Extended Abstracts of the 1995 International Conference on Solid State Devices and Materials, Osaka, 1995, pp. 971-973 **PD-4-4**

Microstructure of Si Surface Epitaxially Grown in SiH_4-H_2 System

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The growth temperature dependence of the Si surface microstructure after epitaxial growth was studied using atomic force microscopy (AFM). The microstructure of the Si surface was observed by AFM for (100) and (111) epi-wafers grown in a SiH_4-H_2 system at 800-1050° C. We found that, by decreasing the growth temperature, the microstructure of the (100) epi-surface changes at 800-1050° C prior to the increase in surface roughness and crystalline defect density at 800-900° C, whereas these three properties changed drastically in the temperature range of 950-1000° C for the (111) epi-wafers.

1. Introduction

The microroughness of Si surface needs to be controlled before gate oxidation to assure good dielectric properties and the reliability of thin gate oxide films. These microstructures have been studied after both wet treatments (Buffered HF, etc.) and dry treatments (H_2 annealing, epitaxial growth, etc.).[1-3] This paper discusses our study on growth temperature dependence of Si surface microstructures after chemical vapor deposition (CVD) epitaxy. We found that, by decreasing the growth temperature, the microstructure of the (100) epi-surface changes gradually before the increase in surface roughness and crystalline defect density, whereas these three properties change in the temperature range of 950-1000° C in the (111) epi-wafers.

2. Experimental

The substrates we used were p-type (100) and (111) Si wafers with diameters of 150 mm and the 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 or 210 nm for the (111) surface. Atmospheric pressure epitaxial growth was performed for the chemically cleaned substrates, and a 0.5-1.0 μm thick epi-layer was grown in a SiH_4-H_2 system at 800-1050° C after pre-baking at 1080° C. We observed the microstructure of the Si surface by atomic force microscopy (AFM, SPA300/SPI3700, SII) for the (100) and (111) epi-wafers using the cyclic contact mode for 1x1 μm^2 or 5x5 μm^2 scanning area. The surface roughness of epi-wafers was read as a haze value (area %) by a laser surface inspector (LS-6000, Hitachi DECO.). We measured the crystalline defect density of epi-layers after chemical defect etching by optical microscopy observation.

3. Results and Discussion

The (100) epi-wafers grown at 850-1050° C showed a terrace structure with mono-atomic-layer steps and growth fingers in the <110> directions on alternating terraces (Figs. 1(a)-1(e)). The step-finger structure we observed is in agreement with previous reports and reflects the double domain reconstruction of (2x1) and (1x2).[2,3] The (100) epi-wafer grown at 800°C showed a featureless AFM image (Fig. 1(f)), probably due to the high-density of the step-fingers and islands on the terrace. We found that the step-finger density increases with decreasing growth temperature between 850-1050°C (Fig. 2, top), indicating that the surface migration is suppressed in low-temperature epitaxial growth. The roughening of a step with surface diffusion was analyzed with the surface diffusion field theory and the Monte Carlo simulation on a relatively simple model.[4,5] For the analysis of the microstructure change we observed, the surface reconstruction and the dependence of surface diffusion constant on growth temperature should be considered.

The dependences of roughness (haze) and crystalline defect (stacking fault) density on growth temperature were respectively observed with a laser surface inspector and by chemical defect etching (Fig. 2, middle and bottom). Note that, on decreasing the epitaxial growth temperature, the step-finger density increased prior to the increase in haze and crystalline defect density. This means that, on decreasing the epitaxial growth temperature, the suppression of surface migration occurs rather gradually, whereas surface roughening (3-dimensional growth) and defect formation (miss-arrangement of addatoms) occur when the surface diffusion constant is decreased to a critical value. Accordingly, the step-finger density is thought to be the most sensitive parameter of epitaxial growth quality for (100) epi-wafers.

The (111) epi-wafers grown at 1000-1050° C show terrace structures with almost parallel mono-atomic-layer steps (Fig. 3(a)). On decreasing the growth temperature, the microroughness of the (111) epi-surface increases drastically and shows micro-hillocks at 950° C (Fig. 3(b)) and twins at 800-900° C (Fig. 3(c)). The increase in the haze and defect density was observed along with the microstructure change in the (111) epi-surface. It is infered here that the microstructure change in the (111) epi-surface occurs prior to the increase in haze and defect density as in the (100) epi-surface within the temperature range between 950° C and 1000° C.

Decreasing the growth temperature, the microroughness (Rms) of the (111) epi-surface increased drastically, whereas the microroughness of (100) epi-surface is almost independent on the growth temperature (Fig. 4). This is because arranging the addatoms on the (100) surface correctly is much easier than arranging them on the (111) surface.[6)]

4. Conclusion

The microstructure of the Si surface was observed by AFM for (100) and (111) epi-wafers grown in a SiH_4-H_2 system at 800-1050° C. On decreasing the growth temperature of CVD epitaxy, the change in surface microstructure occurred gradually prior to the rapid increase in surface roughness and crystalline defect density in the (100) epi-wafers. These three properties, however, changed in the temperature range of 950-1000° C for the (111) epi-wafers.

