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Atomic Step Morphology of Epitaxially Grown and H_2 Annealed Si Surface

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Changes in the Si surface atomic step morphology induced by H_2 annealing after epitaxial growth were studied using atomic force microscopy (AFM). After pre-baking at 1100°C, Si epi-layers were grown in a SiH_4-H_2 system and subsequently annealed in H_2 ambient for 0-30 min at 1000-1100°C. Then, the surface morphology was observed by AFM for the Si (100) and (111) samples at room temperature. The (100) samples showed finger-like step lines. Smooth atomic step-lines on the (111) surface were obtained at 1000-1050°C whereas a zigzag step morphology was observed for the (111) samples annealed at 1100°C.

1. Introduction

To assure ideal dielectric properties and the reliability of thin (< 3 nm) gate oxide films, the atomic step of a Si surface before gate oxidation should be controlled. The atomic scale structure of the Si surface has been studied after H_2 annealing and epitaxial growth[1-3]. However, the effect of H_2 annealing has not been extensively studied with regards to the annealing temperature and time.

This paper describes the changes in the Si surface atomic step morphology induced by H_2 annealing at 1000-1100°C for 0-30 min after epitaxial growth. After pre-baking at 1100°C, Si epi-layers were grown in a SiH_4-H_2 system and subsequently annealed in H_2 ambient. The morphology of the Si surface atomic step was observed by atomic force microscopy (AFM) for the Si (100) and (111) samples. We found that, by annealing the epi-surface in H_2 ambient, the atomic step morphology of the (111) epi-surface can easily be controlled at 1000-1050°C whereas an uncontrollable zigzag step morphology was observed for the (111) samples annealed at 1100°C.

2. Experiment

The substrates we used were p-type (100) and (111) Si wafers with diameters of 150 mm and resistivities of 20-40 Ω cm. The miss-orientations of the substrates were within 0.05° for directions parallel or normal to the orientation flat. The width of the mono-layer-step terrace was calculated at more than 130 nm for the (100) surface and 210 nm for the (111) surface. Atmospheric pressure epitaxial growth was performed for the chemically cleaned substrates, and a 1.0 μm thick epi-layer was grown in a SiH_4-H_2 system at 1000-1100° C after pre-baking at 1100° C. The Si epi-layers were subsequently annealed in H_2 ambient at the same temperature (Fig. 1). After unloading the samples, we observed the microstructure of the Si surface by atomic force microscopy (AFM, SPA300/SPI3700, SII) for the (100) and (111) samples using the cyclic contact mode for 1x1 μm^2 and 5x5 μm^2 scanning areas.

3. Results and Discussion

The (100) epi-wafers grown at 1000°C without H_2 annealing showed a terrace structure with mono-atomic-layer (0.14 nm) steps, and the finger-like steps extended in the <110> directions on alternating terraces reflecting the double-domain reconstruction (Fig. 2 (a)). The observed structure was almost the same as that reported previously[1-3], but the finger was wider than before. This is because H_2 annealing was not performed for this sample. With H_2 annealing for 3 min, which is normally performed to purge the deposition gases before cooling samples, the step-finger width shrunk and the observed structure was exactly the same as that reported[3] (Fig. 2 (b)). With further annealing for 20 min, the etched terrace region was observed (Fig. 2 (c)). The observed structure change with H_2 annealing is almost the same for the growth and annealing temperature range of 1000-1100°C.

The (111) epi-wafers grown at 1000°C without H_2 annealing showed the terrace structure with bi-atomic-layer (0.31 nm) steps with kinks (Fig. 3 (a)). The kinks were probably formed by the inhomogeneous ambient when the ambient changed from SiH_4-H_2 to H_2. With H_2 annealing for 3 min, the kinks disappeared and the step-line was wavy (Fig. 3 (b)) as reported previously[3]. With further annealing for up to 20-30 min, the wave amplitude becomes smaller and the almost parallel step-lines without kinks were observed (Fig. 3 (c), (d)). The dependence of terrace width deviation on H_2 annealing time is shown in Fig. 4. The deviation of terrace width first increases, and then decreases with the annealing time increase through the change in step morphology.

The 1-dimensional theoretical model[4] predicted that the deviation of terrace width decreases exponentially if the step captures the surface atoms from the lower terrace rather than from the upper terrace. However, the observed decrease in Fig. 4 is much faster than the exponential behavior. Obviously this is because the 1-dimensional model does not explain the present situation and a 2-dimensional model should be considered. The step energy increase due to the step curvature (Fig. 3 (b), (c)) will enhance the step motion, and will result in a faster decrease of terrace width deviation. The surface diffusion field theory and the Monte Carlo simulation[5,6] will be useful in analyzing the present results.

The observed step-lines after H_2 annealing for 20-30 min was almost the same for the growth and annealing temperature range of 1000-1050°C. As shown in Fig. 5 (a), the step-line is rather smooth for the samples annealed for 20 min at 1050°C. However, zigzag step-lines are observed for the samples grown and annealed for 0-30 min at 1100°C (Fig 5 (b)). Therefore, with H_2 annealing at 1100°C, it is rather difficult to control the step-line shape of the Si (111) surface.

