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# Strain-engineered self-organized InAs/GaAs quantum dots for long wavelength (1.3 $\mu\text{m}$ -1.5 $\mu\text{m}$ ) optical applications

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**Abstract.** InAs/GaAs quantum dot systems can emit light at the wavelengths above 1.3 $\mu\text{m}$  by covering the InAs quantum dots with an In<sub>x</sub>Ga<sub>1-x</sub>As strain reducing capping layer (SRCL). The presence of the SRCL relaxes the strain in the growth direction while the in-plane compressive strain remains nearly unchanged. This results in an aspect ratio increase of the quantum dot. Both the strain relaxation in the growth direction and the aspect ratio change induce a non-linear red shift. This work studies the dependence of the emission wavelength on the thickness and the indium composition of the SRCL. Experimental topologies have been simulated and a close quantitative match is found.

**Keywords:** Quantum Dots, Electronic structure, Strain, Strain-reducing layer, Wavelength.

## INTRODUCTION

III-V compound semiconductor (GaAs/InAs) quantum dot structures (QDs) are very attractive for their efficient, stable and only slightly temperature dependent emission in the near-infrared region, especially around 1.3 $\mu\text{m}$  and 1.5 $\mu\text{m}$ : the wavelengths important for the fiber optical communication devices such as photo-detectors and lasers. A promising way to red shift the emission wavelength is to use the strain relaxation effect of InGaAs quantum well: covering the InAs QDs with InGaAs strain-reducing capping layers. In the past, several experimental groups [1] have tried to achieve long wavelength emissions by embedding the InAs QDs in In<sub>x</sub>Ga<sub>1-x</sub>As strain-reducing capping layer (SRCL).

The presence of SRCL relaxes the strain in the growth direction keeping the in-plane compressive strain constraint nearly unchanged. This reduces the band gap and increases the aspect ratio (AR) of QD. Both of these effects tend to red shift the emission spectra. The selection of the thickness and the indium concentration of the SRCL is very important to obtain the required emission wavelength. Earlier theoretical studies [2] based on reduced models such as  $\mathbf{k}\cdot\mathbf{p}$  or single band effective mass model have tried to explain this red shift without giving any quantitative contribution of QD size change and reduction of barrier height on the SRCL side, thus leading to wrong conclusions. Our recent study [3] has shown a close quantitative match with the experiment. We explained the quantitative contribution of strain relaxation, the QD volume and the aspect ratio change, and the reduction of the barrier height on the SRCL side in the red shift of emission spectra for various indium fractions in the SRCL. In this work, we have presented

the dependence of red shift of the emission spectra on the SRCL thickness and indium composition. We find that a correct thickness of SRCL to achieve the required emission wavelengths above 1.3 $\mu\text{m}$ .

## SIMULATION APPROACH

This study is carried through atomistic simulations using the NanoElectronic Modeling tool NEMO-3D [4]. The strain is calculated using an atomistic VFF-Keating model over a large domain containing about 15 million atoms to capture its long-range effects. The Atomistic calculation of the strain takes into account the interface roughness effect and the random nature of atoms in the materials. The relaxed inter-atomic positions obtained are used to influence the  $sp^3d^5s^*$  tight-binding electronic Hamiltonian defined in a subdomain containing about 9 million atoms. Smaller electronic domain is used due to the strong confinement effects of the electronic states within and around the quantum dot region. The strain simulations fix the atom positions on the bottom plane to the GaAs lattice constant, assume periodic boundary conditions in the lateral dimensions, and open boundary condition on the top surface. The smaller electronic box assumes closed boundary conditions with passivated dangling bonds. These multi-million atomic simulations run on 60 CPU's for about 15-20 hours.

The InAs dome-shaped QD used in this study (see figure 1a) has a diameter of 20nm and a height of 5nm, positioned on a 1ML thick InAs wetting layer. The QD is surrounded by a “D” nm thick In<sub>x</sub>Ga<sub>1-x</sub>As SRCL, where D is varied from 0 to 5nm and Indium fraction x is varied from 0 to 0.4. Figure 1b (green line) compares the emission wavelength against the

experimental measurements (black lines) for the experimental topology  $D=5\text{nm}$  [3]. Our results closely match with the nonlinear nature of the experimentally measured emission wavelength as the indium fraction in the SRCL is increased.

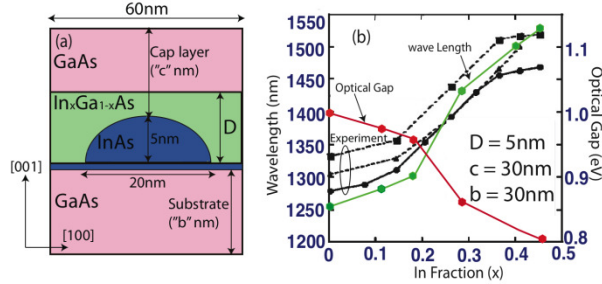


FIG 1: (a) Schematic view of the system simulated, with an InAs dome shaped quantum dot placed on an InAs wetting layer covered by InGaAs SRL. (b) Optical gap (red line) and emission wavelength (green line) as a function of indium fraction  $x$  in SRCL compared against the experimental data (black lines) [3].

