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Atomic-Scale Structure of SiO_2/Si(001) Interface Formed by Furnace Oxidation

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1. Introduction

The atomic-scale structure of the SiO_2/Si(001) interface is an important element in ensuring the good electrical performance of metal-oxide-semiconductor devices. Recently, it was reported that the initial oxidation (< 2 nm) on an atomically flat Si(001) surface takes place in a layer-by-layer fashion [1, 2]. This oxidation manner is an intriguing process to produce an atomically flat SiO_2/Si(001) interface. In this report, we study the atomic-scale structure of the furnace-oxidized SiO_2/Si(001) interface by scanning reflection electron microscopy (SREM) and a profile analysis of reflection high-energy electron diffraction (PA-RHEED) [3].

2. Experiment

SREM and PA-RHEED were carried out using an ultrahigh-vacuum surface analysis system [4]. SREM images were obtained by recording the intensity change in the specular spot. PA-RHEED was performed for (10) spot by using a CCD camera.

The thermal oxide layers were grown on the atomically flat Si(001)-2x1 surface. First, an initial oxide layer of about 0.3 nm was grown at 630°C under $2x10^{-6}$ Torr O_2. Second, the thicker oxide layers were grown under 1-atm O_2 at 900°C in a furnace. Finally, in order to observe the interfacial structure by SREM, as-grown oxide layers were thinned by using dilute HF(1%) solution to less than 1 nm.

3. Results and discussion

The SREM image for initial Si(001)-2x1 surface, shown in Fig. 1 (a), indicates the terrace contrast in which the bright area is a 1x2 surface, and the dark area is a 2x1 surface. Figure 1 (b) shows the 5.2-nm-thick SiO_2/Si(001) interface formed on the Si(001)-2x1 surface shown in (a). Step contrast can be observed even after the furnace oxidation, which indicates that the initial atomic steps are preserved at the SiO_2/Si(001) interface. It should be noted that the SREM image changed from the terrace contrast of the initial surface to the step contrast of the SiO_2/Si interface. The dark protrusion in the right side of Fig. 1 (a) is the SiC island which happened to be formed by the initial flash heating and still remains after the oxidation. The scales between the SiC island and the same step indicate that the interfacial atomic steps do not move laterally during the oxidation. This SREM result indicates that the furnace oxidation is not the step flow type, but the layer-by-layer type.

The change of the SREM image suggests that the small islands (< 10 nm) with atomic-scale depth are formed at the SiO_2/Si(001) interface. In order to examine the atomic-scale roughness, we performed PA-RHEED. Figure 2 shows the CCD images and spot profiles obtained from the atomically flat Si(001)-2x1 surface, initial SiO_2/Si interface, and 5.2-nm-thick SiO_2/Si interface. The streak of (10) spot shown in Fig. 2 (c) indicates that the atomic scale roughness was formed at the 5.2-nm-thick SiO_2/Si interface. In order to evaluate the atomic-scale structure, we calculated the profiles using a diffraction theory that took the stepped surface into account [5]. The profiles were calculated for the SiO_2/Si(001) interface model shown by the inset in Fig. 3. Figure 3 shows the dependence of the (10) profile on the average island size, TL. It is found that the streak reaches a higher wavenumber when TL is decreased. Comparing the measured and calculated streaky profiles, the TL of the SiO_2/Si(111) interface was determined to be about 3 nm.

Our results indicate that the layer-by-layer oxidation caused by the two-dimensional island nucleation [1-3, 6] progresses at the SiO_2/Si(001) interface during the furnace oxidation. In addition, the fact that the atomic-scale roughness remains at the interface suggests that the island nucleation simultaneously occurs throughout a few layers of the SiO_2/Si(001) interface.

4. Conclusion

The atomic steps on the initial Si(001)-2x1 surface were preserved at the SiO_2/Si(001) interface by the layer-by-layer oxidation caused by two-dimensional island nucleation. The SiO_2/Si(001) interface consists of islands which have a diameter of about 3 nm and monolayer depth. Our results indicate that the layer-by-layer oxidation progresses during the conventional furnace oxidation of Si(001) substrate.