4. Conclusion

The microstructure of the Si surface for (100) and (111) wafers was observed by AFM after epitaxial growth and H_2 annealing. For (100) samples, the observed structure was finger-like step morphology and the change with H_2 annealing was almost the same for the growth and annealing temperature range of 1000-1100°C. For (111) samples, the deviation of terrace width first increased, and then decreased with the H_2 annealing time increase through the change in step morphology. The observed step-lines after H_2 annealing for 20-30 min were almost the same for the growth and annealing temperature range of 1000-1050°C, but zigzag step-lines were observed for the samples grown and annealed for 0-30 min at 1100°C. Accordingly, with H_2 annealing at 1000-1050°C, we can easily control the Si (111) epi-surface, and smooth and uniform atomic step morphology is obtained.

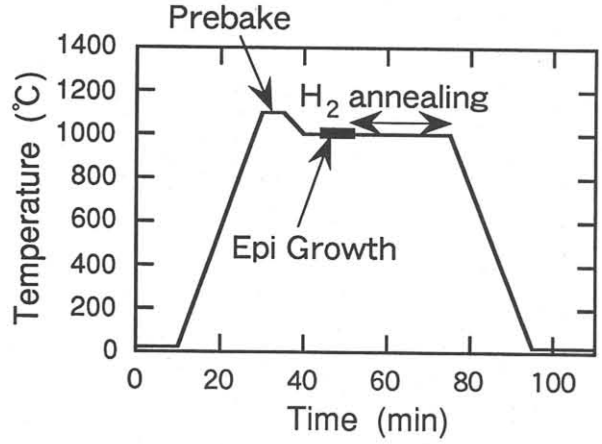

Fig. 1 Epitaxial growth and H2 annealing sequence.

Acknowledgments

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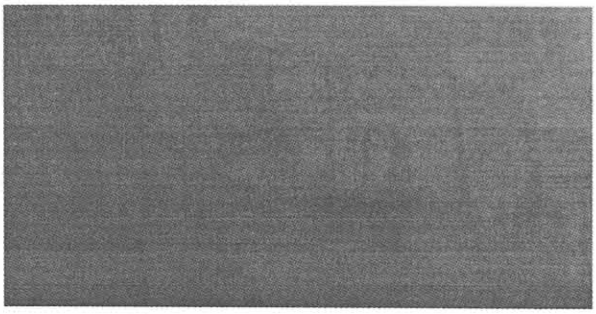
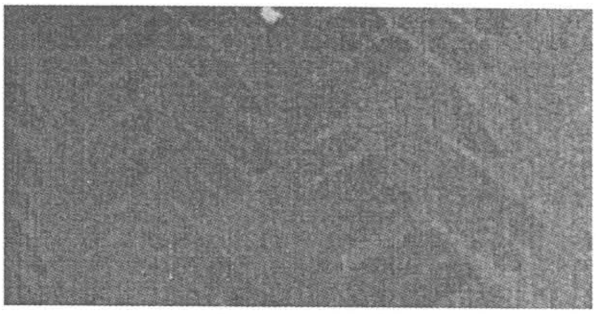
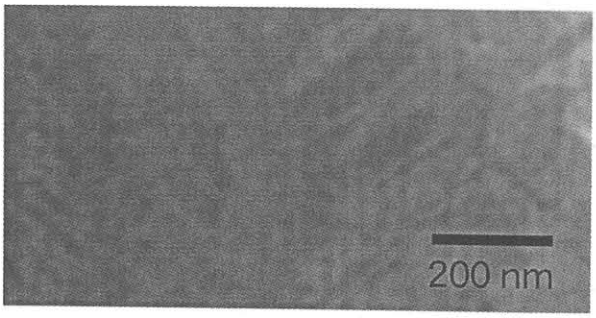


(a) As grown (without H2 annealing).

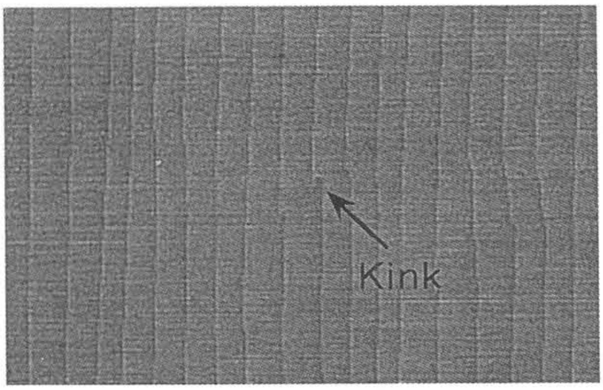


(b) 3 min annealed.

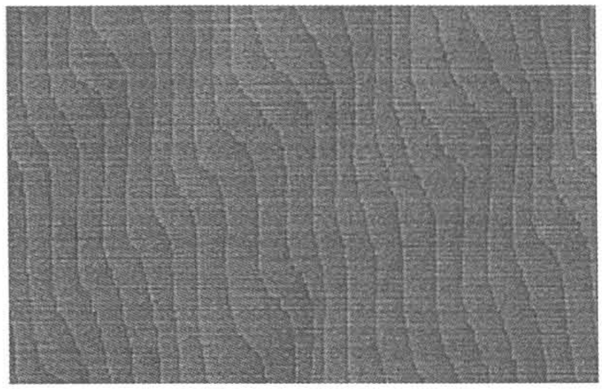


(c) 20 min annealed.

