IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Effect of the Gamma -X crossover on the binding energies of confined donors in single $GaAs/Al_xGa_{1-x}As$ quantum-well microstructures

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1994 J. Phys.: Condens. Matter 6 10025

(http://iopscience.iop.org/0953-8984/6/46/019)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.151
The article was downloaded on 12/05/2010 at 21:07

Please note that terms and conditions apply.

J. Phys.: Condens. Matter 6 (1994) 10025–10030. Printed in the UK

Effect of the Γ–X crossover on the binding energies of confined donors in single GaAs/Al_xGa_{1-x}As quantum-well microstructures

A M Elabsy†

Department of Physics, Faculty of Science, United Arab Emirates University, PO Box 17551, Al-Ain, United Arab Emirates

Received 20 June 1994

Abstract. The present work investigates the effect of the Γ–X crossover pressure at low temperatures on the donor binding energies in single-quantum-well (QW) microstructures. It is found that, at a constant QW thickness, the predicted donor binding energies are enhanced with increasing pressure and then decreased when approaching the crossover pressure between the QW Γ states and the barrier X states. It is noticed that the pressure-dependent donor binding energies are mainly related to the changes in the dielectric constants and the effective masses of both materials.

1. Introduction

The man-made diamond anvil cell [1, 2] and the use of low-temperature photoluminescence measurements made it possible to study the electronic and optical properties of microstructure semiconductors such as GaAs/Al_xGa_{1-x}As under high hydrostatic pressures. These structures have had a considerable number of studies made on their optical and electronic properties under atmospheric pressure [3–9] and high hydrostatic pressures [10–18]. The high hydrostatic pressure changes their band structures from direct to indirect. The dropping of the X conduction band of the Al_xGa_{1-x}As barrier layer under the Γ conduction band of the GaAs quantum well (QW) layer due to the effect of high hydrostatic pressure leads to unconfined electrons to the QW.

The purpose of the present work is to study the effect of the Γ–X band crossing due to the applied hydrostatic pressure on confined donor electrons in single GaAs/Al_xGa_{1-x}As QWs at low temperatures.

2. Theory

Considering a confined donor electron in a finite GaAs QW of height $\mathcal{W}_0$ and thickness $L(0)$, and choosing the origin of the growth direction (z axis) to be at the centre of the QW, the effective mass Hamiltonian of this electron at high pressures, P (kbar) and low temperatures, T (K) can be written

$$\mathcal{H}(P,T) = \mathcal{I}(P,T) + \mathcal{V}(P,T,r) + \mathcal{W}(P,T,z). \tag{1}$$

† On leave from the Department of Physics, Faculty of Science, Mansoura University, Mansoura, Egypt.

0953-8984/94/4610025+06$19.50 © 1994 IOP Publishing Ltd

The first term $\mathcal{I}(P,T)$ in equation (1) represents the pressure-dependent kinetic energy operator at low temperatures which is expressed as

$$\mathcal{I}(P,T) = -[1/2m_{\mathrm{w,b}}(P,T)]\nabla^2. \qquad (2)$$

The two subscripts w and b stand for the QW and the barrier layers, respectively. The QW effective mass $m_{\mathrm{w}}(P,T)$ is given [19] by

$$m_{\mathrm{w}}(P,T) = 1/[\![1 + 7.51\{2/\Gamma_{\mathrm{w}}(P,T) + [\Gamma_{\mathrm{w}}(P,T) + 0.341]^{-1}\}]\!] \qquad (3)$$

where $\Gamma_{\mathrm{w}}(P,T)$ eV is the pressure-dependent QW energy gap at the Γ point and at low temperatures. It is expressed as

$$\Gamma_{\mathrm{w}}(P,T) = 1.519 + \alpha_{\mathrm{w}}^{\Gamma}P - 5.405 \times 10^{-4}T^2/(T + 204) \qquad (4)$$

where $\alpha_{\mathrm{w}}^{\Gamma}$ is the measured pressure coefficient of the QW at the Γ point as given in table 1. The barrier effective mass $m_{\mathrm{b}}(P,T)$ is taken [20] as

