that the binding energies are closely correlated to the sizes of the wire, the impurity positions, and the height of the barrier, and also that their magnitudes are greater than those in comparable two-dimensional quantum wells.

I. INTRODUCTION

In the last few years there has been increasing interest in the study of the electronic properties of ultrathin semiconducting wires, namely quantum-well wires whose dimensions are of submicrometer size. In such structures, the electrons are confined to movement along the length of the wire while the motion normal to the wire is quantized in the two dimensions. By investigating electron transport in GaAs-$Ga_{1-x}Al_xAs$ quantum wires, Sakaki[1] was the first to show that electrons can exhibit very high mobilities because of the suppression of the elastic scattering by ionized impurities. Later, Petroff, Gossard, Logan, and Wiegmann[2] fabricated wires by using these materials and reported some of the luminescence properties which appear to be specific to quantum-well wires of small dimensions. Recently much theoretical work has been done to understand the behavior of electrons and holes in such quasi-one-dimensional semiconductor structures. Degani and Hipólito[3] have calculated the effects of the electron– and hole–optical-phonon interaction on the exciton binding energies and showed that the polaronic corrections are quite significant. Lee and Spector[4] and Lee and Vassell[5] investigated the mobility of electrons scattered by ionized donors as well as by optical and acoustic phonons. The optical absorption due to direct intersubband transitions and the free-carrier absorption for the case where the electrons are scattered by acoustic phonons through deformation-potential coupling have also been studied.[6,7] In a recent calculation Chitta and Marques[8] have obtained the conduction- and valence-subband dispersions along the direction of the wire axis of GaAs-$Ga_{1-x}Al_xAs$ quantum-well wires. They have shown the presence of a very strong conduction–valence-subband coupling in this system.

One of the crucial problems in semiconductor physics and particularly in these new quasi-one-dimensional semiconductor structures is the presence of ionized impurities, which play a fundamental role in transport mechanisms at low temperatures. Their associated electronic bound states are hydrogenlike states similar to those found in the impurity problem in two-dimensional semiconductor structures.[9–11] Though several authors have investigated various aspects of the energy levels of impurities in a quasi-one-dimensional electron gas, theoretical understanding of these bound states and their binding energies is not complete. Lee and Spector[12] first calculated the binding energies for the bound states of a hydrogenic impurity placed on the axis of a cylindrical quantum-well wire of infinite confining potential. They have shown that the binding energy of the lowest state is greatly enhanced over the two- and three-dimensional values by reducing the radius of the wire. In the strictly one-dimensional limit, the binding energy approaches infinity.[13] In a subsequent work, Bryant[14] improved the model calculation by assuming a finite barrier for the confining potential with the impurity on the axis of the cylinder wire. In contrast to the previous result, he found that in a very thin wire, the electrons leak out of the wire and behave as three-dimensional electrons in the barrier-acting material. More recently, Bryant[15] and Brum[16] investigated the case where the hydrogenic impurity could be located in different positions outside of the center of the wire. Their calculations were performed for wires with rectangular cross section and with the infinite barrier model for the confining potential. Because of the use of the infinite barrier potential, such calculations have certainly overestimated the impurity binding energies.

The purpose of this paper is to report the results of the binding energies of a hydrogenic impurity associated with the lowest electron subband in a quantum-well wire of GaAs surrounded by $Ga_{1-x}Al_xAs$. For the calculations described here, the wires are assumed to have rectangular cross section and finite barrier potential to the confined electrons. We will also consider the case where the electrons moving perpendicular to the wire are affected by an asymmetric potential barrier with different values of the height in the two directions. We follow a variational approach and calculate the binding energies as a function of the size of the wire for several values of

the height of the barrier potential and the position of the impurity in the quantum-well wire. In addition, we calculate the binding energies for the infinite-potential-barrier model and compare the results with those previously obtained by Bryant[15] and Brum.[16]

A short description of the theory followed by a review of the calculation procedures are presented in Sec. II. The results and discussion of the impurity binding energies for several values of the barrier height and impurity positions are presented in Sec. II.

II. THEORY

Let us consider a quantum-well wire of GaAs surrounded by $Ga_{1-x}Al_xAs$, which is assumed to have rectangular cross section and finite height for the electron-confining potential. The donor impurity is modeled as a hydrogenic impurity located in the well at $(x_i,y_i,0)$ and screened by the bulk static dielectric constant of GaAs ($\epsilon=13.1$). The electron bound states and the associated binding energies are obtained by solving the effective-mass Schrödinger equation. Since the impurity binding energies (of order of meV) are much smaller than the band gap of GaAs (1.4 eV), the effective-mass approximation is appropriate to treat this problem.

