High crystalline quality of SiGe fin fabrication with Si-rich composition area using replacement fin processing*

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A high crystalline quality of SiGe fin with an Si-rich composition area using the replacement fin processing is systematically demonstrated in this paper. The fin replacement process based on a standard FinFET process is developed. A width of less than 20-nm SiGe fin without obvious defect impact both in the direction across the fin and in the direction along the fin is verified by using the high angle annular dark field scanning transmission electron microscopy and the scanning moiré fringe imaging technique. Moreover, the SiGe composition is inhomogenous in the width of the fin. This is induced by the formation of $\{111\}$ facets. Due to the atomic density of the $\{111\}$ facets being higher, the epitaxial growth in the direction perpendicular to these facets is slower than in the direction perpendicular to $\{001\}$. The Ge incorporation is then higher on the $\{111\}$ facets than on the $\{001\}$ facets. So, an Si-rich area is observed in the central area and on the bottom of SiGe fin.

Keywords: SiGe, selective epitaxial growth, FinFET, replacement fin processing

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1. Introduction

As the downscaling of Si-based complementary metaloxide-semiconductor device is approaching to its physical limit, an alternative way of further improving the device performance is to introduce the high carrier mobility materials, such as epitaxial Ge or SiGe for pMOSFETs and epitaxial Ge, Si or IIIV for nMOSFETs.^[1-3] So far, the potential of high mobility channel integration has been demonstrated in recent years by using the shallow trench isolation (STI) last and the STI first (replacement fin) integration routes on FinFET or nanowire devices.^[4-6] Compared with the STI last approach, the replacement fin scheme is easier and flexible to combine different materials for n- and p-MOSFET devices on one substrate. And several groups have successfully used the replacement fin processing to attain an SiGe fin and trap the misfit threading dislocation defects on the STI sidewall by tuning the growth parameters and applying a high temperature anneal or a laser anneal.^[7–9] The composition of their reported SiGe fins is homogenous in the width of the fin. Moreover, the thin SiGe epitaxial cladding of Si fins to form an SiGe-cladded FinFET exhibits $\sim 2x$ higher hole mobility and $\sim 2x$ better $I_{\rm ON}/I_{\rm OFF}$ than Si control device, and the DIBL is improved compared with Si control device.^[10] This is because of the large valence band offset (VBO) between SiGe shell and Si fin, a hole quantum well is configured in the high-mobility SiGe region as the major conduction path.^[11] However, the extra selective epitaxial growth of SiGe on Si fin brings the complexity to the process. So, fabrication of high crystalline quality of SiGe

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fin with a variation composition in one-step epitaxial growth is essential and a challenge to optimize the device electrical performance. However, so far, there are few reports on it in detail.

In this research, the crystalline quality of SiGe fin will be checked by using the high angle annular dark field scanning transmission electron microscopy (HAADF-STEM) and the scanning moiré fringe (SMF) imaging technique both in the direction across the fin and in the direction along the fin after its replacement fin processing has been developed successfully. Meanwhile, the formation mechanism of inhomogenous composition of SiGe in the width of the fin will also be discussed in detail.

2. Experiment

The fin replacement process began with the generation of an STI template on 200-mm-diameter Si substrates. The Si fin recess was attained by utilizing a tetramethylammonium hydroxide (TMAH) solution to etch post Si fin exposure. Then, the SiGe layer was selectively grown at 650 °C in an RPCVD reactor, and dichlorosilane (SiH₂Cl₂) and germane (GeH₄) in H₂ ambient were used as Si and Ge precursors, respectively. The HCl was utilized as the etchant to obtain selectivity during the epitaxial growth. Finally, SiGe fin formation was realized by utilizing the SiGe chemical mechanical polishing (CMP) and the STI recess process under DHF wet etching.

The scanning electron microscopy (SEM) and HAADF-STEM were used for evaluating the SiGe layers' epitaxial

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growth quality. The electron energy loss spectroscopy (EELS) mapping analysis was used to check the composition of SiGe fin. The SMF imaging technique was also employed to study the lattice plane direction and the quality of the SiGe replacement fin.

