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Mechanism of Defect Formation during Low Temperature Si Epitaxy on Clean Si Substrate

I. Mizushima, M. Koike[1], T. Sato, K. Miyano and Y. Tsunashima
Microelectronics Engineering Laboratory, [1]R&D Center
Toshiba Corporation, Yokohama 235-8522, Japan
Phone: +81-45-770-3662, Fax: +81-45-770-3577, E-mail: mizushima@amc.toshiba.co.jp

1. Introduction

Low temperature epitaxy of Si films is one of the promising technology for the scaled devices. A lot of applications such as epitaxial channels or elevated source/drain have been proposed.[1,2] For the adoption of the epitaxy of Si to ULSI devices, defect elimination is the most important issue. In order to obtain the high quality epitaxial films, special attentions to the surface cleaning method before epitaxial growth have been paid.[3] However, it was found that a lot of defects are formed in the deposited films at a certain condition, even though the surface is sufficiently cleaned.

In this paper, defects in the Si films deposited by LP-CVD are examined in detail. Deposition conditions are important for the suppression of the formation of defects. Mechanism of the defect formation is also described.

2. Experiment

Epitaxial Si films were deposited on the HF cleaned (001) Si substrates. In-situ cleaning was performed by the H_2 bake at 900°C for 3 min. Si films were deposited using SiH_4 with H_2 as a carrier gas. The deposition temperature was typically 700°C, and the total gas flow rate was 10 slm. The pressure and the SiH_4 flow rate were ranged from 5 to 80 torr and from 70 to 900 sccm, respectively. The surface morphology and the defects in the epitaxial layer were investigated by SEM and TEM. SIMS was used to confirm the native oxide removal by the in-situ cleaning.

3. Morphology and Defects of the Deposited Films

SEM photographs shown in Figs.1, 2 and 3 indicates that the deposition condition affects the surface morphology of the deposited Si films. The thickness of each deposited film was about 1 μm. Flat surface was obtained under the deposition condition of low deposition rate of 40 nm/min, as shown in Fig.1. This suggests that no defects were formed in the deposited layer. Defects having the shape of mound were formed when the deposition rate was higher (200 nm/min), as shown in Fig.2. Fig.3 shows that all the surface of the deposited layer was rough under the condition of much higher deposition rate (800 nm/min).

The crystallinity of the deposited Si films having different surface morphology was examined by cross-sectional TEM. No defect was observed in the flat surface sample. In the sample having the mound-shape-defects (Fig.2), isolated defect regions were observed as shown in Fig.4. This defect region consists of high density {111} facets. Since the growth rate of the edge of {111} facet is higher than the rate of (001) plane, the top of the defect is above the epitaxial surface. For the sample with rough surface (Fig.3), the deposited layer was polycrystalline as shown in Fig.5. Such polycrystallization is the result of the connection of many isolated mound-shape-defects.

It was confirmed by SIMS that the residual native oxide is not the reason of the defect formation in the deposited layers. The oxygen concentration at the interface was lower than the concentration in substrate as shown in Fig.6. This indicates that the defect formation is a result of the deposition condition.

The following experiment clearly shows that the deposition condition affects the defect formation. The deposition condition was changed without stopping the SiH_4 flow during the growth. The first layer was deposited under the low rate condition, and the second layer was deposited under the high rate condition. Fig.7 shows that the high density defect region starts at the interface corresponding to the change of deposition condition.

4. Mechanism of the Mound Formation

The surface morphology was examined for various deposition conditions at 700°C, as shown in Fig.8. Deposition rate is also shown in Fig.8. It had been expected that the deposition rate should be the determinant factor of the defect formation. However as shown in Fig.8, the surface morphology is affected by the total pressure rather than by the deposition rate.

In order to obtain an epitaxial layer without defects, the adsorbed SiH_4 has to be decomposed and to migrate until the atoms find the stable substitutional site. When the total pressure is high, the decomposition of adsorbed SiH_4 is suppressed, and accordingly the migration on the surface might be suppressed. Thus, the adsorbed atoms locate at the irregular position, which works as a start of the formation of the mound.

Fig. 9 shows the plane TEM photograph of the mound shown in Fig.2 and 4. This clearly shows that the mound is formed by quadrangular pyramid defects. The side of the square is parallel to the [110] direction of the Si substrate. This suggests that the observed defect is quite different to the well known defects in the epitaxial films, where the {111} stacking fault starts at the interface.[4]

5. Conclusion

Defects having the mound structure are formed during the Si epitaxy by LP-CVD at a low temperature of 700°C even if the surface is atomically clean. Careful attention has to be paid to the deposition condition as well as to the surface cleaning in order to obtain a high quality films.

References
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3) H. Wakabayashi et al., Ext. Abst. SSDM97, p.512 (1997).
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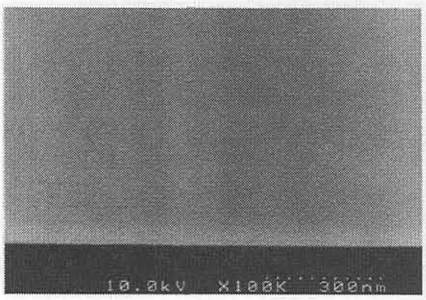

Fig.1 SEM of the Si films deposited under low deposition rate condition.
Total pressure: 5 torr, SiH_4: 350 sccm.
Deposition rate: 40 nm/min.

