Journal of Physics: Conference Series **245** (2010) 012081 doi:10.1088/1742-6596/245/1/012081

Theoretical modelling of quaternary GaInAsSb/GaAs self-assembled quantum dots

J. M. Llorens[1], A. G. Taboada[1], J. M. Ripalda[1], D. Alonso-Álvarez[1], B. Alén[1], J. Martín-Sánchez[1], J. M. García[1], Y. González[1], A. M. Sánchez[3], A. M. Beltrán[2], P. L. Galindo[2] and S. I. Molina[2]

[1] IMM-Instituto de Microelectrónica de Madrid, (CNM-CSIC), Isaac Newton 8, PTM, E-28760 Tres Cantos, Madrid, Spain.
[2] Universidad de Cádiz, Puerto Real, 11510 Cádiz, Spain
[3] Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

E-mail: jose.llorens@imm.cnm.csic.es

Abstract.
InAs/GaAs quantum dots exposed to Sb after growth exhibit spectral changes. We study in the present paper an idealized nanostructure consisting of a homogeneous distribution of the quaternary GaInAsSb surrounded by a barrier of GaAs. We find that the valence band offset is a critical parameter in modelling its electronic structure. Depending on this value, we predict a transition from type-I to type-II band alignment at a different Sb concentration. The addition of Sb to reduce the transition energy while keeping a type-I alignment is only of benefit at low Sb concentration.

1. Introduction

Light sources operating efficiently at 1.55 μm are highly desired by the telecommunication industry. Laser diodes based on semiconductor quantum wells are able to work at high rates, with low power consumption and high temporal and spatial coherence. An excellent candidate technology for lasing at the telecommunication window of interest relies upon InGaAsP/InP multi-quantum-wells. It would be however preferable to replace the InP substrate by an inexpensive one. The most extended approach to achieve this goal consists on growing InAs self-assembled quantum dots (QDs) on top of GaAs substrates. Even though the bandgap of InAs at low temperature lays at ~ 3.0 μm, the emission of InAs/GaAs QDs occurs at ~ 1.3 μm or shorter wavelengths. This blue shift results mainly of confinement and strain effects. The effect of the strain can be partially alleviated using a metamorphic layer [1] or a strain-reducing layer. Alternatively, it is possible to increase the emission wavelength by replacing As atoms by Sb ones, given that InSb presents an even narrower bandgap than InAs. This approach has been very promising, giving rise to room temperature emission at 1.6 μm from InAs/GaAs QDs covered with GaAsSb[2].

We constraint the current study to analyse the impact of Sb on the electronic structure of an InAs/GaAs QD. We leave size effects and the impact of metamorphic and strain-reducing layers for future work. We propose a model for describing such a QD exposed to Sb: a lens shaped volume of 10 nm radius and 8 nm height sited on top of a 0.5 nm wetting layer. Its composition

consists of a homogeneous distribution of the quaternary $Ga_xIn_{1-x}As_ySb_{1-y}$. The amount of Sb in the alloy is limited to 0.5, since higher values are difficult to achieve experimentally. The surrounding barrier material is pure GaAs. Further details on actual samples of InAs/GaAs containing Sb can be found in [3, 4].

2. Method

The whole theoretical study has been performed with the Nextnano++ software package.[5] The strain distribution is computed by minimising the strain energy of the whole structure given the lattice mismatch between the QD material and the barrier. The QD electronic structure is then obtained by means of the 8×8 Kane's Hamiltonian in the framework of the effective mass approximation. Strain effects on the electronic structure are accounted for by adding the Bir-Pikus Hamiltonian to the Schrödinger equation. Further details can be found in Ref. [5].

We have followed the recommendations of Vurgaftman *et al.* [6] to set all material parameters, except the valence band offset (VBO). During the study, VBO has been shown to be critical in determining a type-I or type-II heterostructure band-alignment, which has a major impact on the electronic confinement energies. This has motivated to perform the calculation of the electronic structure for three different sets of VBO values: i) the recommended values of Vurgaftman *et al.* [6], ii) the theoretical values reported by Wei and Zunger [7] and iii) the recently revised VBO of Li *et al.* [8]. In the following, we will refer to these parameter sets as set A, B and C, respectively. The conduction and valence band alignment with respect to GaAs is shown in Figure 1 panels a) and b), respectively. Only GaSb presents a type-II conduction band alignment with respect to GaAs. However, if we introduce the strain due to the lattice mismatch, the band edges shift and the layout changes notably. In Fig. 1 c) can be seen that InSb/GaAs also exhibits a type-II band alignment.