3. Results and discussion

The fin replacement process optimization based on a standard FinFET process is developed to attain an SiGe fin on a silicon substrate. Firstly, a \sim 20-nm-wide top critical dimension (CD) and \sim 200-nm-high Si fin with a vertical profile is obtained under the HBr/O₂/He gas as shown in Fig. 1(a). After a 300nmthick oxide film is deposited as STI oxide, the Si fin exposure is achieved by the Ar plasma bombarding followed by a DHF solution etching as shown in Fig. 1(b). Then, the Si fin recess with a V-shaped profile is achieved by utilizing the TMAH solution at 70 °C as shown in Fig. 1(c). Afterward, the narrow trench is successfully filled with the SiGe material after the pre-baking temperature and growth parameters of SiGe material have been optimized as shown in Fig. 1(d). It is worthy to note that the TMAH etching results in a V-shaped Si recess and the following optimal pre-baking treatment leads to a more rounding V-shaped Si recess profile, which is beneficial to confining the TD defect to the Si_{0.3}Ge_{0.7}/Si-substrate interface in comparison to a flat Si recess. This is because the dislocation network of flat Si recess is less confined to the SiGe/Si substrate interface and the number of threading dislocations reaching the top SiGe fin will be higher.^[12]



Fig. 1. SEM images of (a) Si fin profile, (b) Si fin exposure, (c) Si fin recess, and (d) SiGe's selective epitaxial growth.

One of the major challenges of SiGe fin formation for the replacement fin processing is to attain a high crystalline quality material without obvious structural defects' impact. Figure 2(a) shows the HAADF-STEM image of final SiGe fin fabrication post the SiGe CMP and STI recess process, obtained by utilizing the fin replacement strategy. It can be found

that a less than 20-nm-wide SiGe fin is successfully prepared. And its high resolution images at the top of SiGe fin, in the middle of SiGe fin and at the interface between SiGe and Si substrate are shown in Figs. 2(b)-2(d), respectively. They further confirm that the SiGe/Si-substrate interface is smooth and SiGe fin has no obvious structure defects, such as the misfit threading dislocation, twin boundary, stacking faults, *etc.* The above results prove that our fin replacement process can obtain a good-quality SiGe fin in the direction across the fin.



Fig. 2. HAADF-STEM images for SiGe fin fabrication in narrow trench by using replacement fin strategy, and its high resolution images (a) at top of SiGe fin, (b) in the middle of SiGe fin, and (c) at interface between SiGe and Si substrate.

Although a good crystalline quality SiGe fin is already verified in a direction perpendicular to fin since the STI has a strong confinement effect on the SiGe epitaxial growth, the threading dislocations or stacking fault defects maybe still exist along the fin, therefore, there is big room for the SiGe growth with a weak confinement effect.^[13] The quality of SiGe replacement fin along the fin direction also needs confirming. Based on our TEM experience on epitaxially growing SiGe/Si, the mirror force due to the free surface of crystal structure will cause the misfit dislocation to shift and disappear if the TEM specimen is very thin. So, the TEM specimen along the fin is designed as sandwich into a STI oxide. Figures 3(a) and 3(b) show the TEM and HRSTEM images of SiGe fin of STI oxide/Fin/STI oxide samples along the fin direction post the SiGe selective epitaxial growth (SEG). The TEM result shows no obvious crystal defects found in the SiGe film between the STI oxides. Although there are strong contrast variations in the SiGe between STI oxides, none of them is related to any structure defect. This signature should be related to the stress in SiGe fin causing some bent contours, which may be along the Si (001) direction, and result in the

Bragg diffraction contours' fringes. Moreover the HRSTEM result further confirms that the good crystalline quality of SiGe SEG is attained without obvious crystal defects' impact along the fin direction.



Fig. 3. (a) TEM and (b) HRSTEM images of SiGe fin along fin direction post SiGe SEG.

