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Physica B 339 (2003) 17–22
PHYSICA B
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Binding energies of shallow donor impurities in different shaped quantum wells under an applied electric field

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Received 12 June 2003; accepted 5 July 2003

Abstract

We present a variational method to compute the binding energies for a hydrogenic impurity located at the center of the finite parabolic (PQW), V-shaped (VQW or full graded well) and square (SQW) GaAs–$Ga_{1-x}Al_xAs$ quantum wells under the electric field. The dependence of the ground state impurity binding energy on the applied electric field, the geometric shape of the quantum wells and well width is discussed together with the polarization effect.

PACS: 71.55.−i; 71.55.Eq; 73.20.Dx

Keywords: Parabolic quantum well; V-shaped quantum well; Graded quantum well; Square quantum well; Impurity binding energy; Polarizibility; Electric field

1. Introduction

With the development of the molecular-beam epitaxy growth method, quantum wells can be made into different forms, such as square quantum wells (SQWs), triangular quantum wells, and parabolic quantum wells (PQWs). Such structures have attracted considerable interest since the end of the 1980s [1–4]. In comparison with SQWs, the parabolic potential results in a stronger localization and equidistant energy seperation of eigenvalues. Parabolic structures are well known in designing infrared detectors with low leakage currents and low electric-field sensitivity [5,6]. The effect of an applied electric field on the physical properties of such structures have attracted considerable interest [7,8]. For instance, the application of an electric field in the crystal growth direction causes a polarization of the carrier distribution and shift the quantum energy states, which can be used to control and modulate the intensity output of the device [9].

In this work, we calculate the binding energies for shallow donor impurities in finite SQW, PQW and V-shaped quantum wells (VQW) or full graded $GaAs/Ga_{1-x}Al_xAs$ quantum wells under the parallel-applied electric field to the growth direction using a variational technique. The full graded potential profile is obtained by changing linearly from zero to 0.3 the aluminium

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0921-4526/$ - see front matter
doi:10.1016/S0921-4526(03)00445-9

concentration—x in the $Ga_{1-x}Al_xAs$ layer. As known, one important aspect of electronic band structure engineering is the realization of graded heterostructures, in which the composition is varied continuously in space. Electronic and optoelectronic devices which exploit these effects include, to date; graded-base heterostructure bipolar transistors which promote the egress of carriers through the base; graded separate confinement heterostructure laser active regions which not only confine light to the quantum wells, but may also promote transport within the active region and increase device bandwidth [10,11].

2. Theory

In the effective mass approximation, the Hamiltonian for a shallow-donor impurity under the electric field is

$$H = -\frac{\hbar^2}{2m^*}\vec{\nabla}^2 + V(z) - \frac{e^2}{\varepsilon_0 \vec{r}} + eFz, \tag{1}$$

where m^* is the electron effective mass, ε_0 is the static dielectric constant, $\vec{r}$ is the distance between the carrier and the donor impurity site $\left(r = \sqrt{\rho^2 + (z - z_i)^2}\right)$ and $\rho\left(= \sqrt{x^2 + y^2}\right)$ is the distance between the electron and impurity in the $(x - y)$ plane, F is the electric field strength, $V(z)$ are the finite confinement potentials in the z-direction, The functional forms of the PQW, VQW and SQW are, respectively

$$V(z)^{\mathrm{PQW}} = \begin{cases} V_0, & z < -L/2 \\ \dfrac{4V_0}{L^2}z^2, & -L/2 < z < L/2, \\ V_0, & z > L/2, \end{cases} \tag{2a}$$

$$V(z)^{\mathrm{VQW}} = \begin{cases} V_0, & z < -L/2, \\ \dfrac{2V_0}{L}|z|, & |z| < L/2, \\ V_0, & z > Lz/2, \end{cases} \tag{2b}$$

$$V(z)^{\mathrm{SQW}} = \begin{cases} V_0, & z < -L/2, \\ 0 & -L/2 < z < L/2, \\ V_0, & z > L/2. \end{cases} \tag{2c}$$

