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# Real-Time Observation of Initial Thermal Oxidation on Si(110)-16×2 Surfaces by O1s Photoemission Spectroscopy Using Synchrotron Radiation

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## 1. Introduction

On Si(110) surfaces, the hole mobility is enhanced by a factor of 1.5-2.5 as compared with Si(001)[1], which makes Si(110) a crucially important surface in the next-generation high speed devices. In addition, this surface, in most cases, appears in one of the active layers in the forthcoming three-dimensional CMOS devices such as double-, triple-gated, or Fin FETs. As such, Si(110) surface has been attracting recent technological attentions. Despite the importance, however, knowledge on the kinetics of the initial oxidation, one of the most important surface processes employed in the CMOS technology, has been quite insufficient on this surface. We have conducted real-time observation of initial thermal oxidation on Si(110)-16×2 surfaces by O1s photoemission spectroscopy using synchrotron radiation. Reflecting its unique atomistic structure, the oxidation kinetics on Si(110) is quite different from that on Si(001)[2].

## 2. Experiment

The photoemission-spectroscopy experiments were performed at the surface chemistry end-station of BL23SU in SPring-8 using 687 eV photons. Samples were B-doped p-type Si(110) wafers ( $\rho$ =8-12  $\Omega$ ·cm), cut to 15×15 mm<sup>2</sup>. Sample cleaning consists of *ex-situ* wet cleaning and *in-situ* flash cleaning, with the latter conducted at 1000-1200°C in the UHV ambient for several times. After the flash cleaning, the 16×2 reconstruction, indicative of the atomic cleanliness of the Si(110) surface, is confirmed by a low-electron- energy-diffraction (LEED) pattern. Oxidation was conducted by introducing oxygen molecules into the chamber via a leak valve, whose pressure ranged from  $1.2 \times 10^{-6}$  to  $3.2 \times 10^{-4}$  Pa. The substrate temperature *T* was varied from 495 to 670°C.

#### 3. Results and Discussion

Figure 1 shows a series of O1s spectra after introduction of the oxygen molecules at  $1.1 \times 10^{-5}$  Pa. The foot spectrum corresponds to a very initial exposure of 1.5 L (1L= $1.33 \times 10^{-4}$  Pa·s), which however indicates presence of the oxide amounting a fraction of one monolayer. This clearly indicates occurrence of rapid initial oxidation on Si(110) surface, which is absent on Si(001)[2].



Fig. 1. A series of O1s spectra during oxidation with  $1.1 \times 10^{-5}$  Pa oxygen molecules. *T*=540°C.



Fig. 2. Peak decomposition of O1s spectrum into two subpeaks.

All the spectra in Fig. 1 are successfully decomposed into two subpeaks as shown, for example, for the 1.5-L spectrum in Fig. 2. The one with a lower binding energy (BE) is located at 532.6 eV, while the one with a higher BE is located at 533.1 eV. As seen, the very initial oxide (1.5 L) is dominated by a low-BE state, which is gradually replaced by a high-BE state with the progress of the oxidation. As a result, the O1s peak shows a high-BE shift.

The uptakes for these O1s subpeaks show quite different behavior each other (Fig.3). The low-BE peak (the solid circles), starting from a rather higher initial coverage, grows mildly following a Langmuir-type behavior towards a smaller saturation coverage. In contrast, the high-BE peak (the open circles) starts from a rather lower initial coverage, which however grows steeply, overtakes the low-BE peak, and eventually saturates at a considerably higher coverage.



Fig. 3. Peak intensity uptake for O1s subpeaks at BE=532.6 eV and BE=533.1 eV..

This unique behavior of O1s uptake during oxidation is related to the surface structure of Si(110)-16×2 reconstruction. It is accepted that this reconstruction contains surface adatoms as an important constituent as shown in Fig. 4. As is also shown in the figure, the surroundings of the adatoms quite resemble those of Si(111) surface. Actually, the positions of the O1s subpeaks shown in Fig. 2 agree well with those (533.1 and 533.7 eV) from dry-oxidized Si(111) surface reported by Sakamoto *et al.*[3]. It is likely that the rapid initial oxidation seen in Fig.1 is related to oxidations at or around the adatoms of Si(110)-16×2 clean surface.

### 4. Conclusions

Initial oxidation of Si(110) surface has been investigated by using real-time x-ray photoemission spectroscopy using 687-eV photons. The Si(110) initial oxidation is characterized by presence of rapid oxidation just after the introduction of the oxygen molecules, which is shown to consist of at least two oxidation states.



Fig. 4. Surface structure of Si(110)-16×2 reconstruction..

Comparison with dry-oxidized Si(111) surface suggests oxidation at or around the adatoms of Si(110)-16×2 clean surface as a likely oxidation state in its very initial oxidation.

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#### References

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