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Control of Strain in GaSbAs/InAs/GaAs Quantum Dots

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Abstract. We discuss strain simulations of quantum dot structures covered with a GaSbAs strain reducing capping layer in the presence of Sb segregation. Cross Sectional Scanning Tunneling Microscopy shows strong Sb and In segregation in the material surrounding the quantum dot. Using the three layer model originally proposed for the SiGe system by D. J. Godbey, M. G. Ancona, J. Vac. Sci. Technol. A 15, 976 (1997) we accurately calculate the segregation profile and include a non uniform composition to our models. Using atomistic modeling, we present strain maps of the quantum dot structures that show the propagation of the strain into the GaAs region is strongly affected by the shape and composition of the strain reduction layer.

1. Introduction
The development of semiconductor self assembled Quantum Dot (QD) Lasers [1-2] follows the exploitation of the 3D confinement in self assembled InAs/GaAs Stranski-Krastanow islands and has demonstrated low threshold current and reduced temperature dependent lasing characteristics.

Telecommunication applications dictate that the emission wavelength of InAs/GaAs QDs needs to be in the range 1.31 and 1.55 μm. In order to achieve this QD layers need to be formed as substantially larger islands compared to those used in the first generation of QD laser devices. Such large QDs can be synthesized by overgrowth, epitaxial growth control or by growth on higher index surfaces. However such large islands, when capped with a GaAs layer, tend to develop very large strain fields in the surrounding matrix which result in threading dislocations. [3]

The most viable solution to this problem is to use a “strain reduction layer (SRL)” to embed the InAs (or InGaAs) islands in a material which is an intermediate lattice constant between itself and the substrate. This material, usually grown as a pseudomorphic layer, acts to reduce the band gap and increases the aspect ratio of the QD. Further more the hydrostatic strain present in the island is diffused into the 2D layer and reduces dislocations. The resulting QD/QW combination is called a “dot-in-well” structure (DWELL) [4-8]. Of the various material systems useful as SRLs, Sb alloys are
of particular interest because of the potential type II band alignment which could offer more functionality to the devices. [9]

One technological issue when growing semiconductor epitaxial layers via either MBE or MOCVD is that of elemental segregation. [10-11] The occurrence of segregation has been observed for both group III and group V atoms and generally results in non abrupt interfaces and deviations from the designed properties of the heterostructures. Various theoretical models have been proposed in the years to explain experimental observations for both SiGe and III-V semiconductor alloys. [12-15]

We have recently reported [16] how the Muraki [12], Kinetic [13-15] or Thermodynamic [15] models cannot reproduce satisfactorily the experimentally measured segregation profiles in quantum dot layers covered by a GaSbAs SRL. In fact only the three layer model originally proposed by Godbey and Ancona for SiGe alloys [17] reproduces the long tail of the Sb distribution. Earlier experimental observation by Dorin [18] led to postulate that in films containing Sb, where significant roughening may open paths for Sb segregation, the exchange processes are more likely to take place between at least three layers. This explains the reason for which earlier models, all based on a two layer exchange mechanism, fail to predict the extended diffusion of Sb atoms. Furthermore In segregation appears partially suppressed compared to QD layers covered by GaAs. However it is yet sufficiently present to allow the experimental observation of a GaInAsSb alloy within the SRL.

2. Modelling Strain in the SRL and Quantum Dots

In this section we report our investigation of the influence of the presence of Sb atoms together with In, Ga and As on the strain properties of QDs capped with a SRL. Our intention was to compare our models with direct experimental observation by means of Cross Sectional Scanning Tunneling Microscopy (X-STM), as reported in our previous work [16]. The samples consisted of QD layers capped with GaAsSb, grown by solid source MBE, as follows: an n+ Si doped GaAs [001] substrate was covered by a 200 nm GaAs buffer (590°C), followed by a 2.8 ML InAs layer (500°C), after a 30s growth interrupt a 6 nm GaSbAs (475°C), 10 nm GaAs (475°C) and finally 40nm GaAs (590°C). With the exception of the buffer layer the growth sequence was repeated 3 times but each time changing the nominal Sb content to 12%, 15% and 20%. The sample was finally capped with a further 10nm of GaAs (590°C). The InAs layers were deposited at a growth rate of 0.094 ML/s.