$$m_{\mathrm{b}}(P,T) = m_{\mathrm{w}}(P,T) + 0.083x \qquad (5)$$

where x is the aluminium concentration in the $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ layer. The second term $\mathcal{V}(P,T,r)$ is the Coulomb-potential energy operator which represents the interaction between the donor ion and its associated electron as a function of high hydrostatic pressure and low temperature and is expressed as

$$\mathcal{V}(P,T,r) = -1/[\epsilon_{\mathrm{w,b}}(P,T)r] \qquad (6)$$

where $r = (\rho^2 + z^2)^{1/2}$ and $\rho = (x^2 + y^2)^{1/2}$ is the position of the electron in the x–y plane of the GaAs QW which is parallel to the interfaces. $\epsilon_{\mathrm{w}}(P,T)$ and $\epsilon_{\mathrm{b}}(P,T)$ are the static dielectric constants for QW and barrier materials, respectively, as functions of pressure and temperature. $\epsilon_{\mathrm{w}}(P,T)$ for the QW is determined [21] from the relation

$$\epsilon_{\mathrm{w}}(P,T) = \epsilon(0,T)\exp(\delta P) \qquad (7)$$

where

$$\epsilon(0,T) = \epsilon_0(T_0)\exp[\gamma_0(T - T_0)]. \qquad (8)$$

The values of $\epsilon_0(T_0)$, γ_0 and δ at the reference temperature T_0, and the equivalent temperature range, are listed in table 2. $\epsilon_{\mathrm{b}}(P,T)$ for the barrier material can be expressed [20] as

$$\epsilon_{\mathrm{b}}(P,T) = \epsilon_{\mathrm{w}}(P,T) - 3.12x. \qquad (9)$$

The last term in the Hamiltonian $\mathcal{W}(P,T,z)$ stands for the pressure-dependent potential energy barrier operator which confines the electrons to the QW and its height is given by

$$\mathcal{W}(P,T,z) = \begin{cases} 0 \\ \mathcal{W}_0(P,T) \end{cases} \quad \text{for} \begin{cases} |z| \leqslant L(P)/2 \\ |z| \geqslant L(P)/2 \end{cases} \qquad (10)$$

where

$$\mathcal{W}_0(P,T) = \begin{cases} \Gamma_{\mathrm{b}}(P,T) - \Gamma_{\mathrm{w}}(P,T) \\ \mathrm{X}_{\mathrm{b}}(P,T) - \Gamma_{\mathrm{w}}(P,T) + S_{\Gamma\mathrm{X}}(P) \end{cases} \quad \text{for} \begin{cases} P \leqslant P_1 \\ P_1 < P \leqslant P_2 \end{cases} \qquad (11)$$

and

$$S_{\Gamma X}(P) = S_0 x(P - P_1)/P. \tag{12}$$

In the above equations, P_1 is the crossover pressure between the X_b conduction band and the Γ_b band and P_2 is the crossover pressure between the X_b conduction band and the Γ_w band. In equation (12), $S_{\Gamma X}(P)$ is the pressure-dependent Γ–X mixing strength coefficient and S_0 is an adjustable parameter which is used to match the predicted energy at P_1 with the experimental result. The value of $\Gamma_{w,b}(P, T)$ is determined according to the relation

$$\Gamma_{w,b}(P, T) = \Gamma_{w,b}(0, T) + \alpha^{\Gamma}_{w,b} P \tag{13}$$

where $\Gamma_{w,b}(0, T)$ is the standard value of the conduction Γ minima at atmospheric pressure ($P = 0$) and a low temperature T. $\alpha^{\Gamma}_{w,b}$ is the corresponding pressure coefficient for the two layers. Similarly,

$$X_b(P, T) = X_b(0, T) + \alpha^X_b P. \tag{14}$$

The values of $\Gamma_b(0, T)$, $X_b(0, T)$, T, $\alpha^{\Gamma}_{w,b}$, and α^X_b are given in table 1.

