A single-band constant-confining-potential model for self-assembled InAs/GaAs quantum dots

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Abstract A numerical method for the electronic structure of pyramidal dots is presented and its predictions compared with several experimental photoluminescence spectra: very good agreement is obtained with both energy position and the number of peaks.

1 Introduction

High strain epitaxy has now become a standard technique for the production of quasi-zero-dimensional systems via Stranski-Krastanov growth [1]. The energy levels of such structures cannot be easily calculated, both because of the finite-potential confining barrier (often of the order of 200-500 meV) and the non trivial geometry of the dot. The Schrödinger equation must thus be solved by means of a numerical method.

In our model [2] we expand the envelope function of a pyramidal quantum dot (QD) using a complete orthonormal set of periodic functions, which are solutions for a 3D well with an infinite barrier height and suitably chosen dimensions. The Schrödinger equation is thus reduced to the matrix equation:

$$(M_{mlnm'l'n'} - E\delta_{mm'}\delta_{ll'}\delta_{nn'})a_{lmn} = 0 \tag{1}$$

where the matrix elements $M_{lmnl'm'n'}$ are given by:

$$\begin{aligned} M_{lmnl'm'n'} = & \left[\frac{\hbar^2\pi^2}{2}\frac{1}{m_B}\left(\frac{ll'}{L_x^2}+\frac{mm'}{L_y^2}+\frac{nn'}{L_z^2}\right)+V\right] \\ & \times \delta_{ll'}\delta_{mm'}\delta_{nn'} + \frac{\hbar^2}{2}\left(\frac{1}{m_W}-\frac{1}{m_B}\right) \\ & \times \int_W \nabla\psi^*_{l'm'n'}\nabla\psi_{lmn}\,dxdydz \\ & -V\int_W \psi^*_{l'm'n'}\psi_{lmn}\,dxdydz \end{aligned} \tag{2}$$

The subscript W in the integrals means that the integration is over the pyramidal (well) region. The two main features of this approach are: (i) there being no need to explicitly match the wave functions across the boundary between barrier and dot region, it can be applied to arbitrary confining potentials and thus to structures of arbitrary shape; (ii) all the integrals involved in the matrix elements (Eq. (2)) can be performed analytically.

2 Model

In the envelope function calculations we treat the electrons and holes with separate one-band Hamiltonians and take account of the strain effects both on the confining potentials and effective masses *on average*. This means that we do not account either for band mixing (or coupling) or for the spatial variation of the confining potentials and effective masses due to strain, but decouple the Schrödinger equation for the system into two independent equations, one for the electrons the other for the heavy-holes, and assume constant average (strained) confining potentials and effective masses throughout the dot for both electrons and holes.

For the electron effective mass we used the value $0.04m_0$ as suggested by Cusack et al. [3] (the unstrained value is $0.023m_0$. $V_0^{el,av}$=450 meV, as suggested by Grundmann et al. [4]). For the heavy holes Cusack et al.'s calculations gave $m_{hh,z}$=$0.59m_0$, whereas Grundmann et al. used a value of $m_{hh,z}$=$0.341m_0$. We therefore use both those values, and for each of them we determined one value for $V_0^{hh,av}$ by fitting the theoretical heavy-hole energy data of Cusack et al. [3], and of Grundmann et al. [4], respectively. The average heavy hole confining potential relative to each of the mass values has been determined by performing several calculation sets, for all dot dimensions considered, with different values of $V_{0,hh}$ and choosing the potential value which gave the best agreement with the theoretical results reported in the cited papers. We therefore determined two different parametrisations (i.e. two different pairs $V_{0,hh}$, $m_{hh,z}$), for the heavy holes: C, after Cusack et al., the results of which are well reproduced by this set of values, ($m_{hh,z}$=$0.59m_0$ and $V_0^{hh,av}$=266 meV) and G, for Grundmann et al., this set giving the best agreement with their calculations, ($m_{hh,z}$=$0.341m_0$ and $V_0^{hh,av}$=316 meV).