In the effective-mass approximation, the Hamiltonian describing the interaction of an electron with a hydrogenic impurity placed in a quantum-well wire can be written in the following form:

$$\dot{H}=\frac{p^2}{2m}-\frac{e^2}{\epsilon[(x-x_i)^2+(y-y_i)^2+z^2]^{1/2}}+V(x,y)\ , \quad (1)$$

where $\mathbf{p}$ and $\mathbf{r}=(x,y,z)$ are the electron momentum and coordinates respectively, $(x_i,y_i,0)$ is the impurity position, ϵ is the static dielectric constant of GaAs, m is the electron-band effective mass which is defined as

$$m=\begin{cases} m_1=0.067m_0 & \text{in the GaAs}\ , \\ m_2=(0.067+0.083x)m_0 & \text{in the } Ga_{1-x}Al_xAs\ , \end{cases} \quad (2)$$

m_0 is the free-electron mass, and x is the Al concentration. The electron-confining potential well $V(x,y)$ is taken as

$$V(x,y)=\begin{cases} 0, & |x|<L_x/2, \quad |y|<L_y/2 \\ V_{0x}, & |x|>L_x/2, \quad |y|<L_y/2 \\ V_{0y}, & |y|>L_y/2\ . \end{cases} \quad (3)$$

V_{0x} and V_{0y} are the discontinuities in the conduction-band edge and L_x and L_y are the well widths. The values of the potential heights are determined from the Al concentration x in GaAs-$Ga_{1-x}Al_xAs$ through the expression for the energy-band-gap discontinuity ΔE_G, $\Delta E_G=1.04x+0.47x^2$ eV.[17] The values of V_{0x} and V_{0y} are taken to be 60% of ΔE_G.

In order to calculate the impurity binding energy for the ground electron subband we choose the simplest approximation for the trial wave function that is a product ansatz state,

$$\psi(x,y,z)=(\lambda/2)^{1/2}\Phi(x)\Phi(y)\exp(-\lambda|z|/2)\ , \quad (4)$$

where

$$\Phi(x)=\begin{cases} A_x\cos(K_{1x}L_x/2)e^{K_{2x}L_x/2}e^{K_{2x}x}, & x<L_x/2 \\ A_x\cos(K_{1x}x), & -L_x/2<x<L_x/2 \\ A_x\cos(K_{1x}L_x/2)e^{K_{2x}L_x/2}e^{-K_{2x}x}, & x>L_x/2 \end{cases} \quad (5)$$

$$A_x=\left[\frac{1}{K_{2x}}\cos^2\left[\frac{K_{1x}L_x}{2}\right]+\frac{1}{2K_{1x}}\sin(K_{1x}L_x)+\frac{L_x}{2}\right]^{-1/2},$$

$$K_{1x}=(2m_1E_x/\hbar^2)^{1/2}$$

and

$$K_{2x}=[2m_2(V_{0x}-E_x)/\hbar^2]^{1/2}\ .$$

The parameters K_{1x} and K_{2x} are determined by using the appropriate current-conserving boundary conditions for the wave functions at the interfaces and must satisfy the following relation:

$$m_1K_{2x}=m_2K_{1x}\tan(K_{1x}L_x/2)\ .$$

The wave function $\Phi(y)$ is taken in a similar manner. The variational parameter λ will be determined by minimizing the expectation value of the Hamiltonian $E=\langle\psi|H|\psi\rangle$ which has the following form:

$$E=\frac{\hbar^2}{2m_1}\left[\frac{K_{1x}^2A_x^2L_x}{2}+\frac{K_{1y}^2A_y^2L_y}{2}+\lambda^2\right]+E_C+E_P\ . \quad (6)$$

E_C is the average of the Coulombic impurity,

$$E_C=\frac{-2\lambda^2e^2}{\pi\epsilon}\int dq\frac{F(q)}{\lambda^2+q^2}\ , \quad (7)$$

where $F(q)$ is the form factor for the quasi-one-dimensional system which is given by[3]

$$F(q)=\int dk\frac{G(k)H(q,k)}{(k^2+q^2)^{1/2}}\ , \quad (8)$$

where $G(k)$ and $H(q,k)$ can be explicitly written as

$$G(k)=\frac{2A_y^2\cos^2(K_{1y}L_y/2)}{k^2+4K_{2y}^2}\cos(ky_i)\left[2K_{2y}\cos\left[\frac{kL_y}{2}\right]-k\sin\left[\frac{kL_y}{2}\right]\right]$$
$$+\frac{A_y^2\cos(ky_i)}{k(4K_{1y}^2-k^2)}\left\{\sin\left[\frac{kL_y}{2}\right]\left[4K_{1y}^2-2k^2\cos^2\left[\frac{K_{1y}L_y}{2}\right]\right]+2K_{1y}k\sin(K_{1y}L_y)\cos\left[\frac{kL_y}{2}\right]\right\}, \quad (9)$$

