SiGe epitaxially grown in nano-trenches on Si substrate

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Abstract. SiGe lines epitaxially grown in silicon oxide nano-trenches on Si substrate are characterized by transmission electron microscopy (TEM) based techniques. Due to the high aspect ratio of the trenches most of the extended crystallographic defects are limited to the bottom of the lines. Few of them are still observed at the top of the lines and emerge in the cap above the lines. The SiGe composition is not homogenous in the width of the line and in the cap. This is linked to the formation of {111} facets. This variation of composition is not observed for the lines with an actual width narrower than 20nm.

1. Introduction

In order to increase the electron and hole mobility, co-integration of III-V materials or tensile Si and Ge, respectively, is considered as replacement for the Si channel [1]. The hole mobility in a Ge p-Fin field effect transistor (FinFET) can be even further increased by introducing compressive stress in the Ge channel [2]. This can be achieved by growing the Ge channel epitaxially on top of a SiGe relaxed buffer (SRB).

The aim of this paper is to characterize the SiGe layer epitaxially grown in trenches etched with HCl vapour in shallow trench isolation (STI) structures prepared on (001) silicon wafers. The nominal trench widths are 20-80nm but the actual widths are different, depending on the processing. The nominal width of the lines is mentioned in the rest of this paper except if otherwise specified.

2. Experimental

TEM specimens are prepared parallel and perpendicular to the trenches with the focused ion beam (FIB, Strata, FEI) lift-out technique and characterized with a Tecnai F30 TEM operating at 300kV. A chemical vapour deposited (CVD) glass or an electron beam deposited platinum layer and a FIB induced platinum layer are deposited beforehand on the area of interest in order to protect the specimen during the FIB milling.

Two-beam bright field TEM images are acquired in order to better reveal the presence of extended defects in the SiGe lines.

The composition homogeneity of the SiGe is assessed with energy dispersive x-ray spectroscopy (EDS) chemical analysis and related to the contrast observed in high angle annular dark field scanning TEM (HAADF-STEM) images. The atomic concentration profiles are calculated using the TIA (FEI) software.

3. Results

3.1. SiGe layer grown in shallow trench isolation

Typical TEM images of the nominal 20nm lines perpendicular and parallel to the lines are presented in figures 1a and 1b, respectively. The HCl vapour etch of the trenches results in {113} and {111} facets at the bottom of the trenches in the (001) Si substrate (figure 1a) [3]. The layers exhibiting different contrasts for the parallel orientation (figure 1b) can be explained by the overlap of different materials (e.g. Si-SiGe at the bottom of the trench, SiO_2-SiGe higher in the line) and by the different thicknesses of the materials present in the thickness of the TEM specimen (e.g. SiGe cap vs. SiGe line). Due to the {111} faceting of the bottom of the caps (see paragraph 3.2), voids are present where the caps merge due to the lateral growth of the SiGe on the oxide.

