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Topography change with Multilayer Oxidation at SiO₂/Si(111) interfaces

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1. Introduction

To realize high reliable thin oxide with low leakage current, Si surface topography should be atomically controlled [1]. The authors reported that SiO₂/Si interfaces with wide step/terrace structures were roughened during thermal oxidation [2]. This result provided evidence of breaking a layer-by-layer model at SiO₂/Si interfaces and also suggests that oxidation mechanism needs to be revealed precisely to control roughness of SiO₂/Si interfaces during oxidation. In this study, roughness at the SiO₂/Si interfaces was atomically investigated using AFM in various thicknesses of SiO₂ film to study the oxidation progress at the interfaces.

2. Experimental

We used Si substrates with p-type, (111) oriented, and Czochralski grown Si wafers with a resistivity of 10-20Ωcm. To form step/terrace structures on Si wafer surface, these wafers were dipped into ultra low dissolved oxygen pure water obtained by adding ammonium sulfite monohydrate introduced by Fukidome et al. [3] for 2 hours. After etching, the wafers were subjected to a modified RCA cleaning treatment. Subsequently, the Si surface with the step/terrace structures was thermally oxidized at 1050°C in 2% dry O₂ diluted with argon gas. The SiO₂/Si interface topographies were observed by a tapping mode atomic force microscope (AFM) after removing the SiO₂ film by diluted HF (DHF). It was confirmed that Si surfaces were not roughened by the DHF etching within our experimental error.

3. Results and Discussion

The Si surface before oxidation had a clear step/terrace structure. The height of each step was about 0.3 nm corresponding to the monolayer step height in (111) orientation. The terrace surface was confirmed to have atomic flatness [4]. A topographic image of the SiO₂/Si interface for the thickness of the SiO₂ film of 8.7 nm as determined by ellipsometry is shown in Fig. 1(a). The step configuration was preserved at the SiO₂/Si interface [5, 6]. In Fig. 1(b), dark holes, islands and towers on the islands

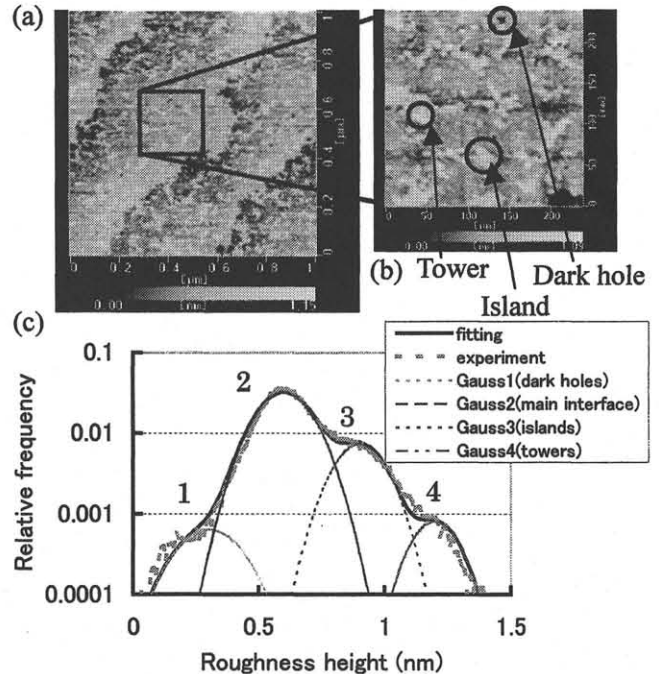


Fig. 1 (a) An AFM image of SiO₂/Si interface for 8.7-nm-thick oxide with the area of 1 μm². (b) There are dark holes, islands and towers on the islands around in the magnified image with the area of 250 nm² (c) The histogram shows the interface consisted of four atomic layers corresponding to four Gaussian peaks.

within each terrace were, however, clearly observed in a whole range of the interface. The depth of the dark holes and the height of the islands and the towers were both about 0.3nm. These seem to correspond to vestiges of two-dimensional oxide-island growth [7]. As discussed in our previous work [4], this result indicates that layer-by-layer oxidation does not progress at SiO₂/Si interfaces strictly. As shown in Fig. 1(c), a histogram was plotted to evaluate roughness quantitatively. The roughness height distribution on this terrace was decomposed into four peaks described with Gaussian distributions. The peaks were separated by 0.3 nm one another. Therefore, Gauss1 peak is due to the dark holes, Gauss3 peak to the islands and Gauss4 peak to the towers. The occupied area ratio, which was obtained by Gaussian peak intensity, for