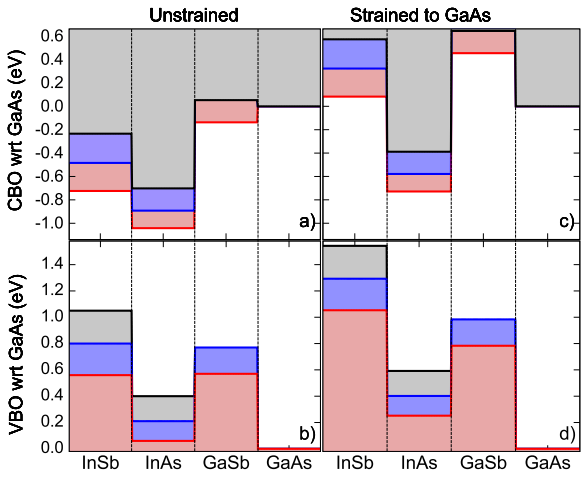

Figure 1. Band edges alignment for the conduction a) and valence b) bands. Three different set values for VBO are plotted: Vurgaftman *et al.* [6] (blue), Wei and Zunger [7] (red) and Li *et al.* [8] (black). The band edges line up under lattice mismatch strain is represented for conduction c) and valence d) bands.

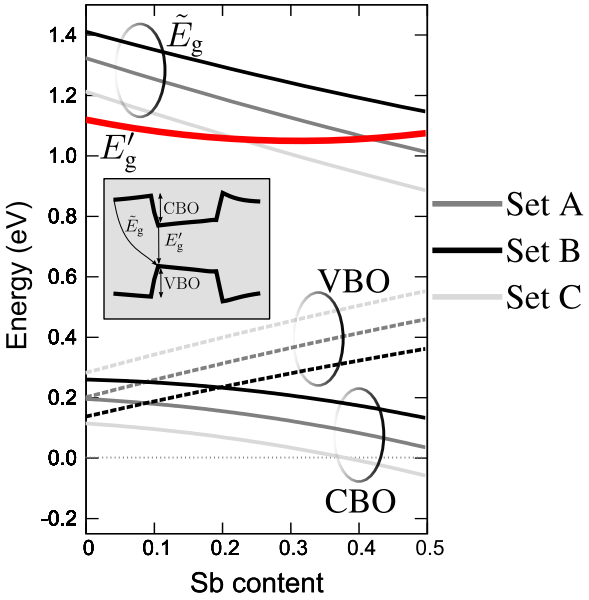

Figure 2. Spatially direct (thick red line) and indirect transitions (upper-half solid lines), and valence and conduction band-offsets (lower-half solid and dashed lines) calculated at the bottom surface of the quantum dot (inset).

The values of the quaternary parameters have been derived by interpolation of the four

ternaries resulting of combining the four binary compounds involved in the alloy. We have taken the bowing parameters from Ref. [6], even for VBO, when available.

3. Results and discussion

To get a first insight into the confinement exerted by the QD on the electron and hole states, it is helpful to analyse the confinement potential at the points where the particle wavefunction tends to localise. In general, the electron wavefunction *fills* most of the QD's volume, while the hole often resides in the lower half of it. Thus, the e-h transition energy can be roughly approximated by the energy difference between the valence and conduction band edges at the centre of the bottom surface of the QD. These values differ from those of Fig. 1 c) and d) in the strain values, which now are the QD local strain ones. The effective energy gap ($E'_{\rm g}$) as a function of the Sb concentration is shown in Fig. 2. The minimum at $y \sim 0.75$ is not related to the minimum of the ternary InAsSb bandgap, since the latter takes place at $y \sim 0.4$ [9]. It results from the increase of the strain net value due to the bigger lattice mismatch associated with the incorporation of Sb. In addition, the spatially indirect transition from the GaAs conduction band to the QD's top valence band is also of relevance here. We have labeled such energy as $\tilde{E}_{\rm g}$ in Fig. 2 [1] The indirect transition crosses the direct one when sets A and C are considered. The crossing indicates at which Sb concentration the nanostructure could exhibit a type-II conduction band alignment. Finally, the effective band offsets are also included in Fig. 2. Within this qualitative picture, the holes are significantly more confined, the more Sb and conversely, the electrons.

