ISSN 1330–0008
CODEN FIZAE4

DONOR BINDING ENERGY IN A PARABOLIC QUANTUM WELL

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Received 10 December 1999; revised manuscript received 30 June 2000
Accepted 11 December 2000

We solved the impurity problem in a parabolic quantum well. The binding energy of a neutral donor in GaAs-Al_x $Ga_{1-x}As$ parabolic quantum well is determined variationally. For a dopant at the well center, and at the edge of the well in the interface region, the changes in the binding energy of donors are calculated, for different well sizes and depths. The 2s excited state is reported.

PACS numbers: 68.65.+g UDC 538.971

Keywords: parabolic quantum well, GaAs-Al_x $Ga_{1-x}As$, neutral donor, 2s excited state

1. Introduction

Confinement impurity states in GaAs quantum wells have recently attracted considerable attention. The binding energies of donors [1,2] and acceptors [3] have been calculated as functions of well width and impurity position. Photoluminescence [4-8], Raman scattering and far-infrared (FIR) magneto-absorption [8] spectroscopies have been used to study the donors and acceptors in these structures. Photoluminescence associated with Si donors in n-type GaAs quantum wells was first reported by Shanabrook and Comas [4,5]. In their work, a donor-impurity associated feature below the ground-state heavy-hole exciton was observed and attributed to transitions between electrons on Si donors at the well centers and heavy holes in the topmost valence-band confinement state [Si (c) $\rightarrow$ VB]. This interpretation yielded donor binding energies significantly lower than the measurements using infrared on samples with similar characteristics, and than the calculated values which are in good agreement with the FIR data.

Here we present a complete study of a donor confined in a parabolic GaAs quantum well. All previous data concerned only impurities in square quantum wells. This parabolic structure is well known in designing infrared detectors with low leakage currents and low electric-field sensitivity [10,11], and in improving the optical confinement factors and enhancing the carrier collection into the thin quantum well to reduce the threshold current density [12,13]. The present work concerns the variation of donor impurity binding energy due to the change in the depth and size of the parabolic quantum well. Also, we considered two different positions of doping: impurity at the center of the well and off-center. The first two excited states of the impurity are calculated.

2. *Theory and calculation*

2.1. *Impurity at the center*

We are seeking for the eigenvalues of the following Hamiltonian for a confinement impurity in a parabolic quantum well

$$H = -\frac{\hbar^2}{2m_e}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)\right] - \frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z_e^2} + V_e(z_e) - \frac{e^2}{4\pi\epsilon_0\epsilon_r}\frac{1}{\sqrt{\rho^2+z_e^2}}\,. \tag{1}$$

We have used a trial wave function in the form of $\Psi_{\rm imp} = N\psi_e(z_e)\,{\rm e}^{-r/\lambda}$.

Here $r = \sqrt{\rho^2+z_e^2}$ is the total distance of the electron from the donor center, N the normalization constant, λ the variational parameter and $\psi_e(z_e)$ is the solution of the following Schrödinger equation for a single particle in a parabolic quantum well [14]

$$\frac{{\rm d}^2}{{\rm d}Z^2}\psi_e(Z) + (\theta^2 - V^2Z^2)\psi_e(Z) = 0, \qquad \text{for} \qquad |Z| \le 1 \tag{2}$$

$$\frac{{\rm d}^2}{{\rm d}Z^2}\psi_e(Z) - W^2\psi_e(Z) = 0, \qquad \text{for} \qquad |Z| > 1$$

where, $\theta^2 = 2m^*a^2E/\hbar^2$, $V^2 = 2m^*a^2V_0/\hbar^2$, and $W^2 = 2m^*a^2(V_0-E)/\hbar^2$. Here $Z = z/a$ and $2a$ and V_0 are the well width and depth, respectively. Substituting $\xi = VZ^2$ and $\Psi(\xi) = \exp(-\xi/2)\Phi(\xi)$ into Eq. (2), the solution of the new differential equation is the confluent hypergeometric function [14], $M(\alpha,\beta,\xi)$, with $\alpha = 0.25(1-\theta^2/V)$ and $\beta = 0.5$. It can be written as

$$\begin{aligned}\psi_e(Z) &= c_1\exp(-VZ^2/2)\,M(\alpha,\beta,\xi), \qquad \text{for} \qquad |Z| \le 1\\ &= c_2\exp[-W(|Z|-1)], \qquad \text{for} \qquad |Z| > 1\,.\end{aligned} \tag{3}$$

