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Facet formation in Si layers selectively grown on patterned substrates studied by different electron microscopy techniques

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ABSTRACT: The growth of Si on substrates patterned with an oxide mask is of considerable technological importance in the fabrication of low dimensional structures. One of the main issues in this kind of epitaxy is the faceting of the Si layers. In this work, the facet formation of selectively grown Si layers was investigated using several different electron microscopy techniques. Surface morphology of these Si films was firstly studied using a high-resolution low-voltage scanning electron microscope (HRSEM) equipped with a field emission gun. The effect of both n-type and p-type doping on the facet formation of selectively grown Si layers, as well as the effect of growth temperature, window orientation and dimensions, was then investigated by cross-section transmission electron microscopy (TEM). On-zone electron diffraction patterns were applied to identify individual facet orientations. Lattice images of the faceted growth front along different orientation were observed in a high-resolution transmission electron microscope (HRTEM) and were used to confirm the facet orientation.

1. INTRODUCTION

The selective epitaxial growth (SEG) of Si on patterned substrates with an oxide mask has attracted a lot of attention in recent years (Fujita et al 1997, Vescan et al 1998). However, it has been found that SEG is usually confronted with the formation of a facet at the edge of the mask (Xiang et al 1996, Vescan et al 1998, Gallas et al 1999). The facet is a very important issue in SEG. Facet formation makes possible the fabrication of new types of vertical metal-oxide-semiconductor (MOS) transistors and nanoscale structures on micrometer scale patterns (Behammer et al 1996). The facets may cause the deterioration of the electrical properties of SEG SiGe devices, such as the heterojunction bipolar transistor (HBT). The facet formation and evolution are due to the growth rate anisotropy among (100), (311) and (111), which is certainly associated with growth conditions, such as temperature, doping, mask size and orientation. Some theoretical models, based on minimising total free energy and surface migration, have also been developed to study the facet formation and competition processes during the epitaxial growth (Li et al 1996). In this study, the facet formation on selective epitaxial growth of Si on patterned substrates using gas source molecular beam epitaxy (GS-MBE) was investigated by transmission electron microscopy (TEM). The main facts, which affect the formation of facets within the unmasked windows, are discussed.

2. EXPERIMENTAL

All the growth experiments were carried out in a VG Semicon GS-MBE system with a base pressure of 5×10^{-11}mbar. The samples were grown on the Si (001) substrates with a SiO_2 mask pattern. The mask window openings with different sizes were aligned along <110> and <100> directions. To investigate the facet formation, Si/SiGe (%Ge=5%) superlattices, doped or undoped, were grown on SiO_2-patterned Si (001) substrate between 700°C and 900°C.

The surface morphology of SiO_2-patterned Si substrates was characterised after the growth using atomic force microscopy (Digital Instrument 3100) and high resolution scanning electron microscopy (LEO 952). The cross-section TEM specimens were made using conventional methods. The sectioned wafers were glued face-to-face and then sliced and mechanically polished, which was followed by dimpling and ion-milling. Prepared specimens were examined using a JEOL 2010 electron microscope operating at 200kV.

3. RESULTS AND DISCUSSIONS

3.1 Surface Morphology

Figure 1(a) shows the arrangement of the patterned windows on a Si (100) substrate and orientation was indicated by the arrows. Figure 1(b) shows an example of the surface morphology obtained after the growth of 500 nm of Si inside a square window etched in SiO_2, enabling us to observe facet formation in all directions simultaneously. Clearly, a film with a facet has been grown in this <110> aligned window. Between the flattened film top and the sidewall, facet formation has occurred as observed by both HRSEM and AFM. Although AFM is powerful for elucidating the morphology and suggesting the possible facet orientation, but it has a problem to differentiate the crystalline and noncrystalline films and some artefacts may occur when examining the facet formed very close to sidewall. Certainly, both AFM and SEM are for not useful for investigating the facet behaviour at the different stages of the growth, in which case the TEM is more powerful to be able to examine the Ge marker layers deep inside the film.

