

## Strain relaxation at HfO<sub>2</sub>/Si interface by post-deposition annealing.

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### Introduction

It is known that HfO<sub>2</sub> is one of material satisfying the conditions required of insulator layers for next generation device. In realization of a metal-oxide-semiconductor (MOS) device using a high-k film as insulator layer, one of key problem is control of strain at HfO<sub>2</sub>/Si interface.

In this investigation, we studied a strain relaxation at an HfO<sub>2</sub>/Si(001) interface by post-deposition annealing with extremely asymmetric X-ray diffraction.

### Experimental

The HfO<sub>2</sub> films were deposited on the H-terminated Si surface by KrF excimer laser deposition from a HfO<sub>2</sub> ceramic target in a 200 mTorr N<sub>2</sub> ambient. Firstly, a sample with a film thickness of 2.5 nm was prepared. Secondly, this as-deposited sample was annealed at 800 °C for 15 s in N<sub>2</sub> ambient after the measurement of strain.

Measurement of the strain at the HfO<sub>2</sub>-Si interface was done by measuring the X-ray rocking curve of the Si 113 reflection of the substrate under grazing incidence conditions at room temperature and atmospheric pressure at beam line 15C, Photon Factory. The experimental setup for this observation was reported elsewhere [1].

### Results and Discussion

Fig.1 shows the dependency of the integrated intensities of the measured curves on the X-ray wavelength. These curves were measured at observation positions on the same sample. For the as-deposited sample, the slopes of the integrated intensity vs. the wavelength are fluctuated for the observation position as shown in Fig.1(a). However, after annealing, this fluctuation disappears as shown in Fig.1(b). Basically, the slope of the integrated intensity vs. the wavelength reflects the strain field induced to the HfO<sub>2</sub>/Si interface [1]. Therefore, from Fig.1, it is thought that the post-deposition annealing refines the nonuniformity of the strain at the HfO<sub>2</sub>/Si interface.

We did a quantitative evaluation of the strain by fitting of the measured curves with curves calculated by a dynamical diffraction theory (Darwin's theory). We used a "distorted crystal model" in the calculation. In this model, a tension or a compression of the (001) spacing along the surface normal is assumed. It was assumed that the magnitude of the strain has its maximum value ( $\epsilon_0$ ) at the topmost surface and attenuates like a Gaussian

function with the depth. And the distorted crystal connects to bulk at a certain depth of  $H$ . Fig.2 shows reliable regions of  $\epsilon_0$  and  $H$  for the as-deposited sample (broken line) and the annealed sample (solid line). In both case, compressive strain was introduced. It is thought that the compressive strain comes from the existence of HfO<sub>2</sub> layer on the substrate. Comparing the reliable regions of the as-deposited and the annealed sample, it is clear that the strain induced by annealing is more compressive than that by deposition alone. From a cross-sectional TEM observation, growth of an amorphous layer was recognized at the interface between the HfO<sub>2</sub> layer and the substrate. From this result, it is thought that the growth of the amorphous layer brings an additional compressive strain and the uniformity of the interface.

### References

- [1] T. Emoto et al., Appl. Surf. Sci., 190, 113 (2002).

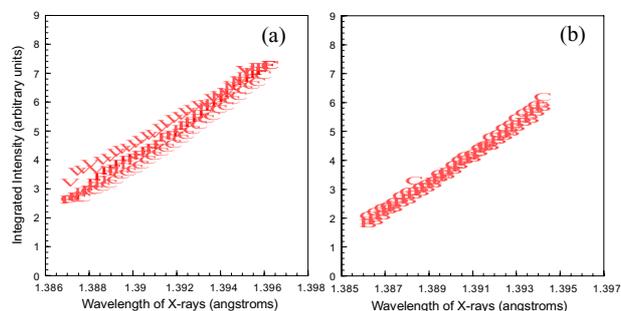


Fig.1: Dependency of the integrated intensity on wavelength for as-depo sample (a), and annealed sample (b).

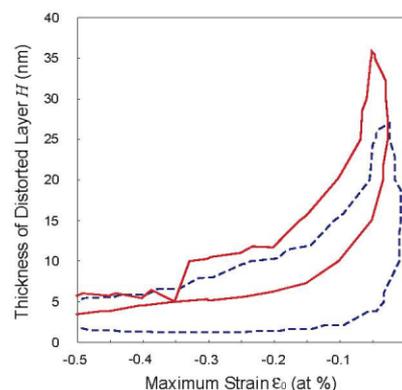


Fig.2: Reliable region of  $\epsilon_0$  and  $H$  for the as-depo sample (broken) and the annealed sample (solid).

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