

P-1-1

Real-time monitoring of initial oxidation of Si(110)-16×2 surface by Si 2p Photoemission spectroscopy

Yoshihisa Yamamoto¹, Hideaki Togashi¹, Atsushi Kato¹, Satoshi Hasegawa¹, Seiiti Goto¹
Takuya Nakano¹, Maki Suemitsu¹, Yuzuru Narita², Akitaka Yoshigoe³, Yuden Teraoka³

¹Center for Interdisciplinary Research, Tohoku University
6-3 Aza-Aoba, Aramaki, Aoba-ku, Sendai 980-8578, Japan
Phone: +81-022-217-5484 E-mail: yamamoto@cir.tohoku.ac.jp

²Kyushu Institute of Technology

1-1 sensui-mach, Tobata-ku, Kitakyushu, 804-8550, Japan

³Synchrotron Radiation Research Center, Japan Atomic Energy Agency.
1-1-1 Kouto, Mikazuki-cho, Sayo-gun, Hyogo, 679-5148, Japan

1. Introduction

Si(110) surface has attracted recent attentions as an orientation gifted with several properties suitable for the next-generation Si-CMOS devices. One of such features is the high hole mobility along this surface [1], which is expected to dramatically improve the performance of the pMOS transistors. In addition, this orientation must be essentially utilized in one of the active layers in the forthcoming 3D-CMOS devices [2].

Despite these growing importance, knowledge on the initial oxidation of Si(110) surface has been quite limited. In this study, we have investigated the initial oxidation of Si(110)-16×2 clean surface by using real-time synchrotron radiation photoemission spectroscopy (SR-PES).

2. Experiments

SR-PES experiment was conducted at the surface chemistry end-station BL23SU in SPring-8, using 687 eV photons as the excitation. Samples were B-doped p-type Si(110) wafers with the resistivity of 8-12 Ωcm, and were processed with *ex situ* wet-chemical and UV-ozone cleanings, followed by an *in situ* flash annealing conducted at 1000-1200 °C in an UHV ambient. Oxidation was performed by introducing oxygen molecules into the chamber in a back-filling mode. The oxygen pressure and the substrate temperature were fixed at 1.1×10^{-5} Pa and 540 °C, respectively.

3. Results and Discussion

Figure 1 shows the Si 2p spectrum taken after the oxidation at 540 °C with the O₂ dose of 1.2 L. The three subpeaks in the figure, α , β , and γ around the bulk Si⁰⁺ peak, have been included in the analysis based on the report by Grill *et al* [4]. The relative shifts of these subpeaks from the bulk position are measured to be +0.42 eV(α), -0.45 eV(β), +0.82 eV(γ), and their presence before the oxidation suggests the intrinsic nature of their origins. Namely, they most likely reflect the atomistic arrangement of the Si(110)-16×2 surface reconstruction, and this is why these shifts are called surface core level shift (SCLS) [4].

The triangles in Fig. 2 present the time evolution of the α peak intensity, which has been normalized with the bulk

Si⁰⁺ intensity. Upon introduction of the oxygen molecules, the normalized intensity shows a sudden decrease, which then turns into a gradual decrease for doses above 1.2 L. Although decrease of SCLS intensities with the progress of oxidation is also observed for other surfaces [3], this rapid initial decrease is quite unique to Si(110) surface. Furthermore, this happens concurrently with the rapid initial oxidation, another unique characteristic of the oxidation on Si(110) surface [5]. The circles in Fig. 2 represent the uptake curve of the subcomponent (532.6 eV) of O 1s spectrum, whose correspondence strongly suggests that the origin of the α SCLS is related to the origin of the rapid initial oxidation.

Temperature dependence of the α peak has also been investigated by Grill *et al.* [4]. By observing a decrease of the α peak (A peak in Ref.4) intensity for temperatures above 730°C, which is close to the transition temperature (~750°C) from 16×2 to 1×1 reconstructions, they related the α peak to the 16×2 reconstruction of the Si(110) surface. As for the atomistic structure of the 16×2 reconstruction, the adatom-tetramer-interstitial (ATI) model, proposed by An *et al.* based on their STM observation [6], seems most promising. This ATI model, supported also by a first principle calculation [7], claims that five-membered rings of Si adatoms (pentagons) are regularly aligned along the <1-12> directions. Our previous STM observation on the rapid initial oxidation of Si(110)-16×2 has actually indicated preferential oxidation at these pentagons [8].

Recently, Kim *et al.* [9] conducted an even detailed photoemission study on the SCLSs of Si(110)-16×2 surface using a high resolution SR-PES. They report two SCLSs at +0.26 (SC₃) and +0.50 eV (SC₄) in the vicinity of the α peak position, for which they assigned the second-layer chain and the top-surface π -bonded chain, respectively, as their origins. It is highly probable, therefore, that the present α peak in Fig. 1 actually consists of a pair of components: SC₃ and SC₄. In this scheme, it is possible to attribute the rapid decrease of the α peak intensity, concurrent with the rapid initial oxidation, to the disappearance of the SC₄ state due to oxidation of the top-surface Si atoms. In the same manner, the subsequent very slowly decreasing behavior of the α peak can be related to the weakening of

the SC₃ state caused by the second layer oxidation. Inclusion of two components in the α peak is already implied in the results by Grill *et al.* [4]. Their observation of the temperature-dependent behavior of the α peak intensity suggests inclusion of at least two components: one that decreases rapidly for temperatures above 730 °C and the other that survives at high temperatures. In view of the loss of the surface reconstructions at high temperature [4], it is possible to relate the decay of the first component to the decay of the top-surface π -bonded chain, SC₄.