Applying the boundary conditions, the following transcendental equation is obtained

$$2M'(\alpha,\beta,V) - (1 - W/V)M(\alpha,\beta,V) = 0\,. \tag{4}$$

Solving Eq. (4), considering the confluent hypergeometric function $M(\alpha,\beta,V)$,we obtain the ground state of the impurity in a parabolic quantum well ($E_{\rm imp}$), which corresponds to the first root. The second root gives the 2s state. That is to say, the function M gives the even states. If we rewrite Eq. (4) in terms of the confluent hypergeometric function $U(\alpha, \beta, V)$, we obtain

$$2U'(\alpha, \beta, V) - (1 - W/V)U(\alpha, \beta, V) = 0\,. \tag{4'}$$

The first root of Eq. (4′) gives the 1p excited state. The donor binding energy is the difference between $E_{\rm imp}$ and the minimum value $E_{\rm min}$ of impurity Hamiltonian H. In our calculations, we considered $m_e = 0.067m_0$ (m_0 is the free-electron mass) and $\epsilon_r = 12.85$.

2.2. Impurity off center

If the impurity is doped at the position $z_{\rm imp}$, Eq. (1) can be written as

$$H = -\frac{\hbar^2}{2m_e}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)\right] - \frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial z_e^2} + V_e(z_e) - \frac{e^2}{4\pi\epsilon_0\epsilon_r}\frac{1}{\sqrt{\rho^2 + (z_e - z_{\rm imp})^2}}\,. \tag{5}$$

The total distance of the electron is $r = \sqrt{\rho^2 + (z_e - z_{\rm imp})^2}$.

3. Results and discussion

In Fig. 1 we plot the impurity binding energy (R_y^*) as a function of the well width, for three different values of Al content. The impurity binding energy has

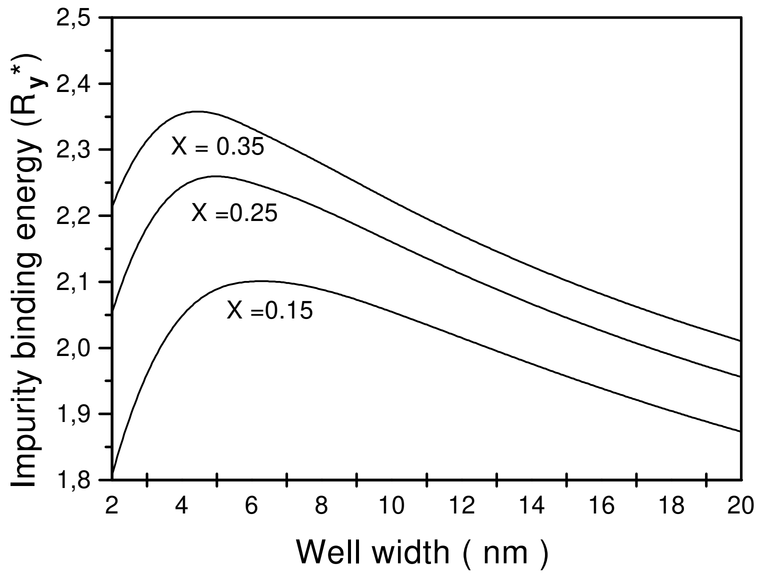

Fig. 1. Binding energy of a centered donor (E_b) in R_y^*, as a function of the well width (in nm*), at $x = 0.15,\ 0.25$ and 0.35.*

a large value as the well depth increases, but it decreases as its width increases. This behaviour is the same as in the square well in qualitatively way but not quantitatively. Here we notice that the impurity binding energy in the parabolic quantum well is higher than in the square well [2] (see Table 1).

Table 1. Binding energy of an impurity located at the well center for well depths of 25 and 50 R_y^* and for six different well widths. The values marked with an asterisk are the results for the square well [2].

Well depth	State	Well width (nm)					
		15	20	30	40	60	80
25 R_y^*	1s	1.92 1.85*	1.902 1.7*	1.773 1.46*	1.685 1.31*	1.570 1.133*	1.49 1.03*
	2s	.0.537 0.335*	0.525 0.323*	0.506 0.303*	0.492 0.290*	0.464 0.262*	0.444 0.244*
	1p	0.622 0.420*	0.614 0.412*	0.596 0.394*	0.580 0.378*	0.552 0.350*	0.532 0.332*
$50R_y^*$	1s	2.120 2.00*	2.020 1.73*	1.884 1.490*	1.794 1.33*	1.668 1.140*	1.585 1.04*
	2s	1.273 0.340*	1.281 0.330*	1.199 0.305*	0.813 0.288*	0.801 0.263*	0.800 0.245*
	1p	0.624 0.423*	0.616 0.414*	0.598 0.396*	0.582 0.380*	0.554 0.351*	0.534 0.330*