The impurity binding energies in PQW, VQW and SQW are calculated by a traditional variational method. The following trial wave function of the ground impurity state for all geometric confinement potentials are given by

$$\psi(r) = \psi(z)\varphi(\rho, \lambda), \tag{3}$$

where the wave function—$\psi(z)$ is exactly obtained from the Schrödinger equation in the z-direction, the wave function in the $(x - y)$ plane—$\varphi(\rho, \lambda)$ is chosen to be the wave function of the ground state of a two-dimensional hydrogen-like atom [12,13]:

$$\varphi(\rho, \lambda) = \frac{1}{\lambda}\left(\frac{2}{\pi}\right)^{1/2} \mathrm{e}^{-\rho/\lambda} \tag{4}$$

in which λ is a variational parameter.

The ground impurity binding energy is obtained as follows:

$$E_{\mathrm{b}} = E_z - \min_{\lambda} \langle \Psi | H | \Psi \rangle, \tag{5}$$

where E_z are the ground-state energies of electron obtained from Schrödinger equation in the z-direction for all geometric confinement potentials without the impurity, respectively.

Apart from the calculations of the well widths and electric field dependence of the impurity binding energies, we also calculated the polarization. Polarization is given by [14,15]:

$$\alpha = -\frac{e}{F}\left[\langle \psi(z)|z|\psi(z)\rangle_{F\neq 0} - \langle \psi(z)|z|\psi(z)\rangle_{F=0}\right]. \tag{6}$$

3. Results and discussions

We have calculated the ground state binding energies for donors in finite PQW, VQW and SQW $GaAs-Ga_{1-x}Al_xAs$. We assume that the effective mass and the relative dielectric constant throughout the whole structures [16–18]. The results obtained for the SQW indicate that the effect of using different effective masses for GaAs and $Ga_{1-x}Al_xAs$ [19] and the effect of the spatial variation of dielectric screening [20] on impurity binding energies is an increase of a few percent except for very small well widths. We use the effective Bohr radius $a_{\mathrm{B}}^* = \hbar^2\varepsilon_0/m^*e^2$ as the length

unit and the effective Rydberg $R^* = m^* e^4/2\hbar^2\varepsilon_0^2$ as the energy unit. For donors in GaAs, these units are $a_B^* \cong 100$ Å and $R^* \cong 5.7$ meV. $m^* = 0.0665\, m_0$ (m_0 is the free electron mass). The depth of the wells is 228 meV, which corresponds to an Al concentration—x equal to 0.3.

The binding energies of a hydrogenic donor impurity located in the centre of SQW, PQW, and VQW under the electric field as a function of the well width for different electric field values are given in Figs. 1–3, respectively. As seen in these figures, when the dimension of quantum wells increases, the impurity binding energy for all geometric confinement potentials increases until it reaches a maximum value, and then decreases. This behavior is related to the change of the electron confinement in quantum wells. When the dimension of well decreases, the confinement of electrons is strengthened, and therefore the impurity binding energy increases. When the dimension of quantum wells is reduced to a small limited value, most of the electronic wave function begins to leak out of the well and therefore the impurity binding energy decreases. As the electric field increases, the Coulombic interaction between the electron and a donor impurity located in the center of the wells decreases since the electron shifts to the left side of the wells. This case can be understood by analyzing the electron wave function under the electric field for all geometric confinement potentials (see the insets in Figs. 1–3). The field dependence of the binding energy in narrow well dimension is very weak, since the geometric confinement is predominant. But in the wider quantum wells, the binding energy is more sensitive to the external electric field.

In order to see the effects of different geometric confinement on the donor impurity binding energy, the variation of the ground state impurity binding energy in SQW, PQW and VQW structures