Figure 3 shows the time evolution of the Si 2p suboxide components during oxidation. Since the separation between the Si¹⁺ and γ peaks is less than the energy resolution of our analysis, only their sums are indicated in the figure. Virtually, however, the intensity of the γ peak, related either to the C peak in Ref.4 or to the SC₅ peak in Ref.9, is estimated to be so small that it may safely be ignored in the present analysis. Anyway, what should be noted in this figure is the significant amount of the higher-oxide component (Si³⁺) from the very beginning of the oxidation. This is in sharp contrast with the oxidation of Si(001) surface, where the initial oxidation is dominated by lower suboxides (Si¹⁺ and Si²⁺), which is followed by a delayed growth of the higher oxides (Si³⁺ and Si⁴⁺) [3].

4. Conclusions

We have investigated the initial oxidation of the Si(110)-16×2 clean surface using real-time SR-PES. We found that the intensity of the surface-related α peak decreases right after the start of the oxidation, which is concurrent with the rapid initial increase of the oxygen uptake. This suggests that the rapid initial oxidation is caused by preferential oxidation at the surface sites related to α peak: the surface π -bonded chain [9] or the pentagon pairs [6]. It is further suggested that part of the α component corresponds to oxidation of the second layer. This surface core-level shift α is therefore expected to be an important probe in understanding the subsurface oxidations, which will be of crucial importance in understanding the oxidation kinetics of ultra thin oxide films on Si(110) surface.

Acknowledgements

The synchrotron radiation experiments were conducted at the SPring-8 with the approval of the Japan Atomic Energy Agency (JAEA) and the Japan Synchrotron Radiation Research Institute (JASRI) (Proposal No. 2006A1651 and 2006B1629).

References

- [1] T. Sato, Y. Takeishi, H. Hara, Y. Okamoto, PRB 4. (1971) 1950
- [2] R. Izawa, T. Kuse, S. Iijima, IEDM Tech. Deg. (1987) 38.
- [3] A. Yoshigoe, K. Moritani, Y. Teraoka, Surface Science. (2004) 1124.
- [4] L. Grill, A. Santoni, S. Prato, L. Petaccia, S. Modesti, Surface Science 474. (2001) 55
- [5] M. Suemitsu, A. kato. H. Togashi, A. Konno, Y. Yamamoto,

Y. Teraoka, A. Yoshigoe, Y. Narita, Y. Enta, SSDM (2006) (JJAP to be published)

- [6] T. An, M. Yoshimura, I. Ono, K. Ueda, PRB 61 (2000) 3006
- [7] A. A. Stekolnikov, J. Furthmuller, F. Bechstedt, PRL 93 (2004) 136104
- [8] H. Togashi, Y. Takahashi, A. Kato, A. Konno, H. Asaoka, M. Suemitsu, IWDTF (2006) (JJAP to be published)
- [9] N. D. Kim, Y. K. Kim, C. Y. Park, H. W. Yeom, H. Koh E. Rotenberg, J. R. Ahn, PRB 75. (2007) 125309.

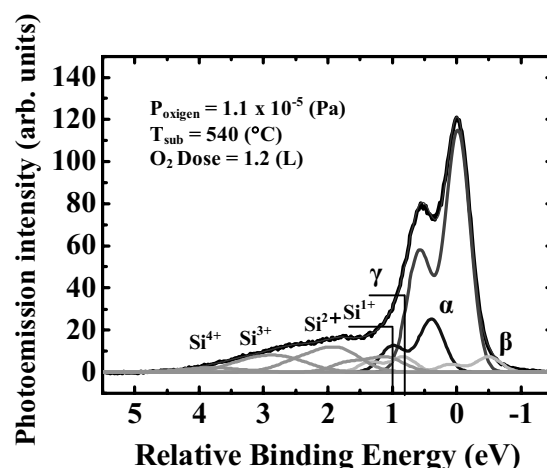


Fig.1 Photoemission spectrum of Si 2p core level after oxygen exposure of 1.2 L.

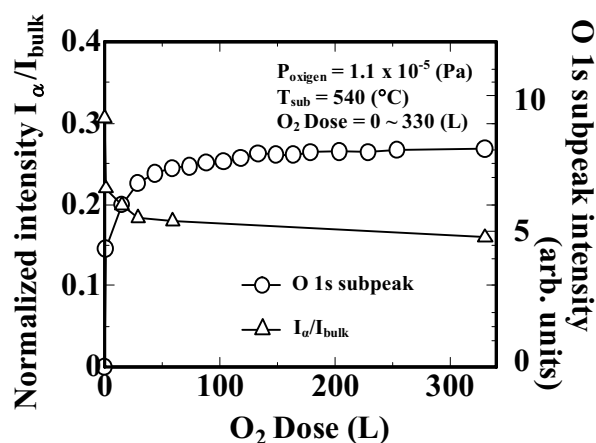


Fig.2 Time evolutions for the normalized intensity of the α peak (triangles) and for the intensity of the O 1s subpeak at 532.6eV (circles).

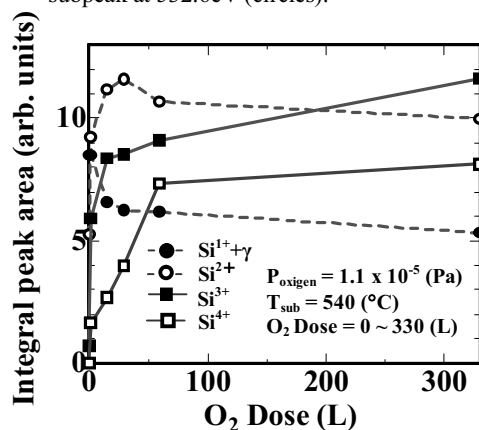


Fig.3 Time evolution of the Si 2p suboxide components during oxidation.