The actual values of the electron-hole (e-h) transition energy are shown in Figure 3. There, we can see that the naive description based upon the confinement potential describes qualitatively well the dependence of the e-h energy on the Sb content. At low Sb content, the transition energy exhibits a red shift. This is followed by either a blue shift (for parameter set B) or a steeper red shift (for parameter set A and C). The latter is associated with the type-I to type-II band alignment transition. This transition takes place at y=0.43 and y=0.4 (y=0.22 and y=15.0) for x=0 and x=0.25, respectively, when set A (C) is considered. The values corresponding to set B have not been computed, being greater than y=0.5. The model predicts an emission at wavelengths greater than 1.2 μm for type-II QDs. For practical applications on light emitters, a type-II heterostructure is undesirable. The e-h overlap gets reduced in spatially indirect transitions and hence the oscillator strength and device performance. One could think that removing the Ga atoms from the QD could help in shifting the e-h transition energy towards red. This is not the case, as it is shown by the dashed lines in Fig. 3. At low y, there is a red shift of $\sim$ 100 meV. However, as more Sb is incorporated in the dot such shift becomes smaller. Although Ga atoms shift the band edges towards blue, the lattice mismatch in the quaternary with x=0.25 is smaller than in InAsSb. Thus, at $y \sim$0.5 the transition energy becomes almost equal, for both Ga concentrations of 0% and 25%.

Ripalda *et al.* reported in Ref. [3] a photoluminescence spectrum peaked at 1.25 μm for InAs/GaAs QDs exposed to Sb and covered with GaAs. Our numerical results are consistent with such experimental observations for QDs with a composition of $Ga_xIn_{1-x}As_ySb_{1-y}$ with $0< x < 0.25$ and $0.1 \lesssim y \lesssim 0.25$. This conclusion should be taken cautiously. We have not computed the excitonic transition energy, which should appear red-shifted with respect to the energies of Fig. 3 as a result of the electrostatic Coulomb interaction. Typically, the excitonic correction is $\sim$ 20 meV in InAs/GaAs QDs[10]. Thus, to our understanding, such corrections would not have a great impact on the above estimation of the quaternary composition. However, an exact calculation should confirm our conjecture.

In conclusion, the optimal Sb concentration to get the narrowest transition energy in a $Ga_xIn_{1-x}As_ySb_{1-y}$/GaAs QD while preserving a type-I band alignment, results from the balance

[1] The conduction band energy in GaAs is taken at the centre of the top surface of the simulation box.

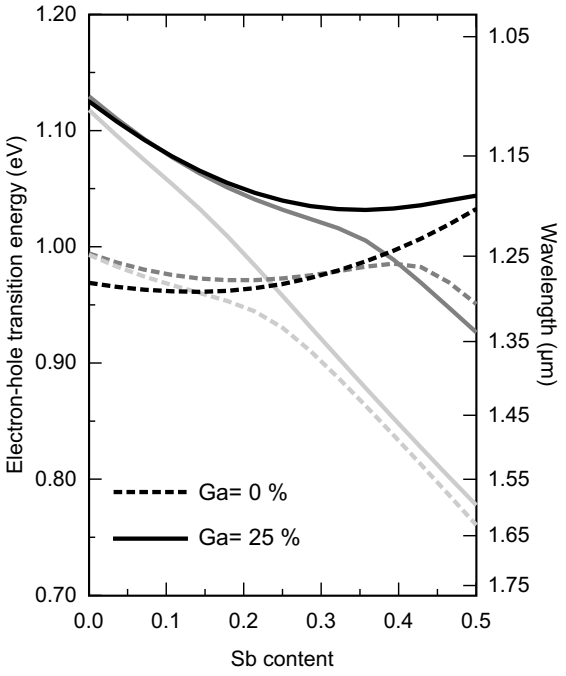

Figure 3. Electron-hole transition energy for a $Ga_{0.25}In_{0.75}As_ySb_{1-y}$/GaAs QD (solid lines) and an $InAs_ySb_{1-y}$/GaAs QD (dashed lines). The grey colour of the lines has the same meaning as in Fig 2.

of two effects: i) the red shift due to the narrower band-gap of InSb and ii) the blue shift associated to the strain induced by the higher lattice mismatch. The VBO parameter plays a critical role in the estimation of the conduction type-I to type-II transition. The results for set C show a type-II band alignment even for small concentrations of Sb. Conversely, the same calculation with set B does not show any type-I to type-II transition for $y \leq 0.5$. Finally, the results for set B show an in-between behaviour.

Acknowledgments
This work was supported by the Spanish MICINN (projects TEC2008-06756-C03-01/02/TEC, CONSOLIDER INGENIO 2010 CSD2006-0019 and CSD2009-00013), the Junta de Andalucía (PAI research groups TEP-120 and TIC-145; project P08-TEP-03516) and Comunidad Autónoma de Madrid S2009ESP-150.

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