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SiO_2/Si(100) Interfacial Lattice Strain Studied by Extremely Asymmetric X-ray Diffraction

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We studied the interfacial lattice strain of SiO_2/Si(100) formed by high-pressure oxidation with extremely asymmetric X-ray diffraction using synchrotron radiation. From the dynamical diffraction calculation, we analyzed that the lattice spacing of oxidized silicon is compressed compared to that of the ideal crystal. By comparing wavelength dependence of integrated intensities of rocking curve obtained by calculations and experiments, we found that the conditions during oxidation influenced the magnitude of the lattice strain. The higher the oxygen pressure was the more compressive strain was introduced. Moreover, for higher temperature, more compressive strain was introduced. The interfacial lattice strain introduced in high pressure oxidation is comparable in magnitude to that introduced in dry oxidation even if the oxidation done at low temperatures.

Key words: SiO_2/Si(100), lattice strain, high pressure oxidation, X-ray diffraction, synchrotron radiation

1. INTRODUCTION

The structure of the interface between an insulator film and semiconductor substrate is an important feature of devices, because the strain introduced into the substrate or defects at the interface may affect the mobility of carriers [1]. Although most oxide films are made by dry oxidation at present, 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. There are many studies on interfacial structures such as the native SiO_2/Si interface [2], the reconstructed Si surface [3], the Ni/Si(100)-H interface [4], etc, by this method. The X-ray optics of this diffraction experiment is an extremely asymmetric Bragg-case under grazing incidence conditions. In this case, the lattice distortion near the crystal surface with respect to the bulk is reflected in the rocking curve because the X-ray penetration is limited to the crystal surface by using a glancing angle smaller than the critical angle of total reflection. 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 absorption effect of the overlayer [3,5].

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 using synchrotron radiation.

2. EXPERIMENTAL

We analyzed samples oxidized by high pressure oxidation and oxidized by normally dry oxidation. High pressure oxidation was done at 600~750°C in oxygen pressure of 1~2 MPa and dry oxidation was done at 750~850°C. The oxide films were etched to a thickness of 10 nm.

The experimental setup which is shown in Fig. 1 is called extremely asymmetric X-ray diffraction technique. In Fig. 1, α is the angle between {100} plane and {311}, and θ_B means 311 Bragg angle. When θ_B equals α, the X-ray wavelength that fulfills the Bragg-condition is ~0.138 nm.

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 from 0.1380 to 0.1386 nm. The experiments performed at beamline 15C, Photon Factory, KEK, Tsukuba, Japan.

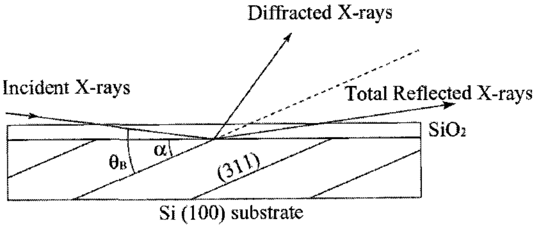

Fig. 1 Experimental setup. α shows the angle between Si {100} plane and {311} plane, and θ_B means 311 Bragg angle.

3. RESULTS

In order to determine the strain near the Si substrate quantitatively, we fitted the measured curves with the calculated curves using a dynamical diffraction theory assuming a strain field near the crystal surface[6]. In this distorted crystal model, a expansion or a compression of the Si(100) spacing along the surface normal is assumed. It was assumed that the magnitude of the strain has its maximum value at the Si topmost layer and attenuates like a Gaussian function with depth. This model is characterized by parameters of ε_0 and H. ε_0 is the strain of the topmost Si(100) spacing with respect to the bulk value and is defined $\varepsilon_0 \equiv (d - d_0) / d_0$ when d is the Si(100) spacing of the topmost layer and d_0 is the Si(100) spacing of the bulk. H is the thickness of the distorted layer. In the calculations, a 10 nm thick SiO_2 layer were assumed for both the samples oxidized by dry oxidation and high pressure oxidation. The quality of the curve fit was evaluated by the chi-square value.

Fig. 2 shows the calculation curves which are fitting to the experimental optimally; solid line is optimum curve assumed compressive strain about 2%. These best fitted curves are obtained by dynamical diffraction calculation with changing wavelength of X-rays and ε_0 in H=10 nm.