Furthermore, the SMF technique is also employed to study the SiGe (110) atomicplane crystalline quality along the fin direction. Figure 4 shows the SMF images of SiGe film from bottom to top along the fin direction. The fast Fourier transform (FFT), mask filter and inverse FFT (IFFT) are used to improve the SMF image quality. The fringe of SMF for Si substrate is adjusted to the horizontal orientation as shown in Fig. 4(a). The SMF of SiGe between the STI oxides is refocused because this part of SiGe is sandwiched into a oxide, which results in some fringes tilted due to the electron magnetic rotation effect as shown in Fig. 4(b). The existence of lattice defects will result in an obvious rotation or distortion of the {110} planes, so, the SiGe between STIs along the fin direction should have a good and acceptable quality without obvious defects. However, there is a minor SMF fringe rotation of about 5.7° from bottom to top, which confirms that the SiGe (110) plane tilts at an angle of about 0.3° from SiGe bottom to top. This is because 1° scan rotation will result in a fringe rotation of 17.1° based on our experiment set-up. This minor tilt of SiGe lattice should be related to the release of the misfit strain from bottom to top along the fin direction. This minor tilt of SiGe lattice cannot be detected by HRSTEM but can be observed by the SMF technique due to its higher sensitivity. So, the SMF result of SiGe between the STIs can further confirm that an acceptable crystalline quality of the SiGe is realized by using the replacement fin processing.



Fig. 4. SMF images of SiGe SEG from bottom to top along fin direction, for (a) Si substrate, (b) SiGe between STI oxides.

In addition, it is found that there is an obvious darker contrast in the fin center and on the bottom in Fig. 2. Although the V-shaped Si recess can help improve the uniformity of the Ge concentration within the SiGe,^[13] the transverse composition in the SiGe fin is still inhomogeneous. In the HAADF STEM image, the contrast is directly related to specimen Z, namely the ordinal number of atom in the periodic table. Consider that the Z of Si is 14 and Z of Ge is 32, the darker area in the middle of SiGe fin may be Si-rich. Moreover, the EELS analysis is employed to check the central darker area composition of this structure and its results are shown in Fig. 5. The average concentration of Ge in SiGe fin is about 30% and about 25% in the darker area. So, the variation of composition qualitatively accords with the variation of contrast observed in the HAADF-STEM image.



Fig. 5. EELS mapping results for dark area of SiGe fin.

At the same time, the HAADF-STEM image of an SiGe material post SEG is presented in Fig. 6(a) and its high resolution image on the bottom of SiGe Fin is shown in Fig. 6(b).

It can be found that the central and bottom Si-rich SiGe truly exist post SEG. And the bottom Si-rich SiGe has a triangular shape and the central Si-rich SiGe has a line shape. Moreover, the bottom triangular shape of Si-rich SiGe has a typical {111} facets signature and it will not further increase as the triangular shape boundary arrives at the interface between STI and Si substrate. The possible formation mechanism of the central and bottom Si-rich SiGe material is as follows: at the initial SiGe epitaxial growth stage, there is a facet compensation and competition on the bottom of the trench. The Ge incorporation is higher on the $\{111\}$ facets than on $\{001\}$ facets because the atomic density of the $\{111\}$ facets is higher, the epitaxial growth in the direction perpendicular to these facets is slower than in the direction perpendicular to $\{001\}$. Namely, Ge incorporation is lower on the $\{001\}$ facets. So, an Si-rich SiGe with a typical {111} facet will grow to form a bottom triangular shape. As its boundary arrives at the interface between STI and Si substrate, the {111} facets' growth of this triangular shape will maintain a balance with $\{001\}$ facets' growth and only central Ge incorporation is lower on the $\{001\}$ facets. So, a central line shape Si-rich area is obtained at the top of the bottom triangular shape Si-rich SiGe till the epitaxial growth is ended. Reference [14] also clearly identified the similar results and the presence of {111} facets during the SiGe growth by adding ultrathin Ge markers.



Fig. 6. HAADF-STEM images for (a) SiGe's selective epitaxial growth in the narrow trench, and (b) its high resolution image at bottom of SiGe fin.

In addition, owing to the VBO existing between SiGe and central Si-rich composition area, the newly developed SiGe fin may possess larger room to finely tune the threshold and leakage performance of device than the homogenous SiGe fin. And we will further investigate the influence of Si-rich area of SiGe fin on its electrical performance after the FinFET device fabrication in future.

4. Conclusions

In this work, a high crystalline quality of the SiGe fin fabrication both in the direction across the fin and in the direction along the fin is realized by using a replacement fin processing. Furthermore, a central area and bottom Si-rich area are observed in the HAADF-STEM images and confirmed by the EELS mapping analysis. The inhomogenous SiGe composition in the width of the fin is induced by the formation of {111} facets during epitaxial growth.

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