Modelling of electronic states in InAs/GaAs quantum dots with GaAsSb strain reducing overlayer

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Abstract. We present results of our 8-band $\vec{k} \cdot \vec{p}$ calculations of the emission energy of InAs/GaAs quantum dots (QDs) covered with GaAs\(_1-x\)Sb\(_x\) strain reducing overlayer (SRO). In agreement with previous experimental observations we find a strong red shift of the emission with increasing Sb content. We explain this effect by: (1) The lowering of the valence band offset between the QD and the SRO with increasing Sb content resulting in the type-II QDs with holes confined in the SRO for Sb concentration above 14%. (2) The reduction of compressive strain inside the QDs. The contributions of these mechanisms to the total red shift are estimated and compared. For realistic shape and size of the QD and a realistic value of the SRO thickness the previously measured photoluminescence data are reproduced with fairly good accuracy.

1. Introduction
Self-assembled InAs/GaAs quantum dots (QDs) have been investigated for their interesting physical properties and potential applications; one of the latter is an efficient light emission on the communication wavelengths of 1.3/1.55 $\mu$m. To tune the emission wavelength towards this range, various strategies can be used. One possibility is to use QDs stacked in vertical multilayers [1]. Another option relies on capping QDs with strain reducing overlayers (SRO); here, ternary materials such as In\(_x\)Ga\(_{1-x}\)As [2] and GaAs\(_1-x\)Sb\(_x\) [3] can be used. The resulting red shift with increasing In content in In\(_x\)Ga\(_{1-x}\)As SROs has been explained as an effect of three mechanisms: the reduction of the hydrostatic strain in the InAs QDs, lowering of the barrier height for both electrons and holes at the side of the SRO, and a change in the dot size during the growth process; the latter two were identified as the decisive contributions [2].

We present here a similar analysis for the GaAs\(_1-x\)Sb\(_x\) SROs. The situation is slightly different since the lowering of the valence band offset with increasing Sb content results in a transition to the type-II QDs occurring at the Sb concentration of approximately 14%. Above this value holes are localized in the SRO instead of the QDs. In previous photoluminescence studies, this transition to the type-II QDs has been attributed to be the dominant cause of the observed red shift [4]. However, a detailed theoretical analysis is still missing.

2. Method
QDs capped by GaAs\(_1-x\)Sb\(_x\) SROs were simulated using nextnano++ software [5]. The structure consisted, from bottom to top, of a GaAs substrate, InAs QD, GaAs\(_1-x\)Sb\(_x\) SRO and a GaAs
capping layer. Our calculations started by finding the strain inside the structure, continued by a calculation of the piezoelectric field, and ended with solving the Schrödinger equation using the 8-band $\vec{k} \cdot \vec{p}$ approximation. All these steps were performed using the nextnano++ built-in solvers. The values of the material parameters have been taken from [6], with the exception of the deformation potentials and the InAs/GaAs valence band offset, taken from [7].

To distinguish between the effects of the reduced strain in the QDs and those of the lowered valence band offset, the following calculations were performed: (1) We have calculated the strain field for the GaAs$_{1-x}$Sb$_x$ SRO and used it subsequently as the input for the piezoelectricity and quantum calculations. Apart from the elastic constants and the lattice parameter, we considered the SRO to correspond to a pure GaAs. In this way we have specified the contribution of the reduced strain within the QDs. (2) We have used the strain field calculated for a pure GaAs overlayer and values of the parameters of the GaAs$_{1-x}$Sb$_x$ SRO (except for the lattice parameter and the elastic constants) in subsequent calculations to obtain the effect of the modified valence band offset. In this case, also other parameters were changed, such as the conduction band offset and effective masses. However, the most pronounced effect is indeed connected with a modified valence band offset.

3. Results and discussion

In our calculations we have varied the dimensions of the QD and the thickness of the SRO, in order to fit the transition energy and its red shift observed in [3]. We have chosen the semiellipsoidal shape of the QD as it is common for InAs dots large in volume. We have obtained the best agreement for the QD height of 5 nm, the QD diameter of 14 nm and the SRO thickness of 3 nm.

