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# THE EFFECT OF STRESS FIELD ON THE FORMATION OF DEFECTS IN SILICON OXIDES

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We have investigated the effect of the stress field on the formation of defects in silicon oxide using a new method recently developed by us, i.e., x-ray photoelectron microscopy (XPS) time-dependent measurements. The Si 2*p* peak energies for samples with and without stress have shifted towards higher binding energies with x-ray irradiation. This phenomenon can be explained by the accumulation of positive charges at the $SiO_2$/Si interface. The positive charges are probably holes generated by the x-ray irradiation and trapped at the interface defects. It was found that the samples with stress show larger energy shift than those without stress, indicating that the stress field has influence on the defect formation process at the $SiO_2$/Si interface.

Key words: stress, chemical oxide, XPS, trap

## 1. INTRODUCTION

With the scaling down of Si-ULSIs, the detrimental effect of the stress in Si wafers on the characteristics of metal-oxide-semiconductor (MOS) transistors has become serious. For example, it is well known that the mechanical stress enhances the leakage current at the local oxidation of silicon (LOCOS) edge.[1] Furthermore, Takahashi et al.[2] reported the successful formation of single electron transistor (SET) taking advantage of stress-induced enhanced oxidation and named PADOX (Pattern-dependent oxidation). In spite of its importance, the effect of the stress field on the Si process chemistry has not been well understood yet.

The scaling of Si-ULSIs in the lateral direction has also requested the reduction in the gate oxide thickness. In fact, n channel MOS transistors with a gate oxide thickness as thin as 15Å were fabricated and found to be promising for future ULSIs in spite of the large leakage currents through the gate oxide.[3] This thickness is almost equivalent to that of the chemical oxide, which is formed in the wet solution to protect the Si surface just before the oxidation process in the furnace. Hence, the quality of the chemical oxide become increasingly important.

In this paper, we have investigated the effect of the stress field on the formation of defects in ultra-thin chemical oxide using a new method recently developed by us, i.e., XPS time-dependent measurements.[4]

## 2. EXPERIMENT

The substrates used in this study were n-type(100) silicon wafers with a resistivity of 8 to 12 Ωcm. We have induced compressive stress to the parallel direction to the wafer surface by growing thick thermal $SiO_2$ film on the back side of the wafer. The thermal oxide was grown at a temperature of 1100℃ for 150 min using pyrogenic system. The thickness of the oxide is about 1 μm. The strain in silicon wafer is originated from the difference between thermal expansion coefficient of Si and that of $SiO_2$, and is estimated to be 0.025 % from the x-ray diffraction measurement. The schematic diagram of the sample with stress is shown in Fig. 1.

Next, we formed chemical oxides on the silicon

substrates with and without stress using a HCl solution ($HCl:H_2O_2:H_2O$=3:3:5 at 65 ℃ for 10 min) after cleaning the substrates by dipping in a $H_2SO_4$ solution ($H_2SO_4:H_2O_2$=1:1) and a HF solution sequentially. The thicknesses of chemical oxides were about 1 nm. Immediately after treating samples in the solution, we transferred them into the XPS chamber. We used VG ESCALAB 220i XL with a monochromatic Al $K_\alpha$ x-ray source ($h\nu$ =1486.6 eV). The power of x-ray was 40 W, and the base pressure of the chamber was $2\times10^{-10}$ Torr. When we measured the Si 2*p* peak energies accurately by XPS, we paid special attention to the elimination of charge-up effect on the silicon substrate. To check whether the silicon substrate was charged up or not, we put a Ag foil on the sample using conductive glue. We found that the Ag 3*d* peak energy remained unchanged during x-ray irradiation, indicating there was no simple charging up on the silicon substrate or the surface of the chemical oxide.

## 3. RESULT AND DISCUSSION

A typical Si 2*p* spectrum is shown in Fig. 1. The peak energy was determined by peak fitting using spin-orbit split peaks (Si $2p_{3/2}$, and Si $2p_{1/2}$). They were separated by 0.61 eV with an intensity ratio of 0.5. The full width at half-maximum (FWHM) of the Si 2*p* peak was 0.41±0.03 eV. A band diagram of the interfaces is shown in the inset in Fig. 1. The measured binding energy corresponds to the difference between the Fermi level of Si at the $SiO_2$/Si interface and the Si 2*p* core-level energy. Thus we determined the band bending feature from the Si $2p_{3/2}$ peak energy.

We measured the Si $2p_{3/2}$ peak energies for samples with and without stress as a function of x-ray irradiation time, and plotted them in Fig. 2. The Si $2p_{3/2}$ peak energies of both samples shifted toward a higher binding energy and were saturated as the x-ray irradiation proceeded. This indicates that the band bending of Si near the interface changes with x-ray irradiation. As we have already pointed out, we also exclude the simple charging in the oxide. Therefore, we conclude that the charging in the oxide is intrinsic to the oxide. We attribute these phenomena to the accumulation of positive charges at the $SiO_2$/Si interface. The positive charges are holes generated by the x-ray irradiation and trapped at the interface defects. Trapping of injected carriers in gate oxides of MOS devices can be considered as one of the causes of reliability problems such as the fluctuation of threshold voltage and the breakdown of gate oxides. Therefore, the characterization of carrier-trapping phenomena in oxides is quite important. The XPS time-dependent measurement is suitable for the characterization of carrier-trapping phenomena in ultra-thin oxides because this measurement is not affected by the tunneling current or sample preparing processes, which are inevitable in the conventional electrical measurements.