Table 1. Values for all parameters used in present work which are taken from photoluminescence measurements [10, 17].

L (Å)	200
x (au)	0.3
$\Gamma_b(0, T)$ (eV)	1.755
$X_b(0, T)$ (eV)	1.918
$\alpha^{\Gamma}_{w,b}$ (meV kbar^{-1})	10.7
α^X_b (meV kbar^{-1})	−1.3
T (K)	4
P_1 (kbar)	13.5
P_2 (kbar)	33.2

Table 2. The experimental values [21] of the static dielectric constant, and its logarithmic temperature and pressure derivatives for the GaAs QW at the reference temperature T_0 and the corresponding temperature range.

T (K)	T_0 (K)	$\epsilon_0(T_0)$ (au)	γ_0 (10^{-5} K^{-1})	δ (10^{-4} kbar^{-1})
$0 \leqslant T \leqslant 200$	75.6	12.74	9.4	−16.7
$T > 200$	300.0	13.18	20.4	−17.3

Since equation (1) cannot be solved analytically, a trial wavefunction is chosen [18] as

$$\Psi(r, z) = \Lambda \exp(-\chi r) \begin{cases} \cos(\zeta z) \\ C \exp(-\kappa |z|) \end{cases} \quad \text{for} \begin{cases} |z| \leqslant L(P)/2 \\ |z| \geqslant L(P)/2 \end{cases} \tag{15}$$

where Λ is a normalization constant, χ is a variational parameter,

$$\zeta = [2m_w(P, T) E_0(P, T)]^{1/2} \tag{16}$$

and

$$\kappa = \{2m_b(P,T)[\mathcal{W}_0(P,T) - E_0(P,T)]\}^{1/2}. \tag{17}$$

The factor C can be obtained by applying the boundary conditions on the longitudinal part of the wavefunction Ψ and its derivative $[1/2m_{w,b}(P,T)]\partial\Psi/\partial z$ [22–24] at the interfaces $|z| = L(P)/2$. The lowest electronic energy $E_0(P,T)$ in the QW can be obtained to satisfy the transcendental equation [9, 18]

$$\tan[\zeta L(P)/2] = \{[m_w(P,T)/m_b(P,T)][\mathcal{W}_0(P,T)/E_0(P,T) - 1]\}^{1/2}. \tag{18}$$

The band crossing-dependent binding energies of the confined donors in the GaAs QW at low temperatures is calculated from the expression

$$E_b(P,T) = E_0(P,T) - \mathcal{E}_{min}(P,T) \tag{19}$$

where $\mathcal{E}_{min}(P,T)$ is the minimum expectation energy of the donor electron which is given by

$$\mathcal{E}_{min}(P,T) = \min\langle\Psi|\mathcal{H}(P,T)|\Psi\rangle. \tag{20}$$

3. Results and discussion

Figure 1 shows a comparison of the predicted pressure-dependent lowest energies $E_0(P,T)$ for both band crossing (solid curve) and neglecting band crossing (broken curve) with the experimental values (full circles) [17]. It is seen from figure 1 that values which neglect band crossing (broken curve) are nearly a straight line while those taking into account the band crossing (solid curve) with an adjustable parameter of $S_0 = 250$ meV and an effective mass of the X band as given in equation (5) are in good agreement with the experimental values. It must be pointed out that large values of the effective mass of the X band such as $m^X(P,T) = (0.85\text{–}0.14)x$ [20] has led to lower values of the predicted lowest energies $E_0(P,T)$, even with large values of S_0. From this finding it is clear that the X band effective mass should not be very heavy relative to the Γ band effective mass which is the same finding as obtained by Mendez *et al* [25], who reported tunnelling through indirect-gap semiconductor barriers under hydrostatic pressure.