Acknowledgments

The authors are grateful to Dr. K. Izumi for his encouragement, to Dr. Y. Omura for critical reading of the manuscript, and to Mr. Y. Imaoka for his contribution to the experiment.

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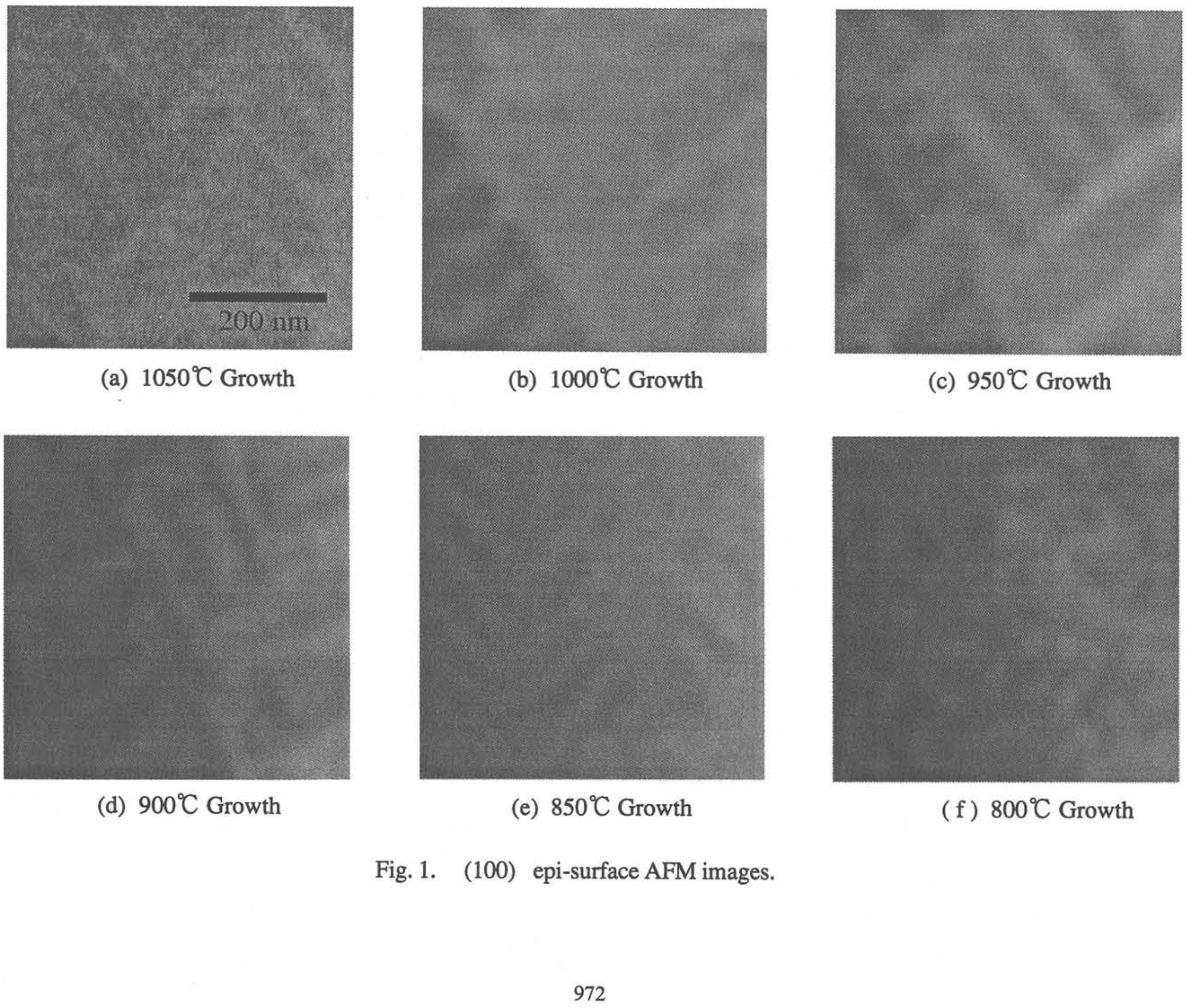


(a) 1050℃ Growth (b) 1000℃ Growth (c) 950℃ Growth

(d) 900℃ Growth (e) 850℃ Growth (f) 800℃ Growth

Fig. 1. (100) epi-surface AFM images.