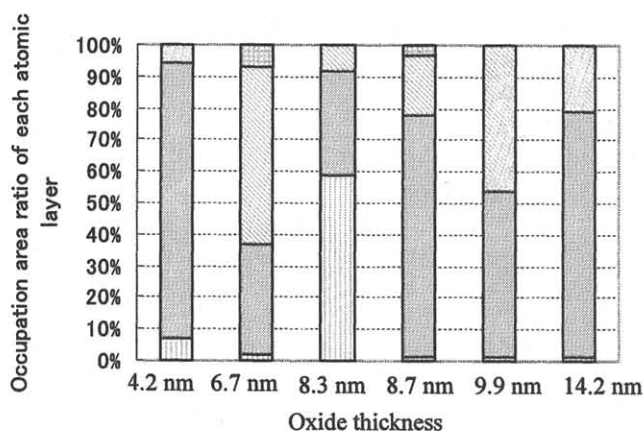


Fig. 2 Occupation area ratio of each atomic layer, such as dark holes or islands, was plotted over each oxide thickness. The SiO₂/Si interfaces consist of at least three atomic layers for every oxide thickness up to oxide thickness of 14.2 nm.

the dark holes was 1%, 19% for the islands, 3% for the towers and 87% for the main interface, which has the most highly occupied area. Fig. 2 shows occupation area ratios of each atomic layer, such as dark holes or islands. The SiO₂/Si interfaces consist of at least three atomic layers for every oxide thickness up to oxide thickness of 14.2 nm. These occupation area ratios of each atomic layer show snapshots of oxidation progress at the SiO₂/Si interfaces. It means that with decreasing the islands on the main interface, the dark holes are creating and growing at the main interface with oxidation. Therefore, whether the interfaces consist of three or four atomic layers seems to be the difference of oxidation phase. This topographic change of the SiO₂/Si interfaces arises from an oxidation rate difference between the directions in the parallel to crystal and in the perpendicular to its. This oxidation rate difference seems to depend on the oxidation conditions, such as oxidation temperature or ambient. Indeed, at the interfaces for the thickness of more than about 50 nm, the step configuration, which was clearly observed at the interfaces for up to 14.2-nm-thick oxide, became vague. No clear step configuration was confirmed by the image with the area of 1- μ m². As shown in Fig. 3(a), faint step configuration can be recognized only by the image with the area of 5- μ m² at the interfaces for 82.9-nm-thick oxide. In Fig. 3(b), there was no dominant atomic layer at the SiO₂/Si interface. Therefore, roughness height distribution on this terrace as shown in Fig. 3(c) cannot be decomposed into each Gaussian distribution corresponding to each atomic layer. However, it seems that roughness of the terrace extends to more than five atomic layers from the roughness height. It means that the oxidation rate difference seems to

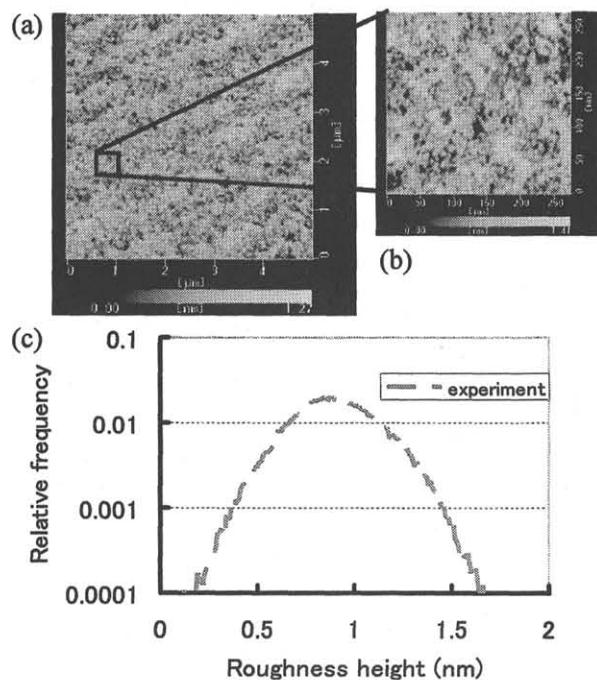


Fig. 3 (a) An AFM image of SiO₂/Si interface for 82.9-nm-thick oxide with the area of 5 μ m². (b) There are no clear dark holes, islands and towers on the islands around in the magnified image with the area of 250 nm² (c) roughness height distributions on this terrace cannot be decomposed into each Gaussian distribution.

be getting small with oxidation.

4. Conclusion

It was found that oxidation occurred across at least three atomic layers at the same time for every oxide thickness up to 14.2 nm. It seems to be closely related to the oxidation conditions.

References

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