Figure 2 exhibits the pressure-dependent binding energies $E_b(P,T)$ at a low temperature of 4 K of confined donors to a single GaAs–$Al_{0.3}Ga_{0.7}As$ QW of thickness $L(0) = 200$ Å. The solid curve takes into account the band crossing with $S_0 = 250$ meV and an effective mass of the X band as given by equation (5), while the broken curve neglects the band crossing. It is seen from the figure that the binding energies of both curves are enhanced with increasing pressure. It is also seen from figure 2 that the energy values of the solid curve are not affected by the first crossover point P_1 between the X_b and the Γ_b valleys. The increase in energies arises because the dielectric constants decrease with increasing pressure and lead to low expectation potential energies. Furthermore the enhancement of the effective masses with increasing pressure leads to a decrease in the expectation kinetic energies which in turn enhance the binding energy values. All these effects due to the pressure dependence of both the dielectric constants and the effective masses overcome the decrease in the lowest energies due to the band crossing and end up with enhancement in the binding energies.

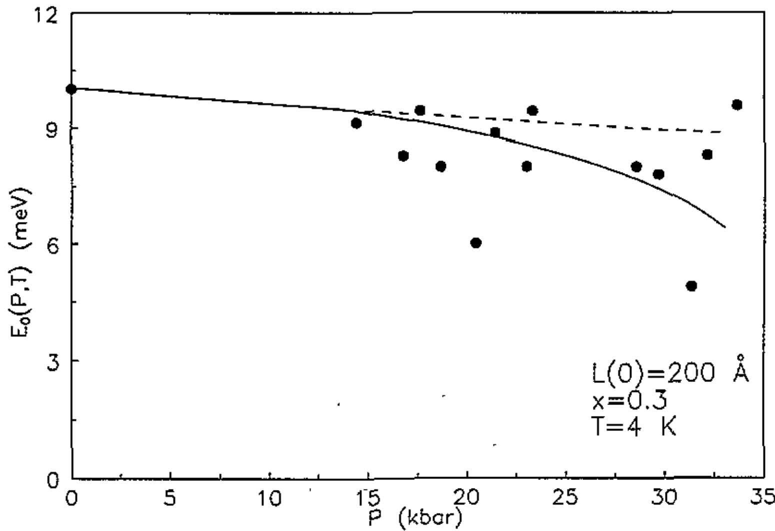

Figure 1. The pressure-dependent lowest energy $E_0(P, T)$ for band crossing (——) neglecting band crossing (– – –) and the experimental results [17] (●) for a 200 Å single GaAs–$Al_{0.3}Ga_{0.7}As$ QW at a low temperature of 4 K.

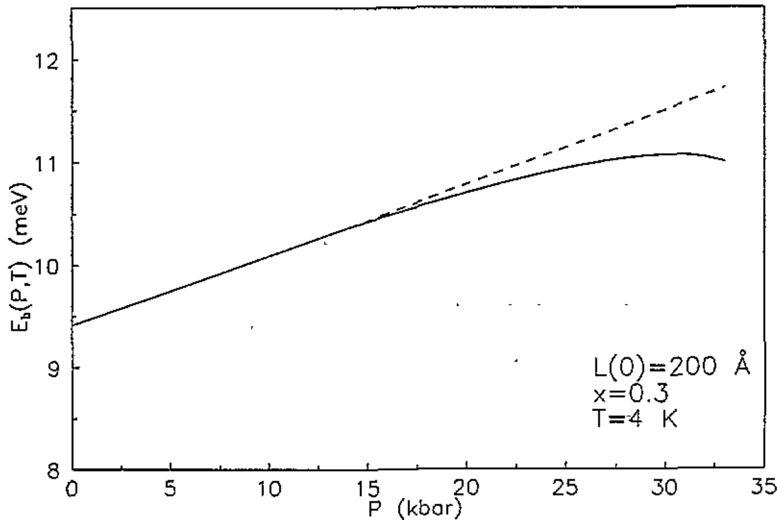

Figure 2. The predicted donors binding energies $E_b(P, T)$ for both band crossing (——) and neglecting band crossing (– – –) versus the high hydrostatic pressure P for a 200 Å single GaAs–$Al_{0.3}Ga_{0.7}As$ QW at a low temperature of 4 K.