The calculated values of the lowest transition energy are shown in Fig. 1. The experimental data measured at 15 K, taken from [3], are shown for comparison. To facilitate the comparison, the calculated data are blueshifted by 20 meV. The shift could be due, e.g., to the fact that the real QDs consist of InGaAs rather than of pure InAs.

The calculated red shift of the lowest transition energy when going from 10 % to 22 % of Sb of 95 meV is in reasonable agreement with the experimental value of 82 meV. We decompose this shift into the contribution of the reduced strain in the QD, and that of the lowered valence band offset between the QD and the SRO. Both contributions are shown separately in Fig. 1.
modified valence band offset accounts for $\sim 45 \text{ meV}$ of the red shift, while the reduced strain accounts for $\sim 20 \text{ meV}$. The difference of $\sim 30 \text{ meV}$ between the sum of the values and the total red shift is a result of the combination of the effects.

Below the Sb concentration of 14 %, both effects contribute nearly equally to the total shift, with a linear dependence on the Sb concentration. Around 14 %, the transition to the type-II QD occurs and increasing the Sb content further enhances the effect of the lowered valence band offset (which becomes negative). Accordingly, we identify the onset of the type-II QDs as the dominant mechanism causing the red-shift of the emission energy, confirming the assumption of Ref. [4]. However, the influence of the $\text{GaAs}_{1-x}\text{Sb}_x$ capping layer on the strain in the structure is responsible for a surprisingly large portion of the red shift as compared to the $\text{In}_x\text{Ga}_{1-x}\text{As}$ SRO [2].

Fig. 2 shows the hydrostatic component of the strain $(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$ along the symmetry axis of the dot. The compressive strain inside the dot decreases by 0.3 % when increasing the Sb content from 10 % to 22 %. This corresponds to the red shift of the conduction band edge by $\sim 20 \text{ meV}$, explaining fully the simulated contribution of the reduced strain to the red shift, shown in Fig. 1.

![Figure 2. Hydrostatic strain $(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$ along the symmetry axis of the QD for —— 0 %, - - - - 10 %, · · · · 22 % of Sb content in the SRO.](image)

The reduction of the compressive strain inside the QD can be explained as follows. The lattice parameter of $\text{GaAs}_{1-x}\text{Sb}_x$ is larger than that of GaAs. The presence of the SRO therefore increases the total strain in the structure. However, the contrast in lattice parameters between the QD and the SRO is reduced as compared to the GaAs overlayer, which results in a reduced strain inside the QD. In particular, the material around the sides of the dot has a lower compressive impact. On the contrary, matching the lattice parameter to the GaAs overlayer enhances the compressive strain in the SRO, as seen clearly in Fig. 2.

There is a pronounced difference in the magnitude of the relaxation of the compressive strain inside the QDs with $\text{GaAs}_{1-x}\text{Sb}_x$ SRO considered here and inside the QDs with $\text{In}_x\text{Ga}_{1-x}\text{As}$ SRO studied in Ref. [2]. The lattice parameters of the SROs are nevertheless comparable. The difference likely originates in the different aspect ratios of the QDs in both cases. The $\text{GaAs}_{1-x}\text{Sb}_x$ covered dots are rather high and the elastic interaction between them and the SRO is more intense than in the flat QDs covered with $\text{In}_x\text{Ga}_{1-x}\text{As}$.
4. Conclusion
In conclusion, we have calculated the emission energy of QDs covered with the GaAs$_{1-x}$Sb$_x$
SRO with various values of the Sb content. We were able to reproduce the observed transition
energies, and their red shift with increasing Sb content. In agreement with previous studies, it
has been found that the red shift is caused mainly by the transition to the type-II QDs above
the Sb concentration of 14 %. Almost one fourth of the red shift is caused by the reduction of
the compressive strain inside the QDs; this is much more than in the case of In$_x$Ga$_{1-x}$As SROs.

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