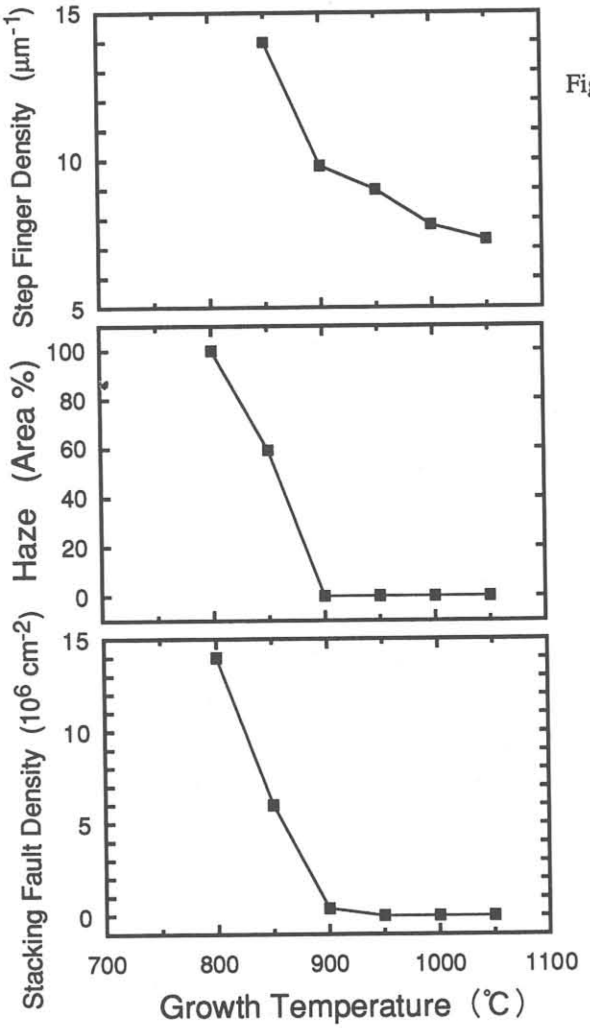
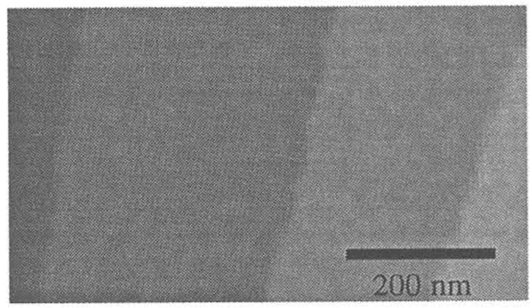
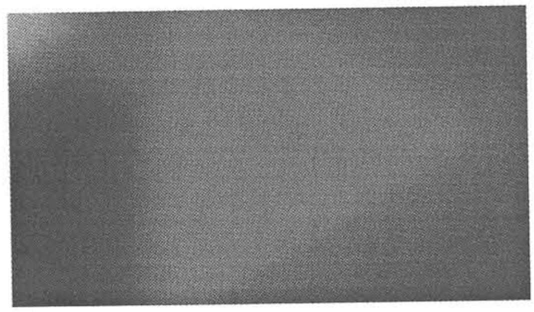


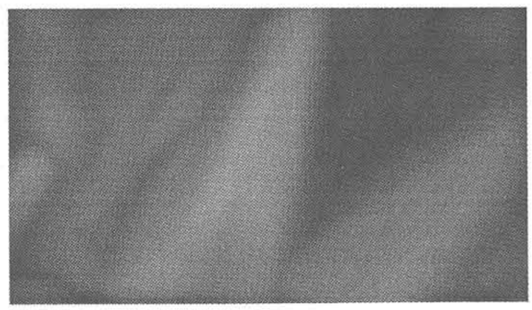
Fig. 2. Dependence of Step Finger Density, Haze, and Defect Density on Growth Temperature for (100) epi-wafers.



(a) 1050℃ Growth



(b) 950℃ Growth



(c) 800℃ Growth

Fig. 3. (111) epi-surface AFM images.

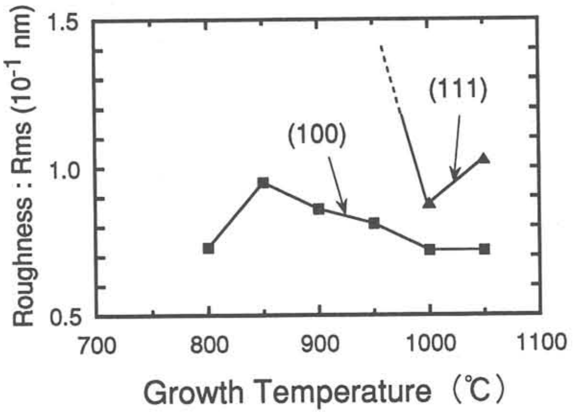


Fig. 4. Dependence of microroughness (Rms) on Growth Temperature for (100) and (111) epi-wafers.