Effect of nonparabolicity of the GaAs conduction band on the binding energy of a hydrogenic donor in a GaAs/$Ga_{1-x}Al_xAs$ quantum dot

A.M. Elabsy [1]

Department of Physics, Faculty of Science, United Arab Emirates University, P.O. Box 17551, Al-Ain, UAE

P. Csavinszky

Department of Physics and Astronomy, University of Maine, Orono, Maine 04469, USA

Received 14 January 1994

The conduction band of GaAs in known to be nonparabolic. The effect of this nonparabolicity on the binding energy of a donor in a $Ga_{1-x}Al_xAs$/GaAs/ $Ga_{1-x}Al_xAs$ quantum well has been found to be significant. Motivated by this fact, we have carried out variational calculations for the assessment of the effect of nonparabolicity on the binding energy of a donor in a GaAs/$Ga_{1-x}Al_xAs$ quantum dot. We have considered a finite confining potential and carried out calculations for Al concentrations of $x = 0.30$ and $x = 0.45$. We find that the effect of nonparabolicity consists in increasing the magnitude of the binding energy of the donor. This result is similar to that found for a donor in a quantum well.

Reduced dimensionality structures, such as a quantum well (QW), a quantum-well wire (QWW), or a quantum dot (QD), can be fabricated by chemical vapor deposition (CVD) [1,2], and molecular-beam epitaxy (MBE) [3–5]. Impurity atoms in these structures are expected to have different binding energies than the same impurity atoms in the bulk semiconductor.

The much studied structures are the following: the quasi two-dimensional QW, such as a GaAs slab sandwiched between two semi-infinite $Ga_{1-x}Al_xAs$ blocks, the quasi one-dimensional QWW, such as a GaAs wire placed in an infinite $Ga_{1-x}Al_xAs$ matrix, and the quasi zero-dimensional QD, such as a GaAs sphere placed in a $Ga_{1-x}Al_xAs$ bulk.

The binding energy of a hydrogenic donor in a $Ga_{1-x}Al_xAs$ QW was calculated by Bastard [6] by a variational approach. The binding energy of a hydrogenic donor

[1] On leave from the Department of Physics, Faculty of Science, Mansoura Universitiy, Mansoura, Egypt.

© J.C. Baltzer AG, Science Publishers

in a $GaAs/Ga_{1-x}Al_xAs$ QWW of circular cross section was calculated by Brown and Spector [7] via a variational approach. The effect of changing the shape of the cross-section of the QWW was studied by Bryant [8]. Recently Porras-Montenegro and Pérez-Merchancano [9] investigated the binding energy of hydrogenic impurities in a $GaAs/Ga_{1-x}Al_xAs$ QD of radius R, also by a variational approach.

The screening of a donor ion by the valence electrons of GaAs in a QW was considered by Csavinszky and Elabsy [10], who used an analytical screening function obtained by Resta [11]. The screening of the donor ion by the valence electrons of GaAs in a QWW of circular cross-section was studied by Csavinszky and Oyoko [12]. Recently, Elabsy and Csavinszky [13] have considered the effect of screening of a donor by the valence electrons of GaAs in a QD. All three of the last references made use of variational formulations of the problems.

In all of the above calculations the donor electron was described by a constant scalar effective mass. It is, however, known that the conduction band of GaAs deviates from the parabolic form. The effect of nonparabolicity on the binding energy of a donor in a $Ga_{1-x}Al_x/GaAs/Ga_{1-x}Al_xAs$ QW was studied by Chaudhuri and Bajaj [14] who considered a finite confining potential. A similar calculation was performed by Csavinszky and Elabsy [15]. Both of these calculations made use of an energy-dependent effective mass for the calculation of the binding energies of hydrogenic donors placed in on-center [14] and off-center [15] positions in the GaAs QW.

In this paper we study the effect of nonparabolicity on the binding energy of a donor in a $GaAs/Ga_{1-x}Al_xAs$ QD. We restrict ourselves to the case of a donor located at the center of a QD of radius R. Our approach is a variational approach, and our units are atomic unites (unit of energy is the hartree, unit of length is the bohr).