## RESULTS AND DISCUSSIONS

The SRCL strongly modifies the electronic structure shifting the emission wavelength to larger values. Fig. 2 (a) shows the emission wavelength for various values of the SRCL thicknesses and indium compositions. For all the values of the SRCL thicknesses  $D$ , the emission wavelength increases as the indium composition is increased. The reduction in the optical band gap resulting in the red shift of the emission spectra can be explained in terms of the strain relaxation in the growth direction. Fig. 2 (b) plots the average value of the hydrostatic strain ( $\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}$ ) at the center of QD for various values of “ $D$ ” and “ $x$ ”. For all the values of the indium fraction, the hydrostatic strain is relaxed by the presence of the SRCL. Significant relaxation is observed for larger values of “ $D$ ” and “ $x$ ”. Hydrostatic strain relaxation directly reduces the optical band gap increasing the emission wavelength.

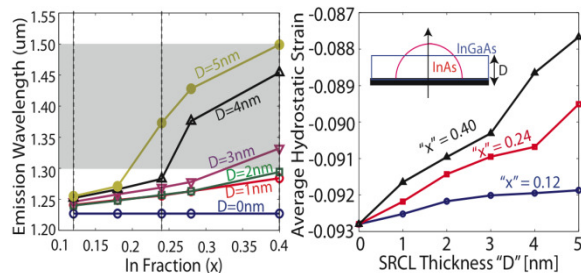


FIG 2: (a) Emission wavelength as a function of SRCL thickness “ $D$ ” and indium composition “ $x$ ”. (b) Average value of hydrostatic strain at the center of QD for different values of indium composition “ $x$ ” and thickness “ $D$ ” of the SRCL in the growth direction. Significant strain relaxation is observed in the growth direction.

Another physical effect which contributes in the red shift of the emission spectra is the change in the

aspect ratio (AR) of the quantum dot. The presence of the SRCL spreads the strain deep into the InGaAs quantum well in the lateral direction. Fig 3 (a) shows the lateral hydrostatic strain plot through the center of the quantum dot with and without SRCL. Large negative values of the hydrostatic strain within the SRCL region are evident from figure 3(a). Since vertical constraint is significantly relaxed and lateral compressive constraint is increased, the base of QD is reduced and the height is correspondingly increased according to Poisson’s ratio. This results in the increase of the aspect ratio of the quantum dot.

Fig. 3 (b) plots the aspect ratio change of the QD as a function of the indium composition for a 5nm thick SRCL. For flat quantum dots ( $AR < 0.3$ ), the increase in the aspect ratio significantly red shifts the emission spectra [5]. We find that strain relaxation and aspect ratio change nearly equally contribute in the red shift of the emission spectra [3].

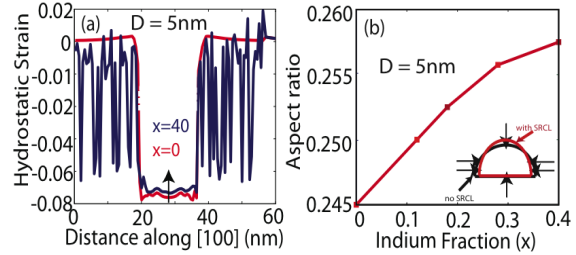


FIG 3: (a) Plot of the hydrostatic strain along [100] direction through the center of the QD as a function of the distance along [100]. (b) Plot of the aspect ratio of the QD as a function of the indium fraction of the SRCL. As the indium fraction increases, the base of the QD decreases and the height of the QD increase, thus increasing the aspect ratio.

We also find that the reduction of the barrier height on the SRCL side only negligibly contribute in the red shift of emission spectra. A detailed physical explanation can be found in reference [3].

## REFERENCES

- [1] Eduard Hulicius *et al.*, J. Crystal Growth (2008); J. G. Lim *et al.*, J. Crystal Growth 275 pp. 415-421 (2005); J. Tatebayashi *et al.* Appl. Phys. Lett. 78, 3469 (2001); A. Hospodkova *et al.*, J. Crystal Growth 298 pp. 582-585 (2007);
- [2] K. Kuldova *et al.*, Phys. State. Sol. (c) 3 (2006) 3811; F. Guffarth *et al.*, Phys. Rev. B 64, 085305 (2001)
- [3] Muhammad Usman *et al.*, submitted to *IEEE Transactions on Nanotechnology* (under review) (13 July, 2008).
- [4] Gerhard Klimeck *et al.*, *IEEE Trans. Electron Devices* 54, 2090 (2007)
- [5] C. Y. Ngo *et al.*, Phys. Rev. B 74, 245331 (2006)

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