Fig.2 SEM of the Si films deposited under medium deposition rate condition.
Total pressure: 10torr, SiH_4: 900 sccm.
Deposition rate: 200nm/min.

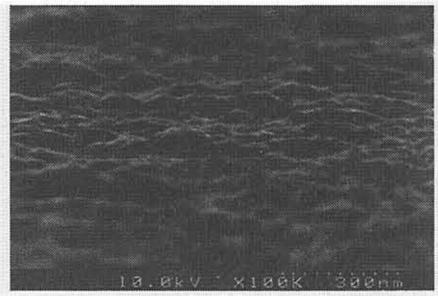

Fig.3 SEM of the Si films deposited under high deposition rate condition.
Total pressure: 80torr, SiH_4: 900 sccm.
Deposition rate: 800 nm/min.

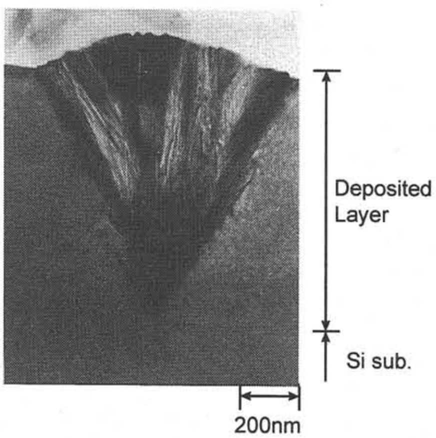

Fig.4 Cross-sectional TEM photograph of the medium-deposition-rate sample, as shown in Fig.2. Mound-shape-defect consists of {111} facets.

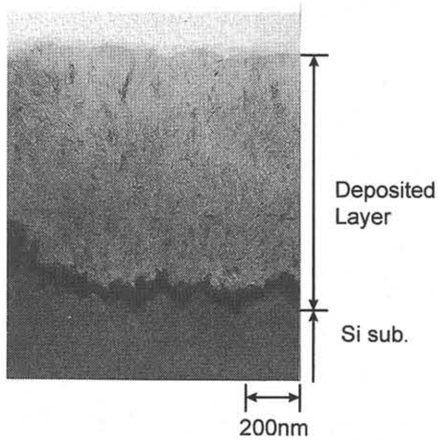

Fig.5 Cross-sectional TEM photograph of the high-deposition-rate sample, as shown in Fig.3. Mound-shape-defects are connected each other, because the density of the defects was very high.

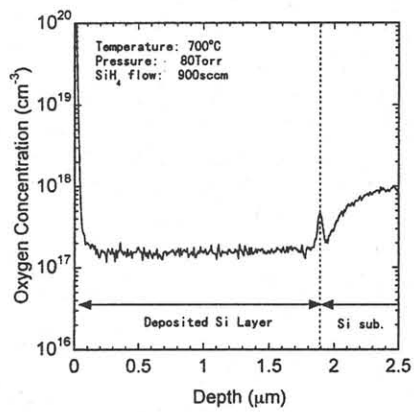

Fig.6 Oxygen profile of the deposited sample, which has a lot of defects in the deposited layer as shown in Fig.3 and 5. The interfacial oxygen concentration was lower than the concentration in the Si substrate.

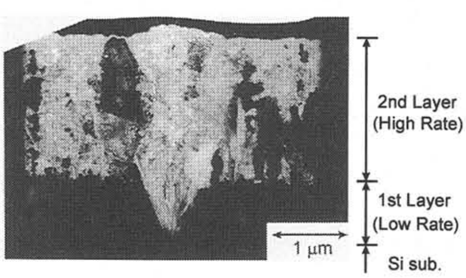

Fig.7 Cross-sectional TEM photograph of the sample, where two Si layers were deposited sequentially. The deposition condition was changed between the 1st and the 2nd layers. High density defects starts not at the surface of the Si substrate but at the interface of the two layers.

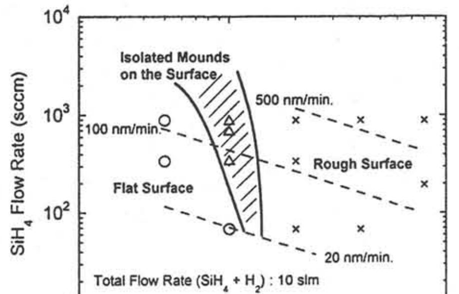

Fig. 8 Surface morphology of the Si films deposited under various conditions. ○, △ and × indicate that the surface of the films was flat, partially rough and rough, respectively.
The solid lines show the boundary between the different surface morphology. The broken lines show the deposition rate.

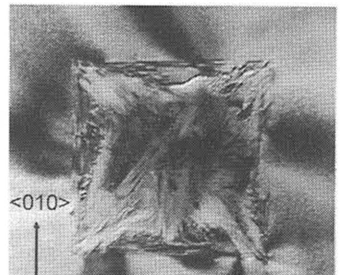

Fig.9 Plane TEM photograph of the mound. The side of the square is parallel to the [110] direction.