

Initial thermal oxidation of Si(100) investigated by Si 2p core-level photoemission

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Introduction

In the previous studies, we measured the time evolutions of the SiO₂ component in the Si 2p core-level spectrum during the initial thermal oxidation of Si(100). We concluded that, at temperatures below 650°C, the oxidation proceeds randomly without formation of two-dimensional (2D) islands by the observation that the growth rate follows a first-order Langmuirian behavior, while at temperatures above 650°C, the oxidation proceeds via 2D nucleation because the growth exhibits some incubation time [1, 2]. Suboxide components in the spectrum, which exist at SiO₂/Si interface, are also very informative. In this study, therefore, we focus on the temperature dependence of the suboxide components to investigate the surface reaction at the initial stage and verify the above oxidation behaviors.

Experimental

The photon energy was set at 135eV. A B-doped Si(100) wafer used was chemically treated with the RCA method and then annealed by resistive heating at 1000°C in the UHV chamber. The 99.99% oxygen gas was used to form the oxide. The overall instrumental energy resolution was estimated at about 0.2eV. The Si 2p core-level spectra are deconvoluted by a least-square fitting procedure using the spin-orbit split Voigt functions.

Results and Discussion

Fig. 1 shows typical Si 2p core-level spectra of oxides on Si(100), which consist of seven components: substrate silicon (Si⁰), three suboxides (Si¹⁺, Si²⁺, Si³⁺), stoichiometric oxide, that is, SiO₂ (Si⁴⁺), and two associated with surface reconstruction (S1 and S2). For 1 min oxidation, in spite of the nearly same intensity of Si⁴⁺, the intensities of Si²⁺ and Si³⁺ at 700°C are much smaller than those at 500°C, while the intensity of S1 shows opposite behavior, as shown in Fig. 2(a). Figs. 2(b) and 2(c) show oxidation-time dependences of the suboxide

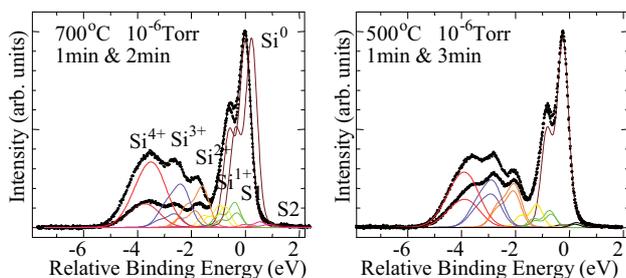


Fig. 1 Si 2p core-level spectra from SiO₂ on Si(100) grown at (a) 700°C and (b) 500°C, with fitted lines.

intensities for 700°C and 500°C, respectively. At the temperature of 700°C, both Si²⁺ and Si³⁺ intensities are almost kept constant, which means they increase in proportion to Si⁴⁺. On the other hand, at 500°C, as the oxidation proceeds, they both decrease monotonically.

As mentioned in the introduction, in the high temperature regime, the oxidation proceeds via 2D nucleation. Once SiO₂ nucleus is formed, it laterally expands on the surface. Therefore, the suboxides exist only at the SiO₂/Si interface. On the other hand, in the low temperature regime, the suboxides gradually change to SiO₂, showing Langmuirian behavior. Since the suboxides exist not only at the SiO₂/Si interface but also on the substrate Si surface, it should be observed that the suboxide intensities at 500°C are higher than those at 700°C as shown in Fig. 2(a). With proceeding of the oxidation, it is obvious that the intensity ratio of suboxide to Si⁴⁺ decrease monotonically at 500°C, while it is kept constant at 700°C because SiO₂ island laterally grows without change of its thickness. This inference is consistent with the results in Figs. 2(b) and 2(c). Thus, the oxidation kinetics mentioned above is reconfirmed by the observation of the change in the suboxide intensity in the Si 2p core-level spectra.

References

- [1] Y. Enta et al., Appl. Surf. Sci. 100/101, 449 (1996).
- [2] Y. Enta et al., Phys. Rev. B 57, 6294 (1998).

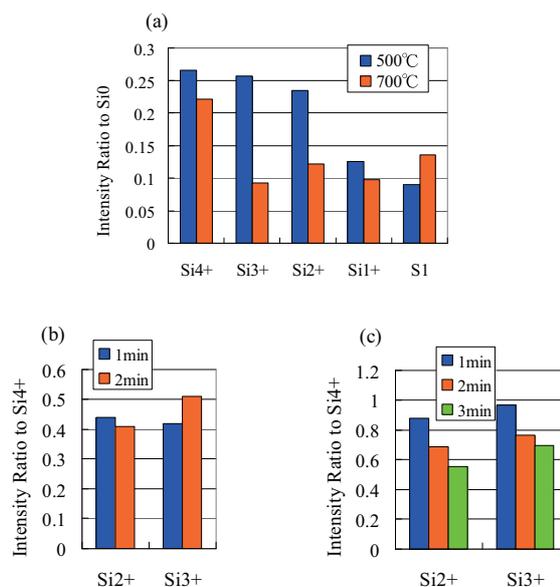


Fig. 2 Intensity ratios of chemical-shift components for Si 2p spectra from SiO₂ grown (a) for 1 min, (b) at 700°C, and (c) at 500°C.