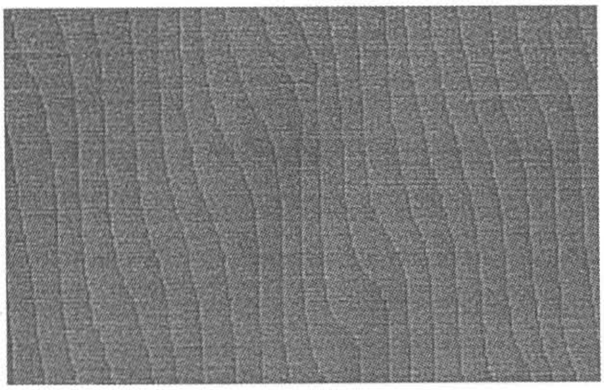
Fig. 2 Change in atomic step morphology of (100) epi-surface with H2 annealing at 1000℃.



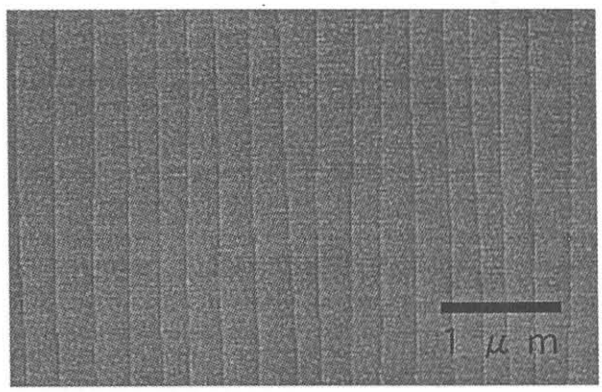
(a) As grown (without H2 annealing).



(b) 3 min annealed.



(c) 6 min annealed.



(d) 30 min annealed.

Fig. 3 Change in atomic step morphology of (111) epi-surface with H2 annealing at 1000℃.

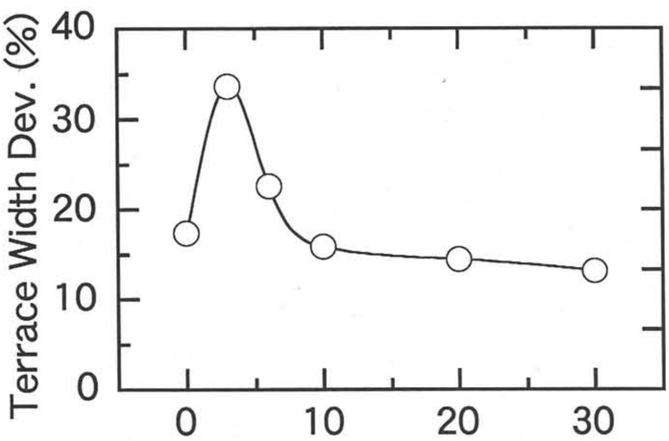
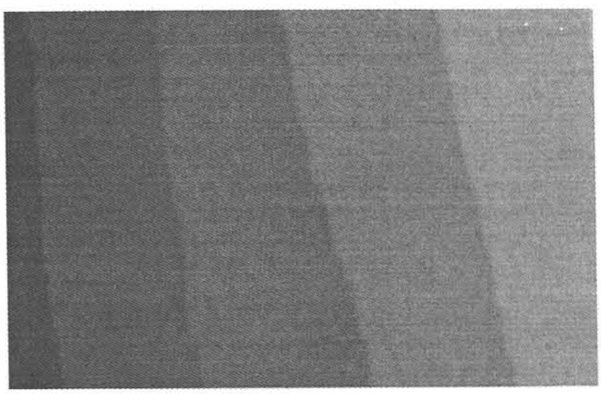
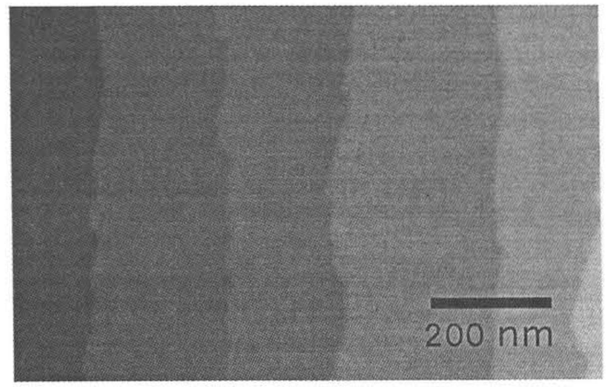


Fig. 4 Change in atomic terrace width deviation of (111) epi- surface with H2 annealing at 1000℃.



(a) 1050℃.



(b) 1100℃.

Fig. 5 Atomic step-lines on (111) surface with H2 annealing for 20 min at 1050℃ (a) and at 1100℃ (b).