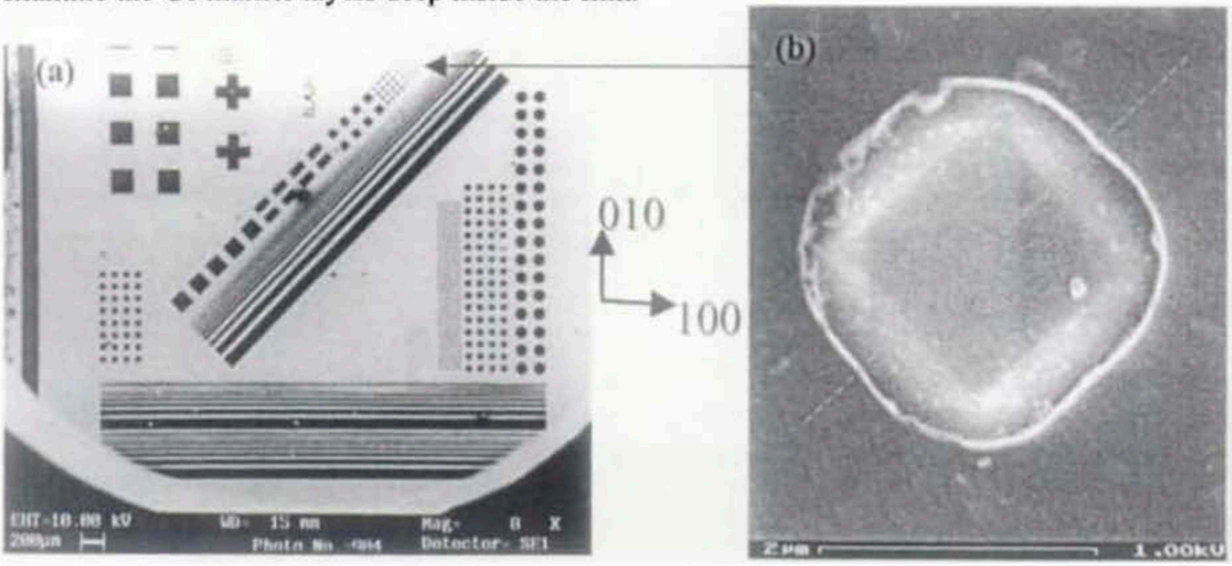

Fig. 1. SEM images of (a) patterned Si (100) substrate and (b) a <110> aligned window. The dotted line in (b) shows the sectioning direction for cross-sectional TEM specimen.

3.2 Effect of Window Orientation and Doping on Facet Formation

Figure 2(a) is a cross-sectional TEM image along the <110> direction. The image shows half of the film grown in a window with <110> orientation. Both the final surface and the inside Ge marker layers suggest that the sidewall facet is {113} and film top facet is {001}. Between sidewall {113} and top {001}, a {119} facet has also been formed. It is usually believed that the facet evolution is due to the growth competition among facets during the SEG growth. In our case, the growth rate relationship has been reported as *R*(100)>*R*(311)>*R*(111) (Hirayama et al 1993), so the {111} facet should be formed as the film becomes thicker. However, in Fig. 1(a), no {111} facet was observed as reported in other literature (Xiang el al 1996), although the film here is significantly thicker than their case. It might be attributed to different mask thickness and the ratio of mask thickness and window dimension. Figure 2(b) shows the cross-section image of a film grown in a <100> oriented window. Different from the <110> orientation, there is no facet formed on the sidewall, as illustrated in Fig. 3, and the film fills almost the whole window trench. The Ge maker layers grown at different thicknesses inside the film are clearly flattened, which also indicates no sidewall facet is formed in the earlier stages of the SEG. This result is similar to previous work (Vescan et al 1998 and Gallas et al 1999).

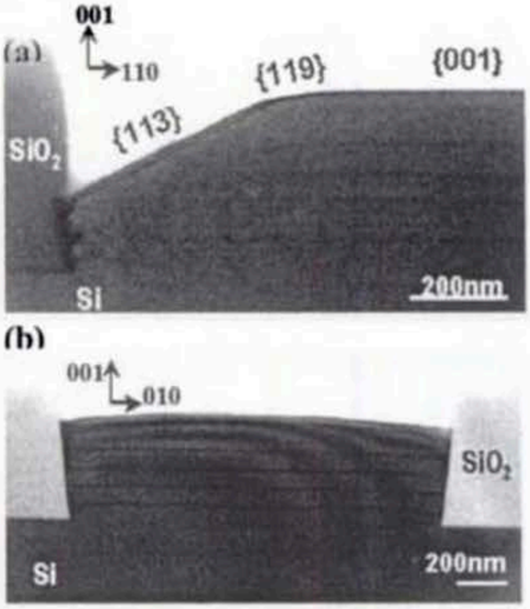

Fig. 2. Cross-sectional TEM images showing undoped films grown in the windows along (a) <110> and (b) <100>.

Fig. 3. Cross-sectional TEM images showing the film and mask interface. The undoped film is grown in the window along <100>.

To compare with the result in Fig. 2(a), a smaller window along <110> is examined by cross-sectional TEM and HRTEM, as shown in Fig. 3. In this case, apart from {113}, {119} and {001}, the {111} facet is also clearly observed at the end of sidewall and {001} becomes smaller. Both selective area diffraction and lattice image (inserted in Fig. 3) have also been applied to confirm the nature of the facets.