It should be noted that the samples with stress show larger energy shift than those without stress, indicating that there are more defects in the sample with stress than those without stress. Using the Poisson equation, we can estimate the net density of hole traps in the oxides from the saturated value of Si $2p_{3/2}$ peak shift. The net densities of hole traps in the HCl oxide for with and without stress samples are calculated to be $4.9\times10^9\,cm^{-2}$ and $3.5\times10^9\,cm^{-2}$, respectively.

The surface charge densities ($Q_S$) are expressed by ;

$$Q_S = w\times N_D = \sqrt{\frac{2\varepsilon_0\varepsilon_r V_{bi}N_D}{q}} \qquad (1)$$

$$Q_S - N_H = \sqrt{\frac{2\varepsilon_0\varepsilon_r(V_{bi}-\Delta)N_D}{q}} \qquad (2)$$

,

where $w$ is depletion-layer width, $N_H$ is estimated trapped hole density, $N_D$ is doner density, $V_{bi}$ is built-in potential, and $\Delta$ is the amount of peak energy shift.

In this way, it was found that the stress field has influence on the defect formation process at the $SiO_2$/Si interface.

## 4. CONCLUSION

We have investigated the effect of the stress field on the formation of defects in silicon oxide using XPS time-dependent measurements. It was found that there are more defects in the sample with stress than those without stress, indicating that the stress field has influence on the defect formation process in ultra-thin chemical oxides.

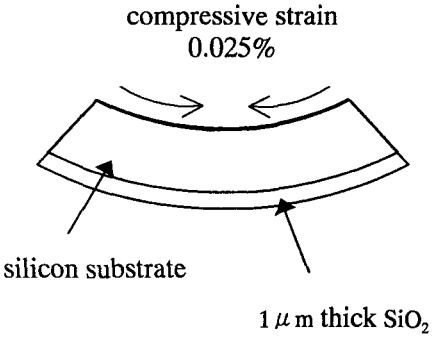


Fig. 1
Schematic diagram of the sample with stress. The strain in silicon wafer is originated from the difference between thermal expansion coefficient of Si and that of $SiO_2$, and is estimated to be 0.025 % from the x-ray diffraction measurement.

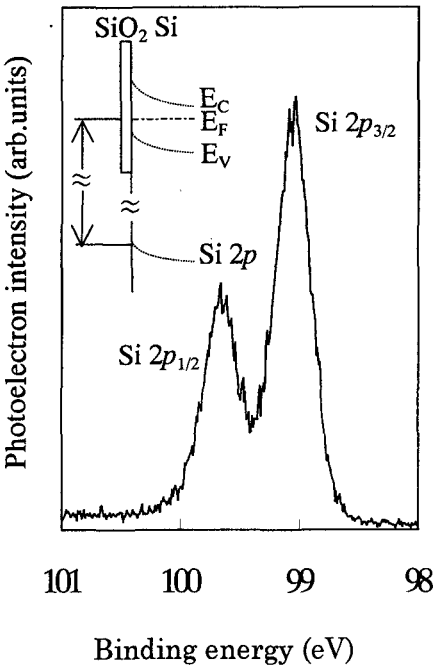


Fig. 2
A typical Si $2p$ spectrum and the band diagram at the $SiO_2$/Si interface. $E_C$, $E_F$, and $E_V$ represent the conduction band minimum, the Fermi level at the interface, and valence band maximum respectively. The measured binding energy corresponds to the difference between the Fermi level and the Si $2p$ core-level energy. We determined the band bending feature from the Si $2p_{3/2}$ peak energy.

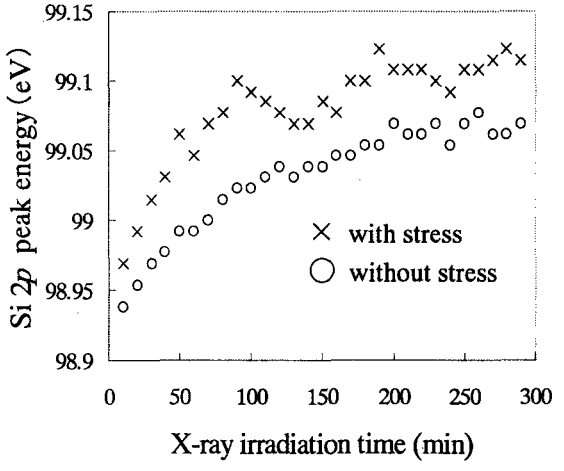


Fig. 3
X-ray irradiation time dependence of Si $2p_{3/2}$ peak peak energy for the samples with and without stress.

## 5. REFERENCES

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