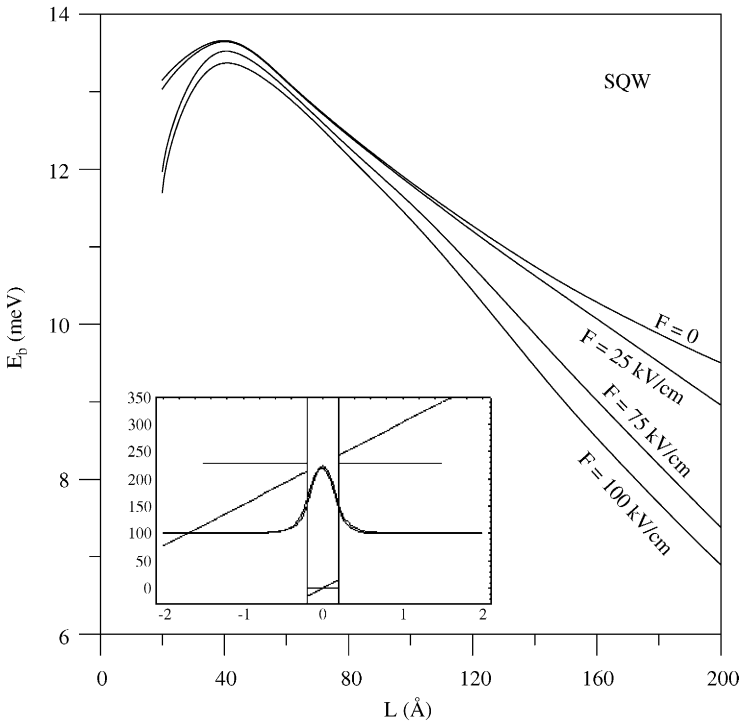

Fig. 1. The variation of the ground state binding energy of a hydrogenic donor impurity located in the centre of SQW under the electric field as a function of the well width for different electric field values. The inset shows the behavior of SQW potential and amplitude of normalized sub-band wave function of electron—$|\psi(\tilde{z})|^2$ versus the normalized position—$\tilde{z} = z/L$ (vertical line indicates the edges of barriers) under the electric field for cases $L = 40$ Å, $F = 0$ and 75 kV/cm.

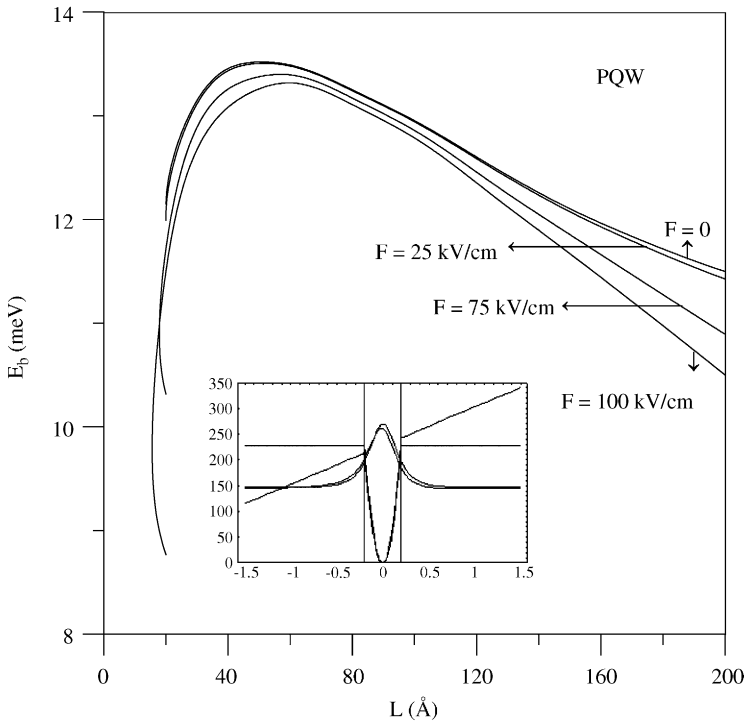

Fig. 2. The variation of the ground state binding energy of a hydrogenic donor impurity located in the centre of PQW under the electric field as a function of the well width for different electric field values. The inset shows the behavior of PQW potential and amplitude of normalized subband wave function of electron—$|\psi(\tilde{z})|^2$ versus the normalized position—$\tilde{z} = z/L$ (vertical line indicates the edges of barriers) under the electric field for cases $L = 40$ Å, $F = 0$ and 75 kV/cm.

as a function of the well width for $F = 0$ and 75 kV/cm electric field values is given in Fig. 4. As seen in these results, for small well dimensions ($20\,\text{Å} \leqslant L \leqslant 40\,\text{Å}$) impurity binding energy for SQW is greater than PQW and VQW, since the wave function of the electron becomes strongly localized in the square well. As the well dimension increases, the wave function of the electron becomes strongly localized in the VQW and PQW in comparison to the SQW and thus the impurity binding energies of VQW and PQW are greater than SQW.