To determine the strain tensor in these structures we have implemented a series of Molecular Statics simulations. The atomistic models are designed as follows: we initially build a GaAs (001) substrate section of dimensions 40x40x10nm followed by a thin InAs 2D layer (wetting layer) of thickness of 2 ML. The pure InAs QD island sits on top of the 2D layer and has dimensions of roughly 28nm in diameter and 10nm in height. The shape of the island is taken from that proposed by Costantini et al [19] where a detailed analysis of the facets observable in STM microscopy was presented.

In the six different models presented here, the region around the island and up to the height of the QD (SRL) is formed by either pure InGaAs, GaSbAs or GaInAsSb, either as a uniform alloy or incorporating a non uniform profile taken from model data of segregation. Such data was already presented in our earlier work [16]. The entire structure is then further capped with a 10nm layer of pure GaAs. Periodic boundaries are used in the [100] and [010] crystallographic directions. The structures comprise usually about 2.8 million atoms and the computational effort is minimized by using a 64-processor parallel implementation of the IMD™ software [20] and using optimally parameterized Tersoff empirical potentials [21-22]. The strain is then directly extracted from the atomic bonds, by comparing the strained lattice to an ideal unstrained one and taking the local composition into account, in a sort of Virtual Crystal Approximation.

3. Results

We present the strain maps for the biaxial and dilation strain, which are obtained from the diagonal components of the strain tensor and express the overall tetragonal distortion and compression of the
unit cells, respectively. In Fig. 1 we show maps of the dilation (i.e. $e_{xx} + e_{yy} + e_{zz}$) and biaxial strain components (i.e. $e_{zz} - \frac{1}{2} (e_{xx} + e_{yy})$), for the case of three uniformly alloyed SRLs with 10% In and 20% Sb, 50% In and no Sb, 30% Sb and no In. Including an SRL during growth is a very effective way of reducing the strain in the GaAs matrix, a fact clearly supported and confirmed in these simulations when compared to results for a GaAs/InAs/GaAs island previously reported [16]. In all cases the change of the propagating strain is evident, as well as having a marked effect on the elastic distortion inside the islands.

![Fig. 1: Strain maps: the SRL is composed by InGaSbAs with 10% In and 20% Sb ((a) and (b)), InGaAs with 50% In ((c) and (d)) or GaSbAs with 30% Sb ((e) and (f)).](image)

![Fig. 2: Strain maps: the SRL is composed by In and Sb segregated layers with a nominal Sb composition of 12% Sb ((a) and (b)), 15% Sb ((c) and (d)) and 20% Sb ((e) and (f)).](image)

However the SRLs of the models used in Fig. 1 is an idealized situation. As previously reported [16] the SRL tends to have very non uniform compositions that are well described by segregation profiles. We therefore also simulated in Fig. 2 the intermixing with In of a GaSbAs SRL with nominally 12%, 15% and 20% Sb, using calculated segregation profiles from our earlier work [16]. All other parameters are kept the same. The experimental X-STM topographies [16] also indicate that the material in the SRL does not form a uniform two dimensional layer. In fact Sb atoms are clearly seen to “wrap” around the island and strongly limit the uniformity of the planes above the tip of the QD. This effect was reproduced in our input models. The results of the simulations shown in Fig. 2 indicate that the strain distribution is altered by the presence of a strongly alloyed SRL compared with having a uniform composition.

Of the three compositions tested we found that the biaxial strain is more strongly reduced in the island for the intermediate Sb content of 15%. The dilation instead appears almost constant in all three
islands. Upon comparing the highest Sb composition in both the uniform and non uniform case, it is manifest that the more strongly alloyed SRL is more effective in reducing the strain in the GaAs regions above and below the QD island.

4. Conclusions

We reported a study of the strain in strongly alloyed GaSbAs/InAs/GaAs QDs and showed how the presence of Sb is able to tune the strain of the structures. Such strain is likely to have a profound influence on the electronic properties as the percentage of Sb controls the amount of internal strain of the islands. Furthermore the strain is also tuned above and below the islands allowing for a more precise morphological coupling should multistacks of QD islands be prepared in such a way.

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