Composition variation of In$_{1-x}$Ga$_x$As epitaxially grown in narrow trenches on Si

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Abstract. In this work we investigate the indium content in In$_{1-x}$Ga$_x$As narrow trenches on Si by transmission electron microscopy (TEM), energy dispersive spectroscopy (EDS) and nano beam diffraction (NBD). We find a higher indium content in wider trenches and by scanning a trench from bottom to top we observe an increase of indium up to a maximum value close to the level of the surface of the shallow trench isolation oxide.

1. Introduction
The use of III-V compound semiconductors as n-type channel replacement materials has attracted great attention because of their excellent bulk electron mobilities [1]. In particular, indium gallium arsenide compounds, with their intrinsically superior electron mobility and high saturation velocity, are considered as candidates for nMOS devices beyond the 14 nm node technology [2].

The material investigated in this work is In$_{1-x}$Ga$_x$As epitaxially grown in narrow trenches on (001) silicon wafers by metal organic chemical vapour deposition (CVD). Different trench widths and nominal In concentrations are considered. The In content is a critical parameter in InGaAs devices because it determines the bandgap of the channel and, as a consequence, the two-dimensional charge carrier density [3]. It is therefore important having an insight on its distribution in the trenches to better understand the device performances. We investigate, by TEM based techniques, how the indium content varies with the width of the trenches and in the lateral and vertical dimension inside the same trench width.

2. Experimental
2.1. Samples and characterisation techniques
TEM specimens were prepared by focused ion beam (FIB Strata, FEI) perpendicular (and parallel) to the trench directions by using the in-situ lift-out technique. In order to avoid damage during FIB ion milling the specimens were protected with a layer of CVD oxide and ion beam deposited platinum. The InGaAs trenches are grown on InP layers deposited over Ge seeds on Si substrate. Specimens with different trench widths as listed in Table 1 were prepared in a single experiment in order to investigate the dependence of the In content on the trench dimensions.

TEM, EDS and NBD analysis were performed on an F30 Tecnai TEM operating at 300kV. The In content was measured using the automatic quantification procedure included in the TIA version 4.5 software (FEI). NBD results were processed by using the TrueCrystal software (FEI), the mismatch is calculated with respect to the Si substrate.
Table 1. Specimens investigated in this study.

| Specimen label | Nominal trench width (nm) | Measured trench width at top (nm) | Cross section | Nominal In concentration (at %) |
|----------------|---------------------------|-----------------------------------|---------------|-------------------------------|
| 1              | 20                        | 10                                | perpendicular | 50                            |
| 2              | 40                        | 27                                | perpendicular | 50                            |
| 3              | 60                        | 40                                | perpendicular | 50                            |
| 4              | 80                        | 58                                | perpendicular | 50                            |
| 5              | 100                       | 76                                | perpendicular | 50                            |
| 6              | 500                       | 500                               | perpendicular | 50                            |
| 7              | blanket on InP            |                                    | wedge         | 53                            |

2.2. Wedge sample: absorption effects and thickness dependence

The blanket InGaAs layer is defect free and shows perfect epitaxy on the InP substrate which implies that it has a In$_{53}$Ga$_{47}$As composition. This is also confirmed by XRD analysis. A specimen with sloped thickness ranging from 100 nm to 300 nm was prepared to understand absorption effects and thickness dependence in the EDS quantification process.

An EDS profile was acquired along the full length of the slope as shown in the upper left corner of Figure 1, with 50s acquisition time per point so that the S/N on the In-K transition is high enough to be well processed by the software. Care was taken to position the TEM specimen in the TEM holder in such way to minimize the Cu stray signal due to the Cu grid and that the sample could be oriented at the optimal angle for best EDS signal detection. The detector take-off angle was 20°. The curves at the bottom of figure 1 represent the ratios between the K In/Ga, In/As peaks (Figure 1d) and the ratios between the In L-peak and the Ga and As K-peaks (Figure 1e). The curves are noisy but on average constant indicating no or little dependence on thickness and absorption for the K peaks, some absorption may be revealed for L-lines in agreement with literature [4].

EDS quantification with the K peaks for this reference sample with nominal 53% In concentration gives ~56%. Therefore a systematic overestimate of the EDS quantification values is to be taken into account but for relative comparison between measurements this is not a limitation.

Figure 1. a) HAADF-STEM image of the FIB prepared wedge sample, b) HAADF-detector intensity profile along the red line in a), c) EDS spectra, d) In/Ga, In/As for K transitions and e) In-L/Ga-K and In-L/As-K ratios.
3. Results and discussion
The specimens investigated in this study are shown in Figure 2. Most 20nm and 40nm trenches are not fully filled while the 60, 80 and 100nm are all well filled and end up with a large facetted cap above the shallow trench isolation (STI) surface. Differently, the 500nm line is facetted but does not develop a cap on top. All trenches are narrower at the STI surface than at the bottom. Also, the wider trenches are more deeply etched in the Si. Misfit dislocations are revealed at the Si/Ge and Ge/InP interfaces and a few nanotwins and stacking faults are also observed in the trench and in the cap.

![Figure 2](image_url)

Figure 2. TEM cross-sectional images of the different trench sizes. The dashed lines indicate the STI surface. The material stack is labelled in Figure 4.

EDS analysis shows that, in the trenches, the In content increases from bottom to top with a maximum value close to the surface of the STI layer and then decreases again as shown in Figure 3a. The average In content depends on the size of the trench: it increases exponentially with the trench width as shown in Figure 3b. The lateral variations of the In content in the trenches are small and vary from trench to trench in a non-systematic way.

NBD measurements are performed to evaluate the variation in lattice parameter due to the In content inhomogeneity. In order to compare NBD and EDS results the horizontal and vertical mismatches measured by NBD are converted to In concentrations by using the Vegard’s law and then averaged assuming a fully relaxed trench as shown in Figure 4b. The NBD measurements confirm the EDS trend but the values do not fully coincide. This is probably due to the presence of a certain degree of strain in the trench as well as to the effect of the lattice defects on the accuracy of the NBD measurements. In fact, for a fully relaxed InGaAs layer we would expect the same values for the horizontal and vertical mismatch. This is not the case and may therefore be the cause for the discrepancy between EDS and NBD results.
Figure 3. a) The In content increases from bottom to top in all size trenches. Curves are aligned to the top of the STI, b) average In content increases with trench width.

Figure 4. a) HAADF-STEM image, the red line indicates the NBD and EDS line profile. b) Indium concentration obtained by averaging the horizontal and vertical mismatch measured by NBD from bottom to top along the red line compared with the Indium content measured by EDS. The peak near 80 nm corresponds to the InP layer.

4. Conclusions
In this study we investigated the In content along the trench height for trenches with different widths. The In content increases from the bottom to the top of the trench up to the STI surfaces and increases with the InGaAs trench width. Awareness of this inhomogeneity can help to better understand the electrical behaviour of InGaAs devices and optimization of the growth process.

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References
[1] International Technology Roadmap for Semiconductors 2011
[2] Heyns M et al., 2011 Proc. IEEE International Electron Devices Meeting (Washington) p 299
[3] Wagner J W 1970 Journal Electrochemical Society 117(9) p 1193-1196
[4] Walther T 2010 Journal of Physics: Conference Series 209 012029