Strain in inhomogeneous InAs/GaAs quantum dot structures

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Abstract. Most Non-destructive experimental approaches for the determination of indium concentration profiles give information about average indium concentration profiles only. Due to this, there is a need to extrapolate the indium concentration profiles in a way that takes into account the geometry of the quantum dots. We here present two extrapolation approaches. In the first approach we assume that the indium concentration profile is constant in the direction perpendicular to the measurement plane, while in the second approach we take into account the symmetry of the structure. Both approaches are compared to a profile with a constant indium concentration inside the dot.

1. Introduction

It is well known that InAs/GaAs quantum dot structures grown based on, for example, the Stranski-Krastanow growth mode [1] do not possess a homogeneous indium concentration inside the quantum dot [2]. Specifically, it has been observed that the indium concentration is highest at the tip of pyramidal quantum dots and decreases as we approach the base of the pyramid. Taking into account the shape of the indium concentration profile is important for accurate prediction of electronic properties for two reasons. First, within the k.p approximation [11] the concentration directly affects the effective masses and confinement potentials resulting in shifts in the energies and dipole transition strengths. Secondly, the concentration profile also affects the strain distribution and through that the piezoelectric potential giving additional shifts in energies and changes in transition strengths.

There exists today many approaches for the determination of concentration profiles in quantum dot structures such as cross-sectional transmission electron microscopy (X-TEM) [3], cross-sectional scanning tunneling microscopy (X-STM) [4], scanning transmission electron microscopy (STEM) [5], X-ray photoelectron microscopy [6], anomalous X-ray scattering (AXS) [7], Scanning-Probe-Microscopy nanotomography [8], and composition evaluation by lattice fringe analysis (CELFA) technique [9]. The ultimate goal of all such approach is to provide information about the full three dimensional concentration profile, however, at present the only way of gaining access to this is by destructive means. The non-destructive methods either provide average information in a give cross-section or the concentration profile on the surface of the structure. In this work we focus on the extrapolation of an average concentration profile obtained using the CELFA technique and study the consequences of a given choice of extrapolation.
2. Concentration Profile

In the paper by Blank et al. [9] information about the indium concentration in InAs/GaAs quantum dots has been obtained using the composition evaluation by lattice fringe analysis (CELFA) technique. The problem with the indium concentration profile found using CELFA is that it only gives information about the average indium concentration profile along one direction (in figure 1a the [010] direction).

In this work we consider the following three different indium concentration profiles extracted based on the average indium concentration shown in Figure 1a. All three profiles has been chosen so that their total indium content is identical.

2.1. Profile 1

We assume the indium concentration to be constant in the [010] direction.

$$C(x, y, z) = \begin{cases} \hat{C}(x, z)/L(z) & \text{inside the pyramid} \\ 0 & \text{outside} \end{cases}$$

where $L(z) = (L_d - 2z)$ for $0 < z < L_d/2$, and zero otherwise. $\hat{C}$ is the average indium concentration shown in Figure 1a, and $L$ is the side length of the pyramid at $z = 0$. We divide by $L(z)$ in order to take into account the shape of the quantum dot, see reference [9] for further details.

2.2. Profile 2

We assume a symmetric indium concentration profile in the [100] and [010] directions. Given the average concentration profile shown in figure 1 the three dimensional concentration profile takes the form

$$C(x, y, z) = \frac{\hat{C}(x, z)\hat{C}(y, z)}{\int \hat{C}(x, z)dx}$$

where again $\hat{C}$ is the average indium concentration. We divide with $\int \hat{C}(x, z)dx$ in order to ensure that $\int C(x, y, z)dx = \hat{C}(y, z)$.

2.3. Profile 3

We assume a constant indium concentration profile throughout the quantum dot.

$$C(x, y, z) = \begin{cases} C_{\text{tot}}/Vol_d & \text{inside the pyramid} \\ 0 & \text{outside} \end{cases}$$
where \( C_{\text{tot}} = \int \hat{C}(x, z) \, dx \, dz \) and \( \text{Vol}_d \) is the volume of the pyramid. We have included this profile as this is the most widespread choice of concentration profile for band structure calculations.

In figure 2 we show the three concentration profiles in the (100), (010), and (001) planes. In the figure we see that the first profile (constant along the [010] direction) gives rise to a higher indium concentration at the top of the structure compared with the symmetric profile. It is clear that in the real structure there is no reason why the indium concentration should be constant along the [010] direction.

### 3. Results

In this work we model strain and piezoelectric effects according to the fully-coupled electromechanical model described in Barettin et al. [10] and the band structure model is the usual Zinc-blende 8 band \( k \cdot p \) model (see e.g. [11]) with parameters taken from the paper by Stier et al. [12].

#### 3.1. Electromechanical Effects

In figures 3 we show the hydrostatic strain component \( H = \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz} \) for the three indium concentration profiles. We clearly see the choice of indium concentration profile reflected in the hydrostatic strain. The most prominent differences are seen in the directions where a constant indium concentration is assumed, i.e., when comparing profile 1 with profile 2 the main differences are seen in the [010] direction. Additionally, we see that for profile 1 the strain is highest at the top of the pyramid, whereas for profile 2 we also see high strains further down in the structure, due to high indium concentration further down in the structure for profile 2.
3.2. Electronic Structure

In figure 4 we show the six first conduction band electron states for the three indium concentration profiles. The corresponding energies are given in table 1 below. From the figures we see that the states
Profile 1 | 0.990 | 1.040 | 1.047 | 1.088 | 1.105 | 1.111
---|---|---|---|---|---|---
Profile 2 | 1.024 | 1.074 | 1.079 | 1.121 | 1.134 | 1.138
Profile 3 | 1.015 | 1.038 | 1.056 | 1.069 | 1.093 | 1.097

Table 1. Conduction band electronic energies for the three profiles. Energies are listed in eV.

for profile 1 and 2 are very similar, the main difference being a small angular rotation of the states. However, the states for profile 3 deviate notable from the states of the two other profile. The states being more spread out and the states 5 and 6 are interchanged compared with the states of the other profiles.

Comparing the conduction band energies of profiles 1 and 2, listed in table 1, we notice that the energy levels of profile 2 is shifted upwards with around 30 meV, however, the spacing of the energy levels of the two profile are more or less the same. Concerning profile 3, we see that here the energy level spacing deviates from the spacings observed for profile 1 and 2. Finally we notice that for profile 2 there are states which are almost degenerate, whereas, none of the states for profile 1 and 3 are close to each other.

The reason for this is that concentration profile 2 is much closer to having inversion symmetry than the other two profiles, and as a result we expect to see more states closer to each other (in the case with an inversion symmetric dot the states would be degenerate).

4. Conclusions

We have studied three possible choice of extrapolated concentration profiles based on an average concentration profile obtained using the CELFA technique. The three dimensional concentration profiles were used in determining the strain and piezoelectric fields in the structure and these were included in 8 band k.p calculations. We observed that there were notable differences between the electronic structure of the different profiles. The most notable being shifts in energy levels and lifting of degeneracies due to inversion asymmetric profiles. We furthermore observed a crossing of excited energy levels in going to a constant concentration profile.

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