# Structural Origin of Carrier Trap Levels at SiO<sub>2</sub>/Si Interface

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## 1. Introduction

As the thickness of  $SiO_2$  films used in MOS devices has decreased, it is indispensable to study structural origin of carrier trap levels at  $SiO_2/Si$  interface, in other words, interface states which give vital effects on the operation of MOS devices. It was found from the combined measurements of the changes in  $SiO_2/Si(111)$  interface structures and the surface microroughness with progress of oxidation that the surface structures are closely correlated with the interface structures.[1] It is the purpose of present paper to clarify the structural origin of carrier trap levels at  $SiO_2/Si(111)$  interface from the combined measurements of the changes in interface state density and interface structures with progress of oxidation.

## 2. Experimental Details

The oxide films used in the present studies were formed as follows on n-Si substrates. Through 0.8 nm thick preoxide formed by treating hydrogen-terminated Si(111)- $1 \times 1$  surfaces in H<sub>2</sub>SO<sub>4</sub>-H<sub>2</sub>O<sub>2</sub> solution (H<sub>2</sub>SO<sub>4</sub>: H<sub>2</sub>O<sub>2</sub> = 4:1) at 80°C for 10min, oxidation was performed in 1Torr dry oxygen at 600-880°C. The interface state densities were measured using the method developed by Lau et al.[2] First, an organic molecules of 2-propanol were adsorbed on oxide film. Second, oxide is charged by electron beam irradiation to produce voltage drop across the oxide film. Third, this charging-induced changes in electrical potentials at surface and interface, which are necessary for the determination of interface state densities, were obtained from the measurements of chemical shifts in C1s level of organic molecules and Si2p core level of silicon substrate. The organic molecules were decomposed during the oxidation. The C1s and Si2p photoelectron spectra excited by monochromatic AlK  $\alpha$ radiation were measured at photoelectron take-off angle of 15, 30 and 90 degrees with an acceptance angle of 3.3 degrees, using high resolution ESCA-300. Other experimental details were described elsewhere. [1]

#### 3. Experimental Results and Discussion

Figure 1 shows the changes in the normalized amount of intermediate oxidation states, so called suboxides and that of Si<sup>4+</sup> with progress of oxidation. Because the total amount of suboxides is in good agreement with that calculated for an abrupt compositional transition, suboxides are localized only at the interface. Although the total amount of suboxides does not change with progress of oxidation, the amount of Si<sup>1+</sup> changes in opposite phase with the amount of Si<sup>3+</sup>. Therefore, the Si<sup>1+</sup> and Si<sup>3+</sup> interface appears alternately with progress of oxidation.[3] Figure 2 shows the interface state densities at and near the midgap of Si for three oxide film thicknesses. For oxide film thicknesses of 1.35 and 1.98 nm, where the amounts of Si3+ take their maximum values, the interface state densities at and near the midgap of Si are almost equal to  $1 \times 10^{13}$  cm<sup>-2</sup>eV<sup>-1</sup>, while for oxide film thickness of 1.62 nm, where the amount of Si<sup>1+</sup> takes its maximum value as shown in Fig. 1, the interface state density near the midgap decrease drastically down to  $1 \times 10^{12}$  cm<sup>-2</sup>eV<sup>-1</sup>. This drastic decrease in interface state density occurs only near the oxide film thicknsess of 1.63 nm as shown in Fig. 3. As shown in Fig. 4, almost the same drastic decrease in interface state density near the midgap appears again only near the oxide film thickness of 2.32 nm, where the amount of Si<sup>1+</sup> takes again its maximum value as shown in Fig. 1. Therefore, the drastic decrease in interface state density near the midgap appears periodically as a result of periodic changes in interface structures and is closely related with the formation of Si1+ interface. It was found from the measurement of surface microroughness of oxide film using non-contact mode atomic force microscope that the protrusions are produced on the oxide surface so as to relax stress produced by the formation of Si<sup>1+</sup> interface.[1] Therefore, the protrusions on the oxide surface indicate the place where interface state density is small. On the other hand, the volume expansion mostly along the interface-plane [1] induced by the formation of Si<sup>3+</sup> breaks a part of Si-Si bonds just below the Si<sup>3+</sup> to produce dangling bonds with density of about 10<sup>12</sup>cm<sup>-2</sup>.

#### 4. Summary

The interface state densities at and near the midgap and interface structures were measured with progress of oxidation of Si(111) surface. It was found that the interface state densities near the midgap exhibits drastic decrease for two oxide film thicknesses, where the amounts of Si<sup>1+</sup> take their maximum values. This strongly implies the close correlation between interface structures and interface state densities. From the close correlation between the interface and surface structures[1] the formation of Si<sup>3+</sup> was found to produce dangling bonds with density of about 10<sup>12</sup>cm<sup>-2</sup>.

### Reference

- [1] M. Ohashi and T. Hattori: Jpn. J. Appl. Phys. 36 (1997) L 397.
- [2] W. M. Lau and X. -W. Wu: Surf. Sci. 245 (1991) 345.
- [3] K. Ohishi and T. Hattori: Jpn. J. Appl. Phys. 33 (1994) L675



Fig. 1 The Upper part shows normalized spectral intensity of Si<sup>4+</sup> and summation of intensities for all suboxides are shown as a function of oxide film thickness. The dashed line shows the normalized spectral intensity calculated for an abrupt interface. The lower part shows dependence of areal densities of Si<sup>1+</sup>, Si<sup>2+</sup>, Si<sup>3+</sup> and Si<sup>4+</sup> on thickness.



Fig. 2 Interface state densities in the bandgap of Si are shown for three oxide film thicknesses.



Fig. 3 Interface state densities in the bandgap of Si at and near the oxide film thickness of 1.63nm, where the amount of Si<sup>1+</sup> takes its maximum value.



Fig. 4 Interface state densities in the bandgap of Si at and near the oxide film thickness of 2.32nm, where the amount of Si<sup>1+</sup> takes its maximum value.