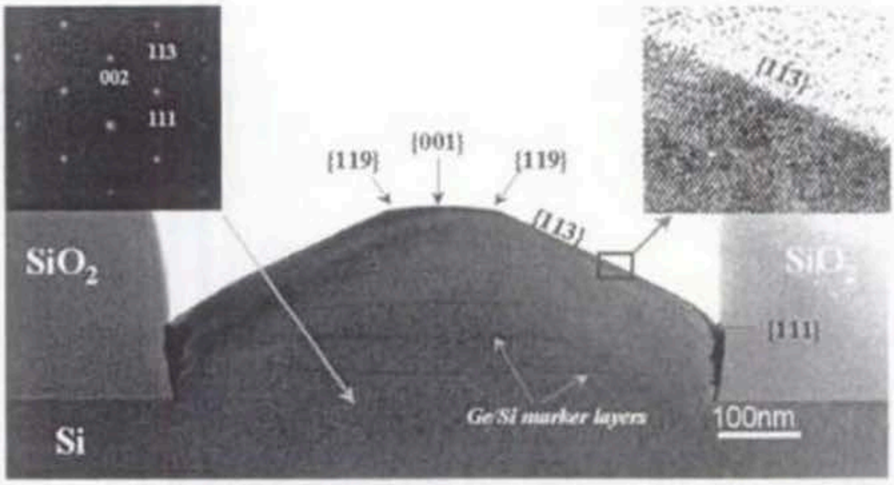

Fig. 4. Cross-section TEM image of an undoped SEG Si film grown in a submicron window along <110> direction. The selective area diffraction and HRTEM lattice image are inserted to reveal the facet orientation.

Both n- and p- doped films have also been examined, as shown in Fig. 5. It is found that there is no significant effect of doping on the facet formation in our case. The facets formed in <110> oriented windows all include {001} and {113^n}, where n=0, 1 and 2, in both doped and undoped films. The only difference observed is that the {119} facet in the As-doped sample is more well-developed than the cases in undoped and the B-doped film and on the other hand the {113} facet in As-doped sample is less-developed. These results might suggest that there is a different growth rate relationship for As-doped film, in which As-doping hinders the growth of {119} and favours the growth of {113}. Certainly, this doping effect needs more careful study; especially the same window dimension should be examined for differently doped films.

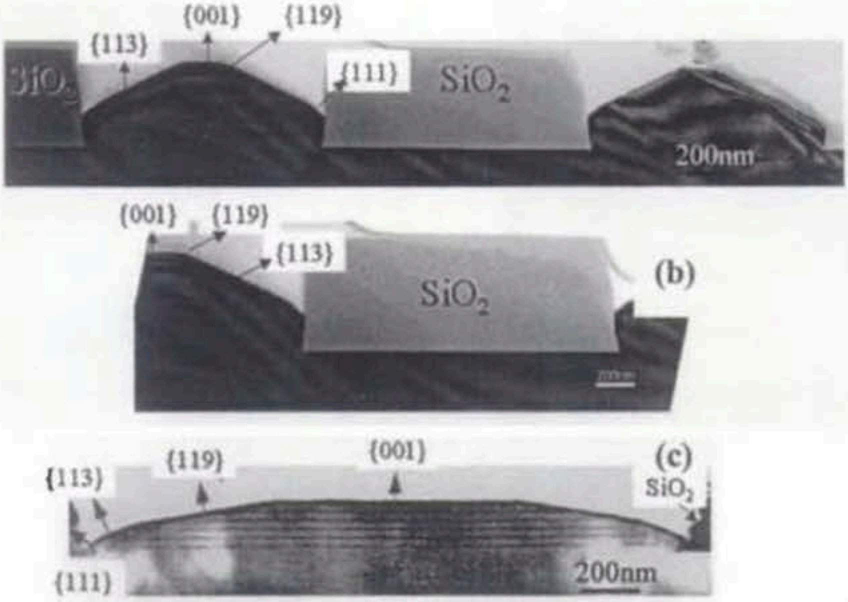

Fig. 5. Cross-sectional TEM images of SEG Si films grown in windows along <110> direction: (a) undoped, (b) B-doped and (c) As-doped.

4. CONCLUSIONS

The microstructure of the SEG Si films were characterised by different electron microscopy techniques, including HRSEM, cross-sectional TEM, on-zone electron diffraction pattern and HRTEM lattice imaging. The facet formation was observed inside the <110> aligned mask windows for both doped and undoped films. The predominating facets includes both {001} and {113^n}, where n=0, 1 and 2. On the other hand, no distinct facet was observed in the doped and undoped films grown in <100> aligned windows. Facet formation and evolution are the result of growth competition among the facets and doping may affect the growth rate relationship between certain facets. In order to obtain more understanding on the facet formation in the SEG Si films, it is also suggested to apply some other advanced TEM based techniques, such as HAADF electron tomography to examine the faceting of the inside of Ge marker layers and electron holography to reveal the doping effect on facet formation.

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