Figure 2 represents a change of the ground state (1s) binding energy as the impurity moves away from the well center. The impurity positions in Fig. 2 are normalized to the well width. We chose two different well widths, 20 and 40 nm and only one well depth (50 R_y^*). We obtained a decrease in the binding energy by almost $0.675R_y^*$ when the impurity moves from the center to a position equal to 0.5 of the well width (at well width of 20 nm). In a wider well (40 nm), the binding energy decreases by 0.794 R_y^* if it is displaced to the same position. That is to say, the binding energy of the ground state (1s), falls down more rapidly in wider wells than in a narrow one when it moves away from the center. However, if the donor is doped at the center, from Fig. 1 we see that the binding energy drops only by 0.21 R_y^* when changing the well dimensions from 4 to 20 nm. In other words, the doping impurity at the center is more confined than the off-center one.

The binding energies of the lower excited 2s and 1p states are shown in Fig. 3. The first excited 1p state takes place inbetween the states 1s and 2s. The binding energies of the excited states 1p and 2s decrease as the well width increases. Also, in the same way as in the ground state, the excited states' binding energies have larger values when the barrier height is increased. As a comparison between the parabolic results and the square well, we list in Table 1 some data for both wells.

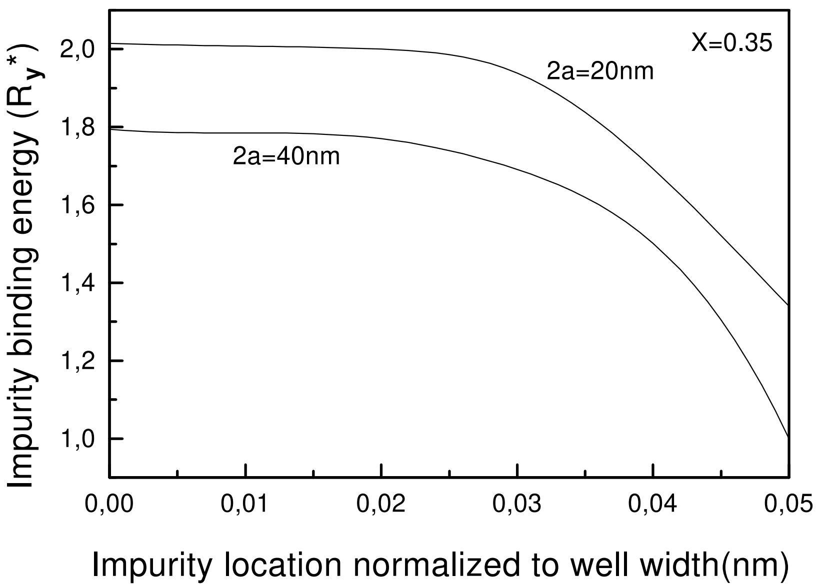

Fig. 2. Variation of E_b with the impurity location normalized to the well width. Here 1s *state is calculated for well widths 20 and 40* nm *and well depth of* 50 R_y^*.

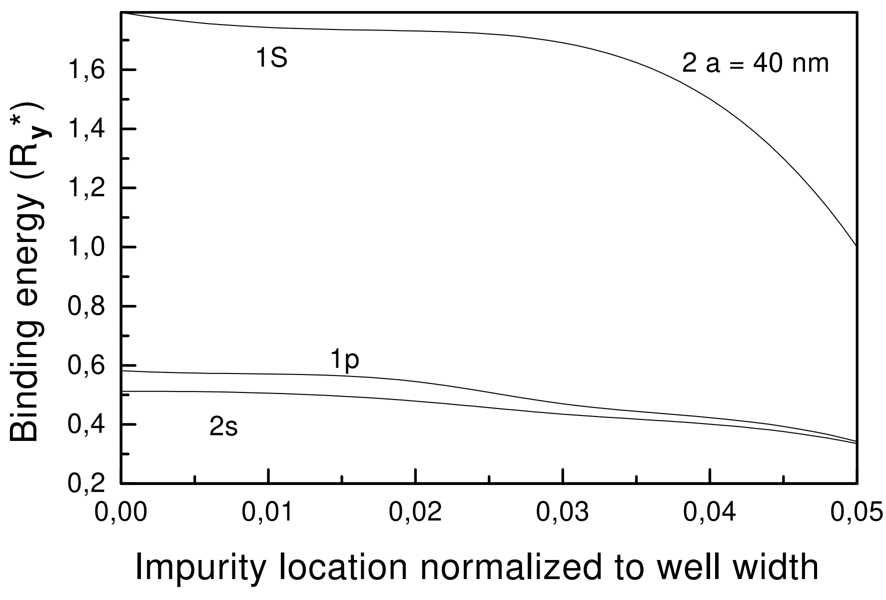

Fig. 3. E_b in R_y^* of 1s, 2s *and* 1p *states is plotted versus the well width for the well depth of* 50 R_y^*.