The variation of the ground state impurity binding energy located in center of the SQW, PQW and VQW as a function of the electric field for two different well widths is given in Fig. 5. As seen in this figure; in the narrow wells, the binding energy in VQW in comparison to the SQW and PQW is weaker and it is sensitive to the electric field strength, since the electron becomes more energetic in narrow wells (see the inset in the Fig. 3). As the electric field increases, the impurity binding energy in the VQW decreases while it behaves nearly constant for SQW and PQW and for large electric field values, the electron penetrates to the left side of the well and bound states for VQW are not found. When the well dimension increases, the energy of the electron becomes weaker and the electron that approaches the well bottom begins to become sensitive to the electric field strength especially in SQW. For large well dimensions, the impurity binding energy decreases, since the probability of finding the electron and impurity in the same plane decreases, while the localization of the electron in the well increase.

The polarization effect depending on the electric field for different well widths of SQW, PQW and VQW is given in Fig. 6. For narrower wells (for example; $L = 40$ Å), the polarization is weaker and nearly constant for SQW and PQW, while the

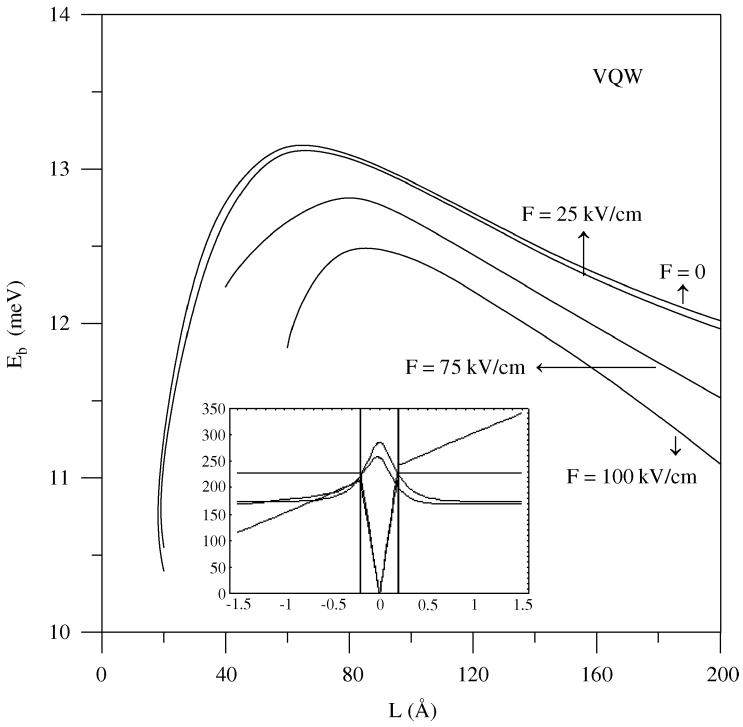

Fig. 3. The variation of the ground state binding energy of a hydrogenic donor impurity located in the centre of VQW under the electric field as a function of the well width for different electric field values. The inset shows the behavior of VQW potential and amplitude of normalized subband wave function of electron—$|\psi(\tilde{z})|^2$ versus the normalized position—$\tilde{z} = z/L$ (vertical line indicates the edges of barriers) under the electric field for cases $L = 40$ Å, $F = 0$ and 75 kV/cm.