$$H(q,K)=\frac{2A_x^2\cos^2\left[\frac{K_{1x}L_x}{2}\right]e^{\frac{-QL_x}{2}}}{(Q+2K_{2x})}\cosh(Qx_i)$$
$$+\frac{A_x^2}{(Q^2+4K_{1x}^2)}\left[\frac{4K_{1x}^2}{Q}+2e^{-QL_x/2}\cosh(Qx_i)\left[K_{1x}\sin(K_{1x}L_x)-Q\cos^2(K_{1x}L_x/2)-\frac{2K_{1x}^2}{Q}\right]+2Q\cos^2(K_{1x}x_i)\right], \tag{10}$$

with $Q=(q^2+k^2)^{1/2}$. E_P is the average of the confining potential, $E_P=\langle\psi\,|\,V\,|\,\psi\rangle$.

Then we obtain the impurity binding energy which is defined as the difference between the lowest value of the energy for the system without the impurity and the minimized value of E, Eq. (6).

III. RESULTS AND DISCUSSIONS

The variational parameter which minimizes the expectation value of the Hamiltonian of the system was calculated as a function of the size of the quantum wire for several values of the barrier heights of the confining potential and for different positions of the impurity inside the wire. With the optimum parameter we evaluated the impurity binding energies.

Figure 1 shows the results we have obtained for the binding energy when the impurity is placed on the center of the wire for two choices of the alloy composition of $Ga_{1-x}Al_xAs$, $x=0.15$ and $x=0.30$. As we can note, by fixing one value of the Al concentration x and one direction of the wire, the binding energy presents the same qualitative behavior as that previously obtained in the two-dimensional quantum wells. The energy increases with the increasing size of the wire, reaches a maximum value and finally decreases monotonically for wider well wires. We also note that the enhancement of the binding energy by the confinement in one dimension is the dominant effect. As the Al content x increases, the confining well depth increases, making the wire more one-dimensional, and as a consequence the binding energy increases.

Figure 2 compares the results of the binding energies for quantum wires with one dimension fixed at $L_y=50$ Å and for different Al concentrations in the two directions perpendicular to the wires. The impurity is located in the center of the rectangular wire. By interchanging the barrier height of the confining potential in the two directions perpendicular to the wire we have obtained distinct values for the binding energies. In the case where the Al content is (0.3,0.15) and (0.15,0.3) in the directions (x,y) we can see from Fig. 2 that for $L_x>L_y=50$ Å the larg-

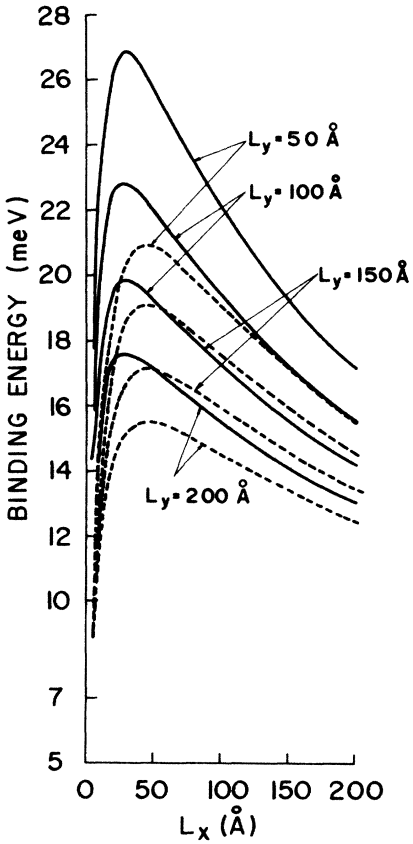

FIG. 1. Binding energy for the ground state of a hydrogenic impurity located in the middle of a GaAs-$Ga_{1-x}Al_xAs$ quantum-well wire for $x=0.15$ (dashed curves) and $x=0.30$ (solid curves).

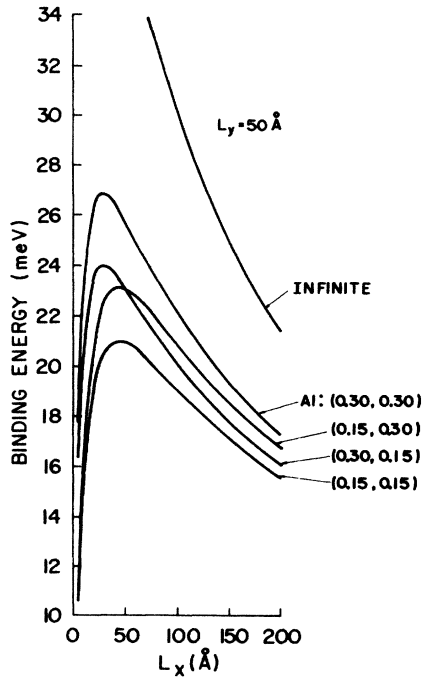

FIG. 2. Binding energy of a hydrogenic impurity placed in the center of a GaAs quantum-well wire as a function of the size (L_x) for different concentrations of Al:(x_x,x_y) in the two directions perpendicular to the wire, for $L_y=50$ Å. Plotted for comparison is the case of infinite-wire barrier potential.