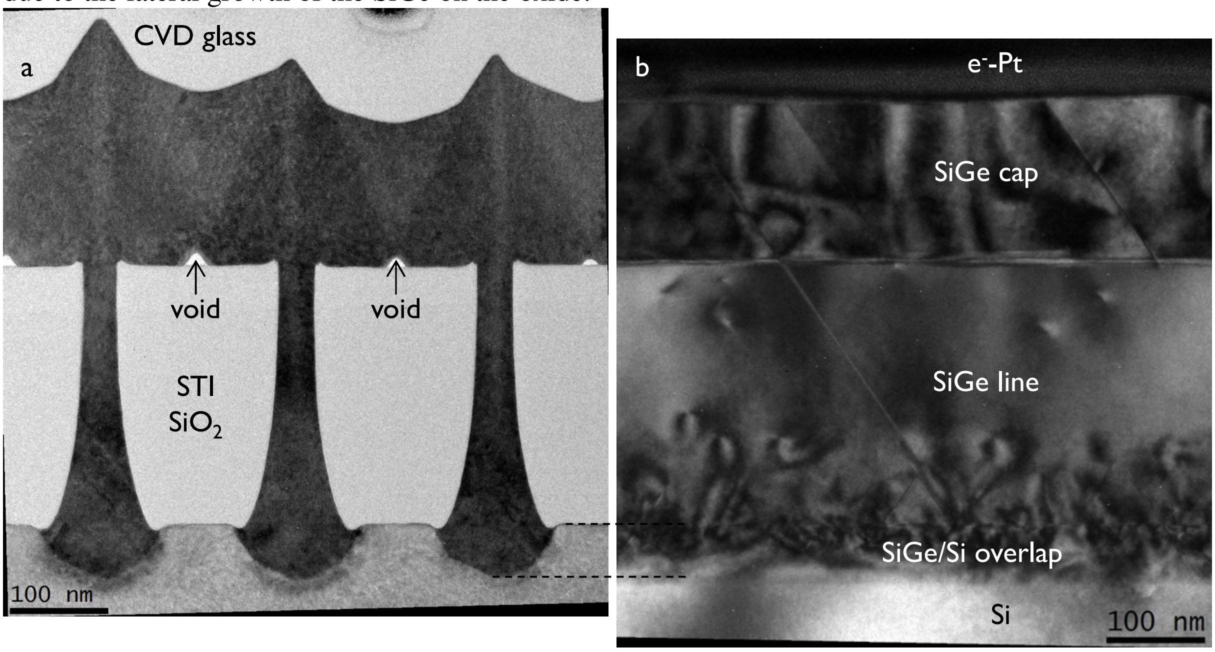

Figure 1. TEM cross-sectional images of the nominal 20nm wide lines perpendicular (a) and parallel (b: BF (220)) to the lines. For the parallel orientation (b) only one 20nm line is present in the thickness of the TEM specimen.

Higher density of {111} defects (stacking faults, nanotwins) and dislocations are observed at the bottom of the lines. Most of these defects start at the SiGe/Si interface and emerge at the sidewalls of the lines leaving the top of the lines with lower defect density. This is induced by the high aspect ratio of the trenches [4]. As can be seen with the trench embedded within the TEM specimen (figure 1b) only few defects propagate through the line and emerge at the top of the cap. Dislocations are also observed higher in the SiGe lines and cap.

Bands exhibiting a brighter contrast are observed in the centre and on the top of the lines in the TEM image (figure 1a). These bands exhibit a darker contrast than the surrounding SiGe in the HAADF-STEM image (figure 2) where the contrast is proportional to about $\langle Z \rangle^2$. It indicates that the SiGe composition is not homogenous in the width of the lines and of the cap.

Energy dispersive x-ray spectroscopy (EDS) is performed across the line (3-4) and across the cap (1-2) as outlined by the white lines on the HAADF-STEM image (figure 2a). The Si and Ge atomic concentration line profiles are calculated using the automatic procedure included in the TIA (FEI) software. The EDS signal is noisy due to the rather short acquisition time (3s), the atomic Si and Ge concentration profiles are therefore also noisy. In the top part of the lines (figure 2c) the Ge content is higher at the sidewalls of the lines (in average $Si_{0.32}Ge_{0.68}$) whereas lower in the central part of the lines (in average $Si_{0.45}Ge_{0.55}$). In the SiO_2 at both sides of the line 100% Si is obtained as only Si and Ge are taken into account for the quantification. In the cap (figure 2b) the Ge content is also lower in the central part above the line (~ $Si_{0.42}Ge_{0.58}$) than on the sides (~$Si_{0.30}Ge_{0.70}$) and then again lower (~$Si_{0.47}Ge_{0.53}$) with faceted frontiers close to {111} in the HAADF-STEM image (figure 2a). The nominal composition of the SiGe layer for these lines is $Si_{0.25}Ge_{0.75}$. It is worth noting that no standard specimen has been used but previous comparisons show that the SiGe quantification is quite accurate (± 5%). The variation of composition is qualitatively in agreement with the variation of contrast observed in the HAADF-STEM image. This composition distribution is not desired since it will create variation of the lattice parameter and strain in the width of the lines.