3 Results and Discussion

Despite the simplicity of our approach the calculated ground state energy eigenvalues of both electrons and heavy holes agree well with those of more sophisticated theoretical treatments [3,4] which take into account band mixing and the microscopic effects of the strain distribution on confining potentials and effective masses (i.e. their spatial variation throughout the dot). The predictions of the model are also compared with several spectra reported in the literature by different authors [5]-[7]. Very good agreement with both position and number of experimental peaks in such photoluminescence (PL) spectra is obtained (see for example Fig. 1 and ref. [2]). Furthermore, our calculated energy splitting $\Delta E^C_{01,hh} = 22$meV, and $\Delta E^G_{01,hh} = 29$meV between the ground and first excited heavy-hole states for a structure with b=200 Å and h=70 Å are also in excellent agreement with the experimentally estimated value of $\Delta E^{exp}_{01,hh} = 27$meV, obtained by Schmidt et al. [5] for their samples by combining capacitance and PL measurements.

The predicted electron energy splitting $\Delta E_{01,e}$ however, is about two times larger (104 meV) than it was determined to

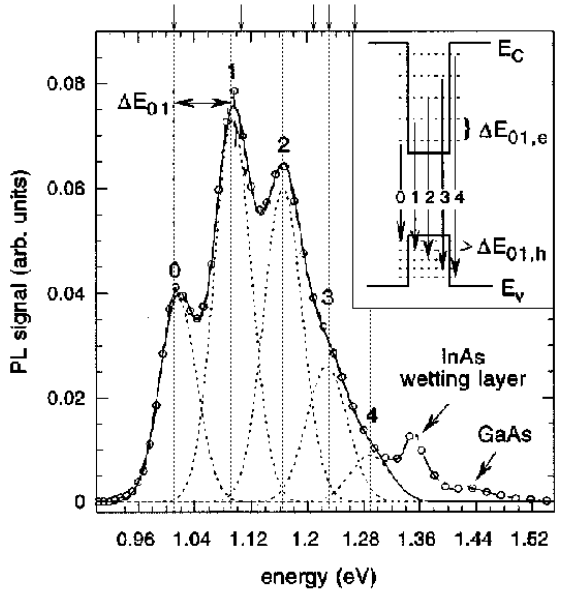

Fig. 1 Comparison between our predicted transition energies (top arrows) and the experimental PL spectrum by Schmidt et al. [5] ["Copyright (1996) by the American Physical Society"].

be by capacitance [5] and far-infrared [8], [9] measurements (i.e. $\approx$ 50 meV) on the same or similar samples.

The values $m_{W,hh}$=0.59, V=266 meV (par. C) have proved to reproduce well the ground state energies of all the experimental spectra considered, whilst the pair $m_{W,hh}$=0.341, V=316 meV (par. G) gives a good agreement with the transition energies between excited states.

We would like to emphasize that although the Schrödinger equation we use does not explicitly include the strain (that is, we do not diagonalize any 8x8 strain Hamiltonian matrix such as that in ref. [10]), its effects are nevertheless accounted for by the choice of strained values for effective masses and average confining potentials (for both electrons and heavy-holes). In order to justify the choice of the parameters used in our calculations we, nevertheless, performed a set of calculations of the strain distribution in pyramidal structures with aspect ratio Q ranging from 1 to 4.5 [11] using a method based on the Green's function technique [12], taking into account the anisotropy of the elastic properties as well. The carriers' strained confining potentials were then calculated as a function of position along the growth direction, in the framework of the 8-band $\mathbf{k}\cdot\mathbf{p}$ theory (see, for example ref. [13]). The results [11] were in agreement with previously published data ([14], [15]), and showed that the confining potentials of both electrons and holes are almost constant throughout the dot for $Q \geq 2$, with average values ranging from about 408 to about 454 meV (for the electrons), and from 228 to 321 meV (for the heavy holes), for the experimental structures considered in the present work, proving our constant-confining-potential approximation as a reasonable choice. The very good agreement obtained by our simple model with so many different experimental transition energies is nevertheless hard to explain. A compensation mechanism in which a positive difference in the confining potential (i.e. between our average strained value of 450 [266] meV and the average strained value calculated for the specific sample) is compensated by a negative difference in the value of the effective mass, (so that when the confining potential is $<$ 450 meV, the effective mass is $>$ 0.04), could be responsible for this little difference in the transition energies.

4 Conclusion

A single-band, constant-confining-potential model has been applied to self-assembled InAs pyramidal dots. It has proved to be suitable not only to predict ground states eigenenergies but also number and energy values of the interband transitions between bound excited states.

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