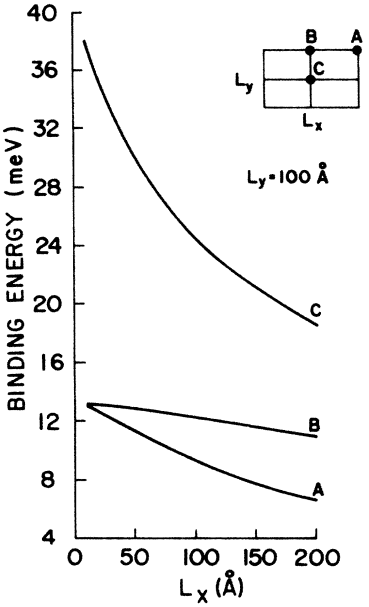

FIG. 3. Binding energy of a hydrogenic impurity placed in three different positions of a GaAs quantum-well wire as a function of the size L_x for $L_y = 100$ Å and an infinite barrier height for the confining potential.

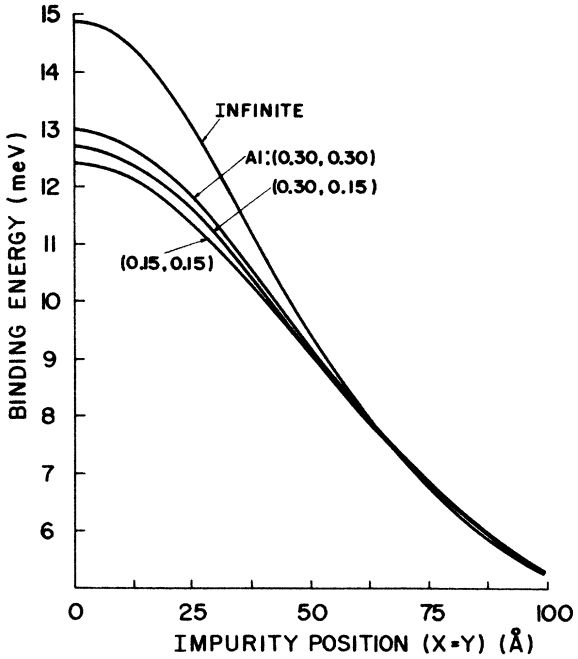

FIG. 4. Binding energy of an impurity as a function of the impurity position along the diagonal of a square (200×200) Å^2 cross-section wire. The curves show the results for different heights of the potential barrier corresponding to the concentration of Al:($\varkappa_x$,$\varkappa_y$) in the two directions perpendicular to the wire.

est binding energy is related to the confinement to the y direction where the potential barrier is higher. On the other hand, for $L_x < L_y = 50$ Å the confinement is more pronounced in the x direction because the Al content is larger in this direction than in the y direction.

In Fig. 3 we show the binding energies for a quantum-well wire of *infinite potential barrier*, $L_y = 100$ Å and for three different positions of the impurity: at the center, at the boundary, and at the corner of the rectangular cross section of the wire. As can be seen, the value of the binding energy corresponding to the case where the impurity is located at the center of the wire is much larger than the other two positions of the impurity. The reason for this behavior is that the wave functions vanish at the boundaries and thus their contributions to the energy when the impurity is at the boundary are smaller than when the impurity is at the middle of the wire.

The results for the binding energies as the impurity moves out along the diagonal of a quantum wire of 200×200 Å^2 are shown in Fig. 4 for several values of the barrier height of the confining potential. From these results we may note that the bound states in the finite-well wires have lower binding energies than the infinite-well wire when the distance of the impurity from the center is smaller than about 60 Å. As the impurity is located at larger distances, more close to the boundaries, the binding energies in the finite-well wires become higher than those in the infinite-well wire. This change occurs because the contributions of the wave functions at the boundary become more significant as the potential barrier height decreases.

In conclusion we have calculated the binding energies for the ground state of a hydrogenic impurity placed in a quantum-well wire of GaAs-$Ga_{1-\varkappa}Al_\varkappa As$ of rectangular cross section. The calculations have been performed for several values of the barrier height of the confining potential and for different positions of the impurity in the wire. We have shown that the binding energy is dramatically dependent on the sizes of the wire and also its magnitude is greater than that in comparable quasi-two-dimensional quantum-well structures. We have also shown that boundary effects strongly influence the quantitative results.

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