The Hamiltonian for a donor in the center of a spherical QD of radius R is given by

$$H = -\frac{1}{2m^*}\nabla^2 - \frac{1}{\epsilon_0 r} + V_b(r)\,, \tag{1}$$

where m^* is an energy dependent effective mass, $\epsilon_0 = 12.58$ is the static dielectric constant of GaAs, and $V_b(r)$ is the confining potential which is given by

$$V_b(r) = \begin{cases} 0, & r \leqslant R\,, \\ V_0, & r \geqslant R\,. \end{cases} \tag{2}$$

By assuming that 60% of the energy band gap discontinuity is related to the conduction band [16], Batey et al. obtained with this assumption

$$V_0 = 0.60\,\Delta E_g^{\Gamma}\,, \tag{3a}$$

where ΔE_g^{Γ} is the difference in the band gaps of $Ga_{1-x}Al_xAs$ and GaAs at the Γ-point

$$\Delta E_g^\Gamma(eV) = 1.247x; \quad x \leqslant 0.45 . \tag{3b}$$

For the effective mass m^*, Hrivnak [17] obtained the expression

$$m^* = m^{*\Gamma} + \frac{E}{\gamma} . \tag{4}$$

In eq. (4), $m^{*\Gamma}$ is the electronic effective mass at the Γ-point, $m^{*\Gamma} = 0.0665$, E is the energy expressed in eV units, and $\gamma = 9.41$ eV.

Our variational trial function for the case of a finite confining potential is of the form

$$\Psi(r) = \begin{cases} \dfrac{N \sin(\zeta_{10} r)}{r} \mathrm{e}^{-\lambda r}, & r \leqslant R , \\ N \dfrac{1}{r} \sin(\zeta_{10} R) \mathrm{e}^{\chi_{10}(R-r)} \mathrm{e}^{-\lambda r}, & r \geqslant R , \end{cases} \tag{5}$$

where N is a normalization constant given in ref. [10], and λ is a variational parameter. Finally, $\chi_{10} = [2m^*(V_b - E_{10})]^{1/2}$ and $\zeta_{10} = \pi/R$.

The binding energy, $E_b(r)$, of a donor is defined as the ground-state energy, E_{10}, minus the impurity ground state energy, $\zeta_{min}(R)$, which is given by

$$E_b(R) = E_{10} - \zeta_{min}(R) . \tag{6}$$

In eq. (6), E_{10} is given by solving the transcendental equation [18]

$$-[(V_b/E_{10} - 1]^{-1/2} = \tan(\zeta_{10} R) . \tag{7}$$

By extremalizing $\zeta(R)$, the expectation value of H in eq. (1), with respect to the variational parameter λ, we obtain $\zeta_{min}(R)$.

The results of our variational calculations for $x = 0.30$ and $x = 0.45$ are given in figs. 1 and 2. Note that the figures are drawn in meV and Å units.

It is seen from both fig. 1 and fig. 2 that the conduction band nonparabolicity of GaAs has a significant effect on the binding energy of a donor placed at the center of a spherical QD. It is also seen from these figures that the effect increases as the radius of the QD decreases. It is also evident from the figures that the binding energy, both for the parabolic and for the non-parabolic cases, increases at first as the QD radius decreases, reaches a maximum, and then starts decreasing as the QD radius decreases further. The figures permit yet another observation, namely they show that the maxima in the binding energy do not occur at the same value of R for the parabolic and for the non-parabolic cases. A similar conclusion has been reached earlier, when comparing the binding energy of a donor in the parabolic and non-parabolic cases [15].

To conclude, we point out that ~ 100 nm structures can now be grown and, for these, the effect of the nonparabolicity of the GaAs conduction band on the binding energy of a donor becomes important.

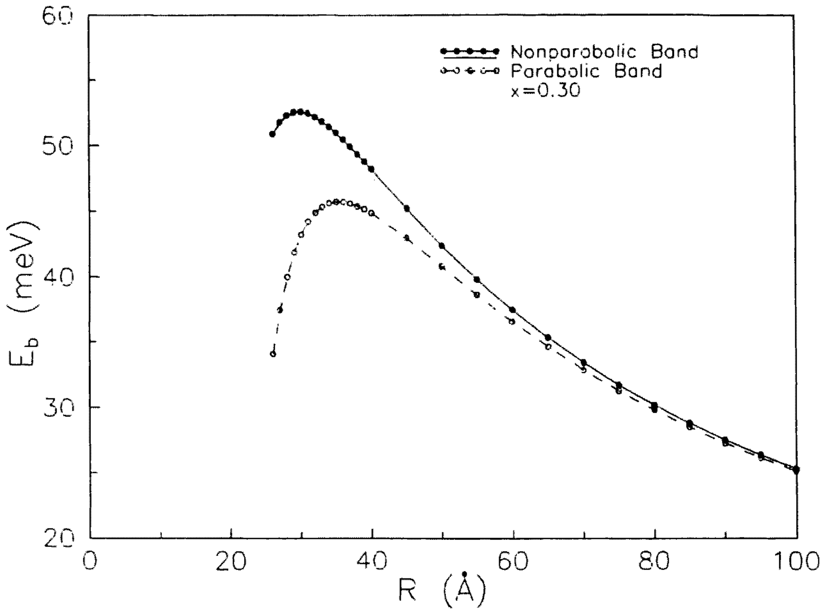
Nonparabolic Band
Parabolic Band
x=0.30
60
50
40
30
20
0
20
40
60
80
100
E_b (meV)
R (Å)

Fig. 1.