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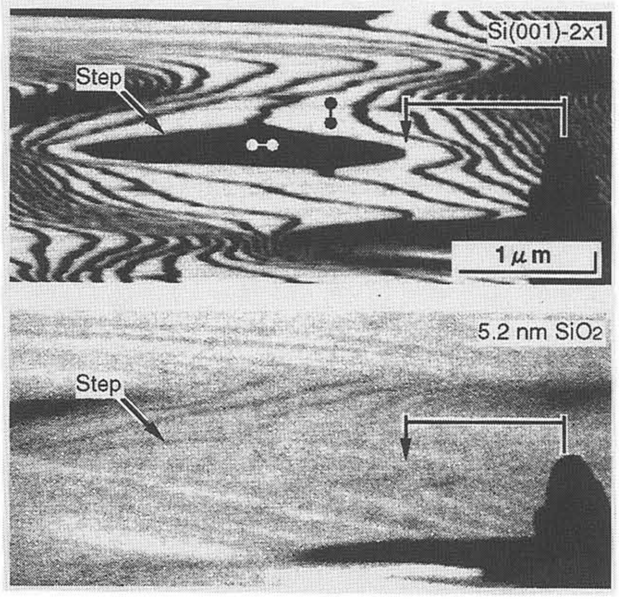

Fig. 1. Scanning reflection electron microscopy image. (a) Atomically flat Si(001)-2x1 surface. (b) 5.2-nm-thick SiO_2/Si(001) interface formed on the atomically flat Si(001)-2x1 surface, (a).

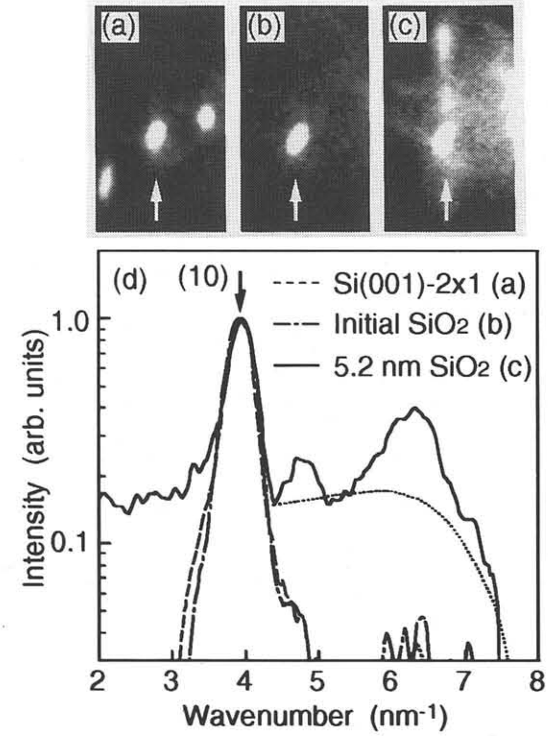

Fig. 2. (10) spot profiles. (a) Si(001)-2x1 surface. (b) Initial SiO_2/Si(001) interface. (c) 5.2-nm-thick SiO_2/Si(001) interface formed on the Si(001)-2x1 surface. (d) Spot profiles obtained by cutting along the arrows in CCD images (a), (b), and (c). The dotted line indicates the streak profile subtracted by the intensity of Si substrate.

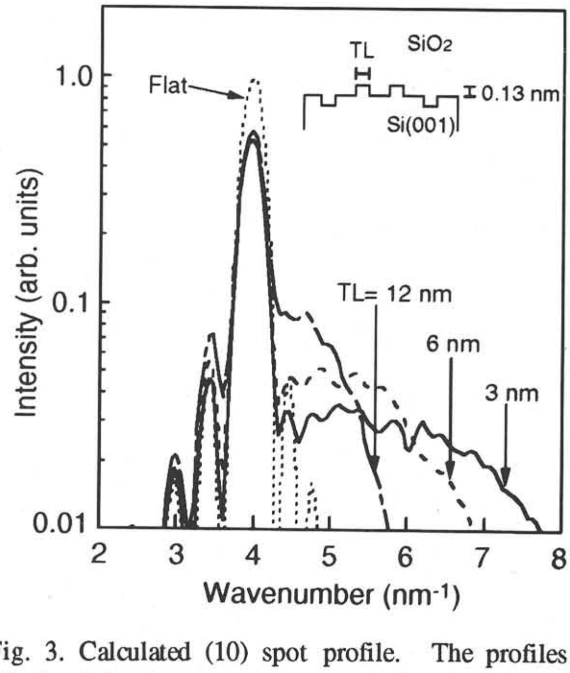

Fig. 3. Calculated (10) spot profile. The profiles were calculated for the monolayer step SiO_2/Si(001) interfaces (0.13 nm in height).