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1 Introduction

Recent experimental studies of low-temperature photoluminescence in InAs self-assembled quantum dots (SAQDs) embedded in GaAs matrix have been performed under hydrostatic pressures P up to 70 kbar [1–4]. Reference [5] has been devoted to a theoretical study of the photoluminescence peak energies as a function of the hydrostatic pressure in SAQDs modelled by a parabolic cylinder-shaped. Nevertheless, the experimental shape and dimensions of the InAs SAQDs are not always well determined and a degree of freedom remains. It is well known that different shapes yield different results, as shown in Ref. [6] when comparing the electronic properties between a cylindrical and a lens shape SAQD. Therefore, it is important to study theoretically the influence of the hydrostatic pressure on a SAQD when the shape is characterized by a full lens symmetry with maximum height b and circular cross section of radius a with $b < a$. This is the purpose of the present work.

Previous theoretical studies in a lens shape [7–9] considered infinite wall potential. Nevertheless, the variation of the band offset is a fundamental parameter when considering the variation of the hydrostatic pressure. Then, it is necessary to extend the model to one which includes a finite barrier potential. This work is also advanced in this case. The results are compared with the case when infinite barrier is considered and the results show that it is possible to use the simple infinite hard wall model introducing an effective dot radius as a fitting parameter.

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2 Effect of the pressure

2.1 Finite barrier model

The eigenvalue problem of the Schrödinger equation in a 3D lens shape with infinite barriers in the effective mass approximation has been solved elsewhere [7]. In our case, the problem for a finite barrier will be modelled including a lens-shape well potential with height V_0 in a hard-walls semi-spherical region has shown in Fig. 1. The semi-spherical region is divided in two regions, D_{out} with potential V_0 and region D_{in} where is zero. The distance Δ between the contour C_1 and C_2 should be large enough to guarantee that the obtained eigenvalue corresponds to finite barrier case. On the other hand, in first approximation, we will consider the same effective mass in both regions D_{in} and D_{out}. Hence, we have the equation:

$$-\frac{\hbar^2}{2m^*}\nabla^2\Psi + V(r,\theta)\,\Psi = E\Psi, \qquad (r,\theta,\phi)\in D = D_{\text{in}} + D_{\text{out}}\,, \tag{1}$$

where the potential $V(r,\theta)$ is zero in D_{in} and V_0 in D_{out}. The solution of Eq. (1) is seek in the form of an expansion

$$\Psi^{(a,b)} = \sum_i C_i \Psi_i^{(0)}\,, \tag{2}$$

and the set of functions $\{\Psi_i^{(0)}\}$ are a complete set of functions in the semi-sphere (see Ref. [7]). We implemented a diagonalization procedure to obtain the electron and hole ground states. With the former expansion the functions $\Psi^{(a,b)}$ satisfy the boundary condition of infinite barrier in the contour C_1 because the set of functions $\{\Psi^{(0)}\}$ does. It can also be shown that the matching conditions at the contour C_2 are also satisfied, but only at those points where it is well-defined the derivative of the wavefunction. This does not occur at the corner and, generally speaking, the problem is then not well-defined. The obtained eigenvalues constitute only an estimation of the real problem but we accept this solution as the better one. Full details of the present model will be discussed in a future paper.

2.2 Effect of the hydrostatic pressure on the parameters

When considering the effect of the pressure on the energy levels, the three main factors to be considered are the change in volume, the change in the band offset of the lens-well and the change in the value of the effective masses.

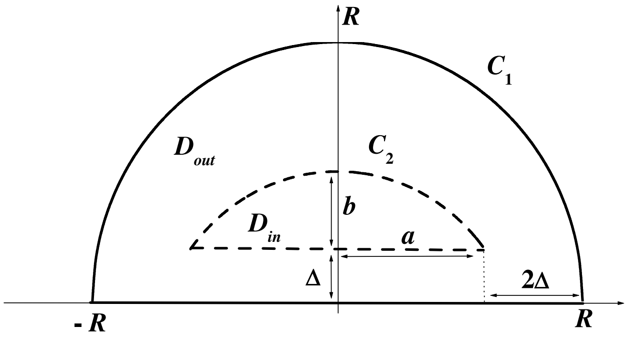

Fig. 1 Finite lens-well D_{in} with barrier height V_0 and contour C_2 inside an infinite semispherical-well with contour C_1. Contours C_1 and C_2 are separated by a distance equal or greater than Δ along the perpendicular axis.