The results for the binding energies of the ground state for an off-center impurity, and for the lower excited 2s and 1p states, are listed in Table 2 as a function of the normalized impurity location.

We notice from Table 2 that 2s and 1p levels merge especially for wider wells, as is seen in Fig. 3.

As a comparison between our results with the avaliable data of the donor in a parabolic quantum well, Table 3 contains our results and the results of Ref. [15] for the same well.

Table 2. Variation of impurity binding energies versus impurity location (normalized to well width). Well depth is 50 R_y^* for all well widths.

Width (nm)	State	Normalized location					
		0	0.1	0.2	0.3	0.4	0.5
20	1s	2.020	2.008	2.000	1.939	1.693	1.340
	2s	0.545	0.533	0.502	0.449	0.421	0.401
	1p	0.614	0.591	0.576	0.554	0.483	0.468
30	1s	1.884	1.832	1.770	1.700	1.652	1.590
	2s	0.526	0.525	0.482	0.435	0.386	0.287
	1p	0.598	0.585	0.563	0.533	0.475	0.381
40	1s	1.794	1.785	1.770	1.691	1.651	1.544
	2s	0.512	0.506	0.479	0.435	0.401	0.335
	1p	0.582	0.571	0.545	0.470	0.423	0.342

Table 3. The variation of the impurity ground state in a parabolic quantum well, as a function of the well width. The asterix values are given from Fig 1 in Ref [15].

Well depth	State	Well width (nm)				
		15	20	30	40	60
36 R_y^*	1s	1.990	1.981	1.799	1.723	1.592
		2.106*	2.0*	1.84*	1.74*	1.6*

We see a good agreement between our results and those give in Ref. [15].

4. Conclusion

We have determined the binding energy of a donor at the center of the GaAs parabolic quantum wells. The binding energy of the off-center impurity is also calculated. Finally, we give the binding energies of excited states of a doped impurity at the well center. Our results for binding energy of excited states for a donor confined in a parabolic quantum well are qualitatively in a good agreement with the previous results [2] for the square quantum well, and those of the parabolic quantum well. The doping at the well center gives a larger binding energy than the off-center one.

References

[1] R. L. Greene and K. K. Bajaj, Phys. Rev. B **31** (1985) 913.

[2] H. Hassan and N. El-Meshad, phys. stat. sol.(b) **201** (1997) 381.

[3] W. T. Masselink, Y. C. Chang and H. Morkoc, Phys. Rev. B **32** (1985) 5190.

[4] B. V. Shanabrook and J. Comas, Sufr. Sci. **142** (1984) 504.

[5] B. V. Shanabrook, Sufr. Sci. **170** (1986) 449.

[6] Y. Nomura, K. Shinozaki and M. Ishii, J. Appl. Phys. **58** (5) (1985) 1864.

[7] B. V. Shanabrook et al., Phys. Rev. B **29** (1984) 7096.

[8] D. Gammon, R. Merlin, W. T. Masselink and H. Morkoc, Phys. Rev. B **33** (1986) 2919.

[9] A. A. Reeder, B. D. McCombe, F. A. Chambers and G. P. Devane, Superlatt. Microstruct. **4** (1988) 381.

[10] R. P. G. Karunasiri and K. L. Wang, Superlatt. Microstruct. **4** (1988) 661.

[11] D. Ka Samet, C. S. Hong, N. B. Patel and P. D. Dapkus, IEEE. J. Quantum Electron. Q. E. **19** (1983) 1025.

[12] G. Bastard, Phys. Rev. B **24** (1981) 4714.

[13] C. Mailhiot, Y. C. Chang and T. C. McGill, Phys. Rev. B **26** (1982) 4449.

[14] Wu-PenYuen, Phys. Rev. B **48** (1993) 17316.

[15] E. C. Niculescu, Phys. Lett. A **213** (1996) 85.

ENERGIJA VEZANJA DONORA U PARABOLIČKOJ KVANTNOJ JAMI

Riješili smo problem primjese u paraboličkoj kvantnoj jami. Energija vezanja neutralnog donora u GaAs-Al_x $Ga_{1-x}As$ paraboličkoj kvantnoj jami se rješava varijacijski. Izračunali smo energije vezanja donora ako je u sredini jame i ako je uz rub u međusloju, za različite širine i dubine jame. Izvješćujemo o uzbuđenom stanju 2s.