The variation of Ge content is due to the formation of {111} facets at the edges of the lines compared to the centre of the lines. Due to the higher atomic density of the {111} facets the growth perpendicular to these facets is slower than perpendicular to {001}. The Ge incorporation is then higher on the {111} facets.

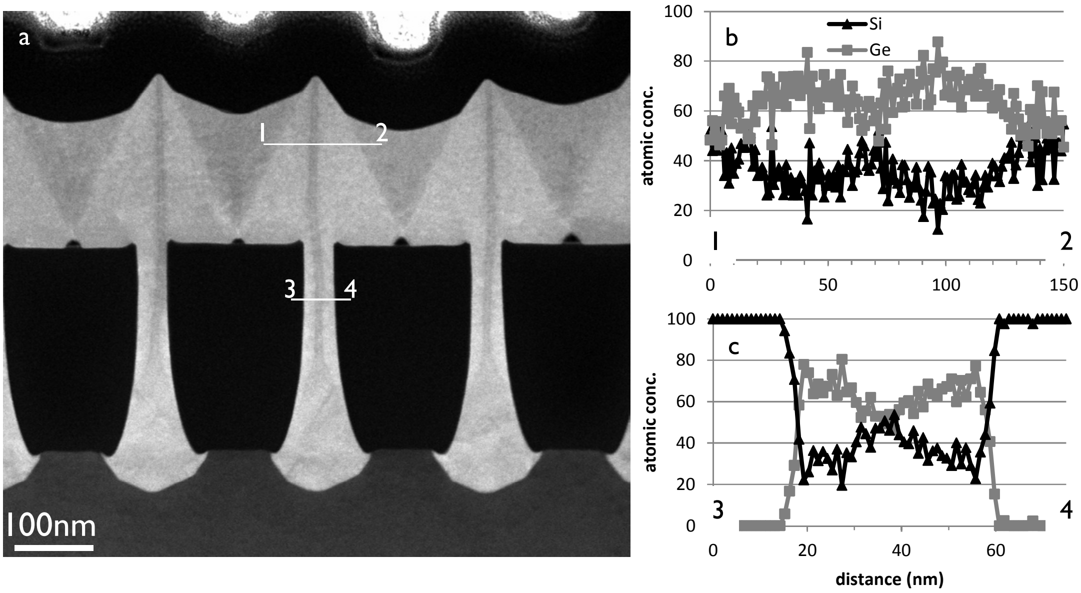

Figure 2. HAADF-STEM image of the 20nm wide lines (a) and Si and Ge atomic concentration profiles calculated from EDS obtained along the lines 1-2 (b) and 3-4 (c).

3.2. SiGe layer grown in shallow trench isolation with Ge marker layers

In order to better observe the correlation between the formation of the {111} facets and the composition variation in the width of the lines the growth of the SiGe layer is interrupted and 5 thin Ge marker layers are grown (figure 3). For the narrowest trenches the Si substrate is less deeply etched than for the wider trenches. It is worth noting that the growth rate of the first SiGe layer on top of the Si is higher for the wider than for the narrower lines.

For the lines wider than nominally 40nm, the 1st Ge marker is {111} faceted at both sides of the lines whereas rounded in the centre. The variation of composition in the width of these lines is clearly observed (figures 3b and c) between the 1st and 2nd marker layer. For the 40nm (actual width: 18nm) line (figure 3a) the first marker layer is rounded and no clear facets are observed at both sides of the lines. No variation of contrast is observed in the width of this line, indicating that the composition of the narrowest lines, the technologically most important ones, is more constant in the width of the lines than for the wider lines.