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The hydrostatic pressure effect on the geometric dimension of the InAs quantum lens is obtained from the fractional change in volume:

$$\delta V/V = -3P(S_{11} + 2S_{12}) , \tag{3}$$

where $S_{11} = 1.946 \times 10^{-3}$ kbar^{-1} and $S_{12} = -6.855 \times 10^{-4}$ kbar^{-1} are the compliance constants [5]. In our case it is kept constant the b/a ratio and the variation of the volume only means a variation of the radio a. The gap energy E_g for low temperature, pressure dependent at the Γ-point is [5]

$$E_g(P,T) = E_g^{(0)} + \alpha P + \frac{\kappa T^2}{T + c} , \tag{4}$$

where $E_g^{(0)}$ is the gap energy at $T = 0$, $P = 0$ and α is the pressure coefficient [5]. The parameters used are shown in Table 1 and the symbol * in $E_g^{(0)}$(InAs) means that it is already taken into account the tension of the InAs material in the GaAs matrix. The band offset of the strained InAs/GaAs quantum lens where taken, for the conduction (valence) band, as 54% (46%) of the total band difference [5]. The temperature considered is $T = 20$ K. The variation of the effective masses was evaluated in terms of the fundamental gaps according to the Kane model [10–12]. The following variations are obtained:

(i) electrons:

$$\frac{m_0}{m_e} = 1 + 2\left(\frac{P_0^2}{m_0}\right)\frac{E_g + \frac{2}{3}\delta}{E_g(E_g + \delta)} , \tag{5}$$

(ii) light holes:

$$\frac{m_0}{m_{lh}} = -\left[1 - \frac{4}{3E_g}\left(\frac{P_0^2}{m_0}\right)\right], \tag{6}$$

(iii) heavy holes:

$$\frac{m_0}{m_{hh}} = \gamma_1 - 2\gamma_2 , \tag{7}$$

where E_g is the gap energy given by (4), γ_1 and γ_2 are the Luttinger parameters and δ is the spin–orbit splitting. Parameter P_0 is the interband momentum matrix element between conduction and valence bands [12]. The values used are shown in Table 1. Taking into account these expressions, the valence effective mass will be calculated taking the effective reduced mass according to:

$$\frac{1}{m_v} = \frac{1}{2}\left(\frac{1}{m_{hh}} + \frac{1}{m_{lh}}\right). \tag{8}$$

Table 1 Values of the parameters used in the calculation of the ground energy level for the InAs/GaAs quantum lens under pressure.

	$E_g^{(0)}$ (eV)	α (meV/kbar)	κ (eV/K)	c (K)	γ_1	γ_2	δ (meV)	$2(P_0^2/m_0)$ (eV)
InAs	0.533*	7.7	2.76×10^{-4}	83	20.4[a]	8.37[a]	380[a]	19[a]
GaAs	1.519	10.8	5.405×10^{-4}	204	6.85[b]	2.1[b]	341[b]	12.9[c]

[a] Ref. [13], [b] Ref. [14], [c] Ref. [15]

2.3 Results

In Fig. 2 it is reported the variation with the pressure of the transition energy between electron and hole ground states for four samples of InAs/GaAs. In the left panels it is fixed the value of $b/a = 0.91$ and we have used $a = 9$ nm and $a = 15$ nm while in the right panels is it fixed the ratio $b/a = 0.51$ and it is used the same radius. The straight line is obtained considering finite barrier while the dashed line represents the transition energy considering the infinite barrier model with the same configuration. In all the calculations we used $\Delta/R = 0.3$ and a 500×500 matrix in the diagonalization procedure.

In all cases the transition energy increases with pressure P and the values obtained considering infinite barrier are higher with respect to the finite barrier model, as could be expected. In the case where $b/a = 0.51$ and $a = 9$ nm the infinite barrier model gives values of the transition energy higher than the band-off set for $P < 40$ kbar and they are not shown. Only for $P > 40$ kbar this model gives appropriate results for this lens configuration. This occurs because when P increases the combined effects over the volume, effective masses and band offset produce a decreasing of the ground electronic and hole levels. The increasing monotonic behavior shown in Fig. 2 is produced by the increases of the InAs energy gap.

