SiO₂/Si Interfacial Lattice Strain Studied by Extremely Asymmetric X-ray Diffraction

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Introduction

Growth of SiO₂ on Si introduces stress or strain into the Si substrate near the interface. This strain can influence the device characteristics. At present, most oxide films are made by dry oxidation. As another oxidation method, the high pressure oxidation can be used to make thick oxide films at comparatively low temperatures.

Recently, the extremely asymmetric X-ray diffraction method was established as a new method for studying interfaces [1]. In this case, the lattice distortion near the crystal surface with respect to the bulk is reflected in the rocking curve. It has been reported that the wavelength dependence of the integrated intensity of the rocking curves is not only sensitive to the strain fields, but is also insensitive to the effect of absorption by the overlayer [2].

In this research, the interfacial lattice strain of $SiO_2/Si(100)$ formed by high-pressure oxidation was examined by extremely asymmetric X-ray diffraction.

Experimental

We analyzed samples oxidized by high pressure oxidation and oxidized by normally dry oxidation. High pressure oxidation was done at $600 \sim 750^{\circ}$ C in oxygen pressure of $1 \sim 2$ MPa and dry oxidation was done at $750 \sim 850^{\circ}$ C. The oxide films were etched to a thickness of 100 Å.

Observation of the strain field near the interface was done by measuring the X-ray rocking curve of the Si (311) reflection of the Si substrate under grazing incidence conditions (about 0.2°) at room temperature and atmospheric pressure by changing the X-ray wavelength in the range $1.38 \sim 1.386$ Å.

Results

Fig. 1 shows the dependence of the integrated intensities on the X-ray wavelength calculated by dynamical diffraction theory. ε_0 is the strain of the topmost (100) spacing with respect to the bulk value and is defined as $\varepsilon_0 \equiv (d - d_0) / d_0$, where d is the (100) spacing of the topmost layer and d_0 is the (100) spacing of the bulk. In this calculation, we assumed that the strain has its maximum value at the interface and attenuates like a Gaussian function with depth. The oxide film thickness was taken to be 100 Å and the distorted layer was 200 Å. From Fig. 1, it is found that the slope decreases when a compressive strain exists. Table I gives the slopes of the integrated intensity versus X-ray wavelength curves. The slopes have errors about 40 arb.unit / Å.



Figure. 1. The dependence of the integrated intensities on the X-ray wavelength calculated by dynamical diffraction theory.

Table I. Slopes of the integrated logarithmic intensity versus wavelength curves for different temperatures and pressures.

| Temperature [°C] | Dry | 1 MPa | 1.5 MPa | 2 MPa |
|------------------|------|-------|---------|-------|
| 850 | 2430 | | | |
| 750 | 2570 | | | 2130 |
| 700 | | 2600 | 2210 | 2320 |
| 650 | | | | 2340 |
| 600 | | 2680 | | |

Discussion

From Table I we can see the tendency that for the high pressure oxidation samples the higher the oxidation temperature and oxygen pressure were the smaller slope became. This indicates that the higher the oxygen pressure was the more compressive strain was introduced.

Further working is needed to fit the experimental results into the absolute strain values.

References

[1] T. Emoto, K. Akimoto, A. Ichimiya, Surf. Sci., **438** (1999) 107–115.

[2] T. Emoto, K. Akimoto, Y. Yoshida, A. Ichimiya, T. Nabatame, A. Toriumi, Appl. Surf. Sci., **244** (2005) 55–60.

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