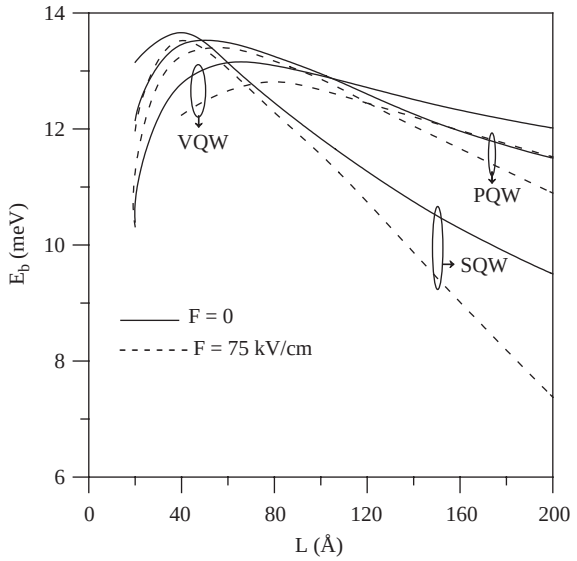

Fig. 4. The variation of the ground state impurity binding energy for SQW, PQW and VQW(or full graded) structures as a function of the well widths for $F = 0$ and 75 kV/cm electric field values.

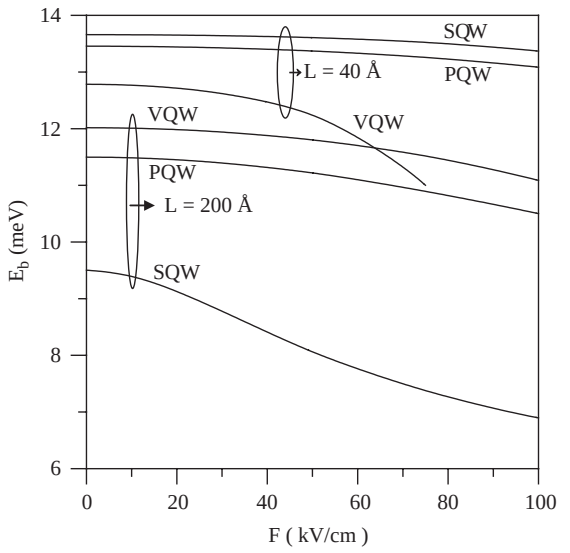

Fig. 5. The variation of the ground state impurity binding energy located in center of the wells (SQW, PQW and VQW) as a function of the electric field for two different well widths.

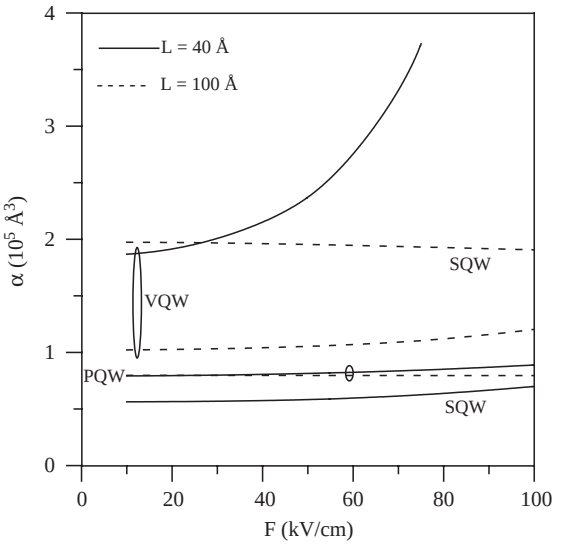

Fig. 6. The polarization effect depending on the electric field for different well widths of SQW, PQW and VQW. Solid curve: for $L = 40$ Å; dashed curve: $L = 100$ Å.

polarization is very sensitive to the electric field for VQW, as expected. We also find that the polarizibility increases as the well dimensions increase. But the polarizibility for PQW is nearly independent from both electric field strength and well width.

In summary, we have studied the binding energy of the hydrogenic impurities located at the center of different shaped quantum wells (SQW, PQW and VQW) under the electric field. The calculations were performed within the effective-mass approximation and by using a variational method. The dependence of the ground state impurity binding energy on the applied electric field, geometric shapes of the wells and well width was discussed together with the polarization effect. The results we obtained for SQW and PQWs are in good agreement with previous results. To the best of our knowledge, this is the first study for hydrogenic donor impurities in VQW. We expect that this method will be of great help for theoretical studies of the physical properties of VQW. Furthermore, the simplicity of the method will provide an interesting insight into the main physical properties of carriers in VQW.

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