On the other hand, each panel shows in dotted line the calculation with the infinite barrier model keeping the ratio b/a and using and effective radius a_{eff} as a fitting parameter at $P = 0$. It can be seen that it is possible to estimate the values obtained by the finite barrier model with this procedure for small values of P while the estimation error increases with pressure. This behavior is expected because when a and b are such that the electron and hole states have values close to the barrier height, the infinite barrier model are less suitable to describe the system. Nevertheless in case of soft deformations ($b/a \sim 1$) and large values of radius a, the electron and hole energies are close to the bottom of the lens-well and the fitting is very robust for all values of P. This situation can be seen for the configuration given by $b/a = 0.91$ and $a = 15$ nm.

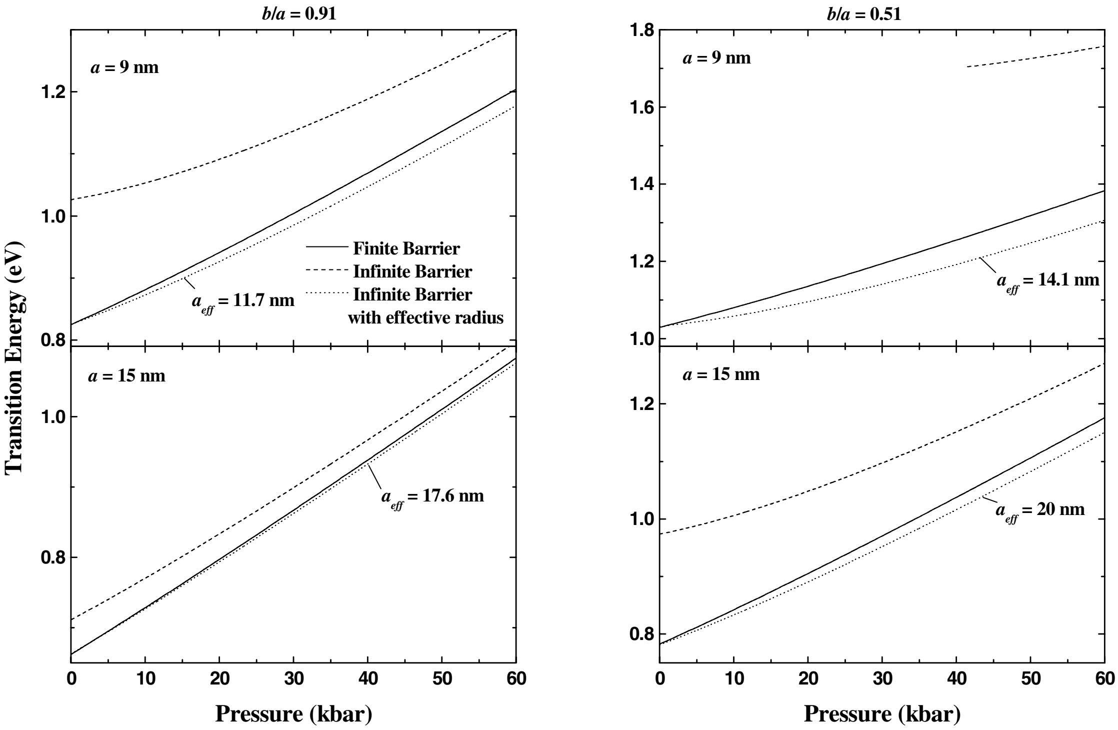

Fig. 2 Transition energy as a function of the pressure between the electron and hole ground states for different lens configurations. In left panels we have $b/a = 0.91$ with $a = 9$ nm and $a = 15$ nm while in right panels we have $b/a = 0.51$ and same radius. Straight lines are obtained considering finite barrier, dashed lines with infinite barrier and dotted lines represent the result with infinite barrier using an effective radius a_{eff} as a fitting parameter.

3 Conclusions

In the present work it has been generalized the results of Refs. [7] and [8] to evaluate electronic energies in SAQDs with lens shape geometry taking into account the finite band offset. The present model was used to study the effect of the hydrostatic pressure on the energy transition between electron and hole ground states. The obtained results remark the importance of the hydrostatic pressure over optical properties in SAQDs with lens symmetry.

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