

## Residual Order in the Interfacial SiO<sub>2</sub> Layer between a High-k Material and a Si Substrate

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### Introduction

Exceptionally low density of trap charge at the interface between a thermal oxide layer and a Si substrate is one of the principal reasons for the enormous development of semiconductor industries based on silicon metal-oxide-semiconductor (MOS) devices. It is incredible that the trap density at the interface is no more than  $10^{11} \text{ cm}^{-2} \times \text{eV}^{-1}$  despite a large structural difference between an amorphous oxide layer and a crystalline silicon substrate. It is roughly estimated that only one defect, such as a dangling bond, exists in  $10^4$  atomic bonds at the interface.

High-k gate dielectric materials are forthcoming instead of SiO<sub>2</sub> in MOS devices in order to reduce the gate leakage current. However, a very thin interfacial SiO<sub>2</sub> layer is still indispensable to reduce the interface trap density between the high-k material and the Si substrate. Therefore, it is still important to understand the SiO<sub>2</sub>/Si system.

One of the major research subjects for high-k gate dielectric technology is the control of this interfacial layer, because thermal annealing is accompanied by an increase in the electrical thickness of the gate insulator due to growth of an interfacial oxide, even when annealed in a ultrahigh-vacuum (UHV) ambient environment. Therefore, it is important to investigate the oxidation mechanism between the high-k material and the Si substrate.

In this report we present preliminary results for the observation of ordered oxide in the interfacial SiO<sub>2</sub> layer [1].

### Experimental

A stacked structure of HfSiOx/HfO<sub>2</sub> layers was formed by an atomic-layer deposition (ALD) technique, after a 0.5-nm thick SiO<sub>2</sub> layer was formed on Si wafers (HfSiOx/HfO<sub>2</sub> sample) [2]. The thicknesses of the HfSiOx and HfO<sub>2</sub> layers were nominally 1.0 and 1.5 nm, respectively. The high-k gate dielectrics were nitrided using nitrogen radicals, and annealed in a N<sub>2</sub>-diluted oxygen atmosphere (O<sub>2</sub> concentration of 0.004%) at a high temperature of 1000°C (HfSiON/HfON sample). Some of the samples were annealed in a 100% nitrogen atmosphere at 800°C for 3.5 min (annealed HfSiON/HfON sample).

X-ray diffraction experiments using synchrotron radiation were performed on BL4C of the Photon Factory

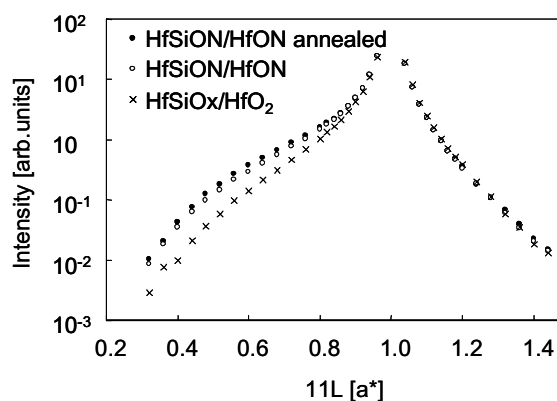


Fig. 1 Intensity distributions along the CTR scattering around the 111 Bragg point for the HfSiOx/HfO<sub>2</sub>, HfSiON/HfON, and annealed HfSiON/HfON samples.

(KEK) by employing a four-circle diffractometer with an Si(111) crystal analyzer.

### Results

In Fig. 1, the intensity distributions along the CTR scattering around the 111 Bragg point are shown for the three samples. Sharp diffraction peaks are not observed on the CTR scattering, because the thickness of the interfacial SiO<sub>2</sub> layers is very small. However, the intensity of the low angle side of the CTR scattering clearly increases after the nitriding and post-nitriding annealing, although the intensity of the high angle side of the CTR scattering does not change. This indicates that the oxide layers with the ordered structure are really formed at the interface between the high-k layer and the Si substrate. The intensity of the ordered oxide slightly increased for the annealed HfSiON/HfON sample compared to that for the HfSiON/HfON sample. This also indicates additional oxidation at the interface.

### References

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