For all the line widths, the Ge marker layers are clearly {111} faceted in the cap and rounded at the intersection while the outer shape is sharper. For the 40nm lines (figure 3a) the different layers in the cap are rougher, leading to a widening of the Ge marker layers due to the projection of the roughness. Variation of contrast due to the variation of the Ge content is clearly observed in the caps.

The steps on the SiO_2 layer at both sides of the SiGe lines are most likely at the origin of the bottom {111} facets resulting in voids when the caps merge.

It can also be remarked that the growth of the Ge marker layers introduced a perturbation. On top of each Ge marker layer the SiGe area poorer in Ge is wider than below and above. The width of this area increases after each Ge marker layer, corresponding with the enlargement of the rounded top surface.

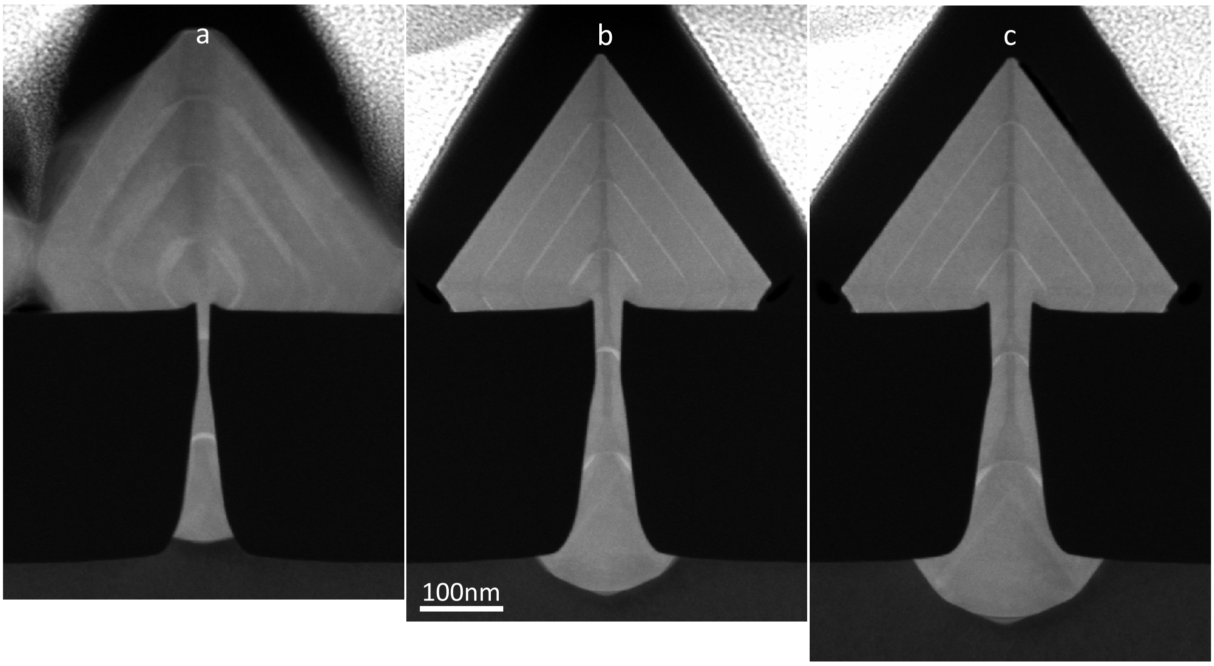

Figure 3. HAADF-STEM images of the nominal 40nm (a), 60nm (b) and 80nm (c) wide lines.

4. Conclusions

20-80nm nominal SiGe lines epitaxially grown in shallow trenches between silicon oxide are characterized by TEM based techniques. Due to the beneficial effect of the high aspect ratio of the trench a lower density of extended defects is observed at the top than at the bottom of the lines. A variation of composition linked to the formation of {111} facets is observed in the HAADF-STEM images and detected by EDS in the width of the lines and in the cap. This undesirable effect is not observed for the lines with an actual width narrower than 20nm.

Acknowledgements

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References

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