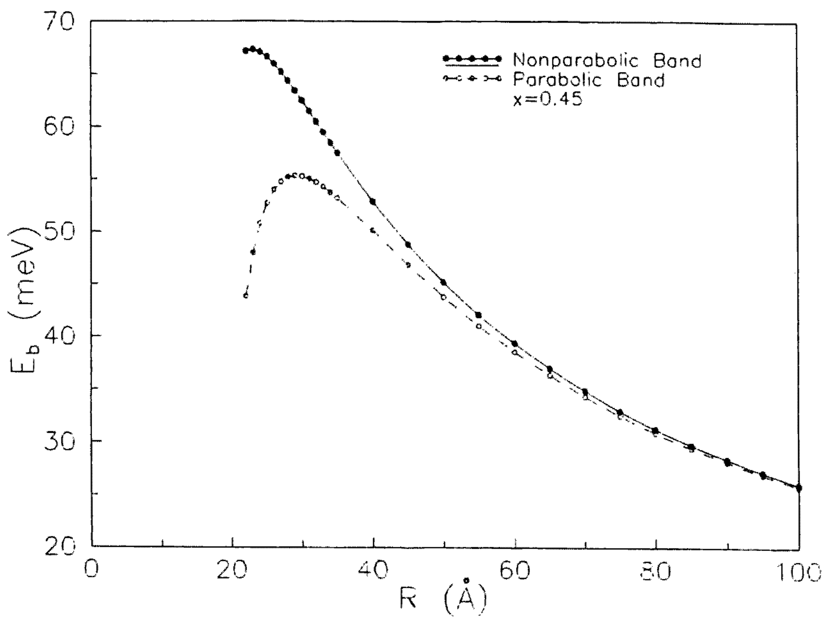
Nonparabolic Band
Parabolic Band
x=0.45
70
60
50
40
30
20
0
20
40
60
80
100
E_b (meV)
R (Å)

Fig. 2.

References

[1] H.M. Manasevit, J. Electrochem. Soc. 118 (1971) 647.
[2] R.D. Dupuis and P.D. Dapkus, in: *7th Int. Symp. on GaAs and Related Compounds*, St. Louis, 1978, ed. C.M. Wolfe (Institute of Physics, London, 1979) pp. 1–9.
[3] A.Y. Cho, J. Appl. Phys. 42 (1971) 2074.
[4] E.H.C. Parker, *The Technology and Physics of Molecular Beam Epitaxy* (Plenum Press, New York, 1985).
[5] J. Cibert, P.M. Petroff, G.J. Dolan, S.J. Pearton, A.C. Gossard and J.H. English, Appl. Phys. Lett. 49 (1986) 1275.
[6] G. Bastard, Phys. Rev. B24 (1981) 4714; Surf. Sci. 113 (1982) 165.
[7] J.W. Brown and H.N. Spector, J. Appl. Phys. 59 (1986) 1179.
[8] G.W. Bryant, Phys. Rev. B31 (1985) 7812.
[9] N. Porras-Montenegro and S.T. Merchancano, Phys. Rev. B46 (1992) 9780.
[10] P. Csavinszky and A.M. Elabsy, Phys. Rev. B32 (1985) 6498.
[11] R. Resta, Phys. Rev. B16 (1977) 2717.
[12] P. Csavinszky and H. Oyoko, J. Math. Chem. 9 (1992) 197; Phys. Rev. B43 (1991) 9262.
[13] A.M. Elabsy and P. Csavinszky, Croat. Chem. Acta, accepted for publication.
[14] S. Chaudhuri and K.K. Bajaj, Phys. Rev. B29 (1984) 1803.
[15] P. Csavinszky and A.M. Elabsy, Int. J. Quant. Chem.: Quant. Chem. Symp. 22 (1988) 25.
[16] J. Batey and S.L. Wright, J. Appl. Phys. 59 (1986) 200.
[17] L. Hrivnák, J. Appl. Phys. 71 (1992) 4370.
[18] In ref. [9], this equation has the exponent $1/2$ but the correct exponent is $(-1/2)$. We have also found misprints in eqs. (19), (22), and (23). In the second term of the denominator of eq. (19), the term ζ_{10} should be ζ_{10}^2. In eq. (22), the exponential is not $e^{-2\lambda R}$ but $e^{-2\lambda r}$. In eq. (23), the numerator is not $e^{-2}(\chi_{10} + \lambda)r$ but $e^{-2(\chi_{10}+\lambda)r}$.