For the solid curve the behaviour of the increased binding energies continued until the applied hydrostatic pressure approaches the second critical crossover pressure P_2 between the X_b band and the Γ_w band and then starts to decrease. This decrease in fact is related to the continuous decrease in the barrier height that confines the electrons to the QW, which becomes shallower as the P_2-value is reached as seen from figure 2. The discrepancy

between the two curves arises because the barrier height that confines the electrons to the QW becomes shallower with increasing pressure when the band crossing is included than when it is neglected. The behaviour of the predicted binding energies of the present work is in good agreement with that reported in the recent work by Dutisseuil *et al* [26] who have found a decrease in the current with increasing pressure in $GaAs/Al_xGa_{1-x}As$ superlattice oscillators.

4. Conclusion

The donor binding energies in single QWs at low temperatures are pressure dependent. The Γ–X crossing changes the binding energy of donor dramatically, especially when the hydrostatic pressure reaches the Γ_w–X_b crossover point P_2. The barrier effective mass in the crossing region is an effective parameter in determining the binding energies of donors in single-QW microstructures.

References

[1] Welber B, Cardona M, Kim C K and Rodriguez S 1975 *Phys. Rev.* B **12** 5729
[2] Jayaraman A 1983 *Rev. Mod. Phys.* **55** 65
[3] Bastard G 1981 *Phys. Rev.* B **24** 4714
[4] Greene R L and Bajaj K K 1983 *Solid State Commun.* **45** 825
[5] Csavinszky P and Elabsy A M 1985 *Phys. Rev.* B **32** 6498
[6] Shanabrook B V and Comas J 1984 *Phys. Rev.* B **29** 7096
[7] Liu X, Petrou A, McCombe B D, Ralston J and Wicks G 1988 *Phys. Rev.* B **38** 8522
[8] Elabsy A M 1992 *Phys. Rev.* B **46** 2621
[9] Kopf R F, Herman M H, Schnoes M L, Perley A P, Livescu G and Ohring M 1992 *J. Appl. Phys.* **71** 5004
[10] Wolford D J and Bradley J A 1985 *Solid State Commun.* **53** 1069
[11] Wolford D J, Kuech T F, Bradley J A, Gell M, Ninno D and Jaros M 1986 *J. Vac. Sci. Technol.* B **4** 1043
[12] Venkateswaran U, Chandrasekhar M, Chandrasekhar H R, Vojak B A, Chamber F A and Meese J M 1986 *Phys. Rev.* B **33** 8416
[13] Lefebvre P, Gil B and Mathieu H 1987 *Phys. Rev.* B **35** 5630
[14] Wolford D J, Kuech T F, Steiner T W, Bradley J A, Gell M A, Ninno D and Jaros M 1988 *Superlatt. Microstruct.* **4** 525
[15] Masumoto Y, Kinoshita Y, Shimomura O and Takemura K 1989 *Phys. Rev.* B **40** 11 772
[16] Wang L, Jia W, Tang R, Wang Y, Zhou J, Ge W and Wang B 1990 *Superlatt. Microstruct.* **7** 175
[17] Burnett J H, Cheong H M, Paul W, Koteles E S and Elman B 1993 *Phys. Rev.* B **47** 1993
[18] Elabsy A M 1992 *Phys. Scr.* **46** 473
[19] Aspnes D E 1976 *Phys. Rev.* B **14** 5331
[20] Adachi S 1985 *J. Appl. Phys.* **58** R1
[21] Samara G A 1983 *Phys. Rev.* B **27** 3494
[22] Morrow R A and Brownstein K R 1984 *Phys. Rev.* B **30** 678
[23] Liu H C 1987 *Superlatt. Microstruct.* **3** 413
[24] Einevoll G T and Hammer P C 1988 *J. Phys. C: Solid State Phys.* **21** L1193
[25] Mendez E E, Callejia E and Wang W I 1986 *Phys. Rev.* B **34** 6026
[26] Dutisseuil E, Sibille A, Palmier J F, Aristone F, Mollot F and Thierry-Mieg V 1994 *Phys. Rev.* B **49** 5093