Fig. 3 shows the dependence of the integrated intensities on the X-ray wavelength calculated by dynamical diffraction theory. It is known that these integrated intensities are not influenced by absorption of an overlayer and that their slopes are correlated to the interfacial lattice strain. From Fig. 3, it is found that the slope decreases when a compressive strain exists. In this analysis, the integrated intensities are obtained by integrating the logarithms of rocking curves intensities.

The dependence of the experimental integrated intensities on the X-ray wavelength is shown in Fig. 4(a) for dry oxidation and Fig. 4(b) for high pressure oxidation done at different oxidation temperatures, Fig. 4(c) for high pressure oxidation done at different oxygen pressures. Table I gives the slopes of the integrated intensity versus X-ray wavelength curves. The slopes have errors about 4000 arb.unit / nm.

4. 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. Moreover, for higher temperatures, more compressive strain was introduced. It is concluded from the fitting by the dynamical diffraction calculation that Si near the SiO_2 interface is compressed about 2%. Therefore the higher the oxidation pressure and temperature were the more the strain would be introduced. The strain may affect the carrier mobility [1] and the performance of LSI devices.

In addition, because the high pressure oxidation can make thick oxide films at comparatively low temperatures than dry oxidation, it should be possible to produce at low temperature samples with a similar strain to samples produced at high temperatures with dry oxidation.

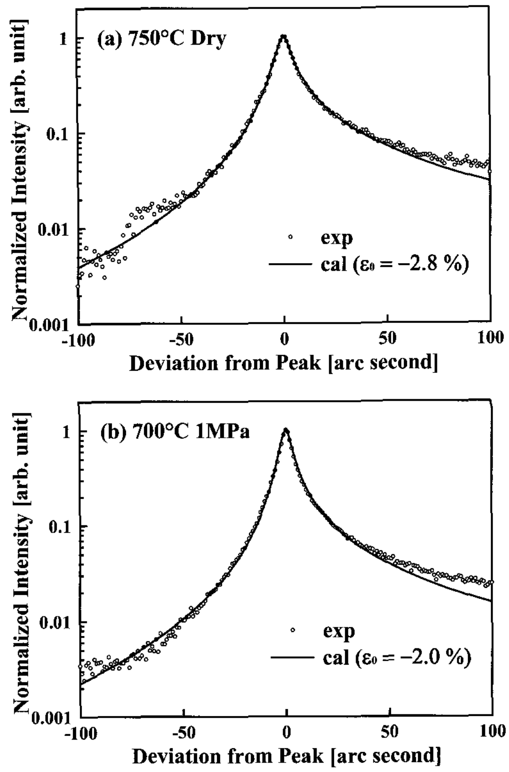

Fig.2 The calculated optimum curve for experimental data from the samples formed (a) by dry oxidation at 750°C and (b) by high pressure oxidation at 700°C in oxygen pressure of 1MPa.

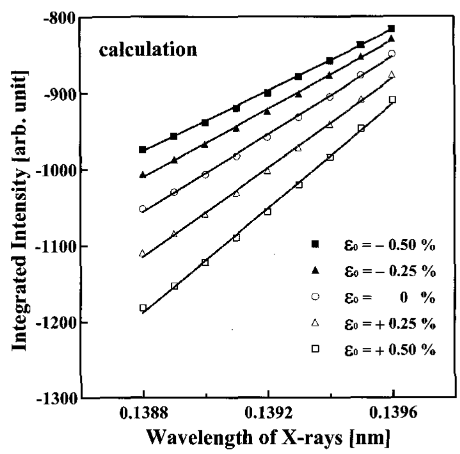

Fig. 3 The dependence of the integrated intensities on the X-ray wavelength calculated by dynamical diffraction theory.

5. SUMMARY

In this research we examined the interfacial lattice strain of SiO_2/Si (100) formed by high-pressure oxidation by extremely asymmetric X-ray diffraction using synchrotron radiation. The experiments show a correlation between the interfacial lattice strain and the oxidation conditions. The higher the oxygen pressure was the more compressive strain was introduced. Moreover, for higher temperature, more compressive strain was introduced. The interfacial lattice strain introduced in high pressure oxidation is comparable in magnitude to dry oxidation even if the oxidation is done at low temperature.

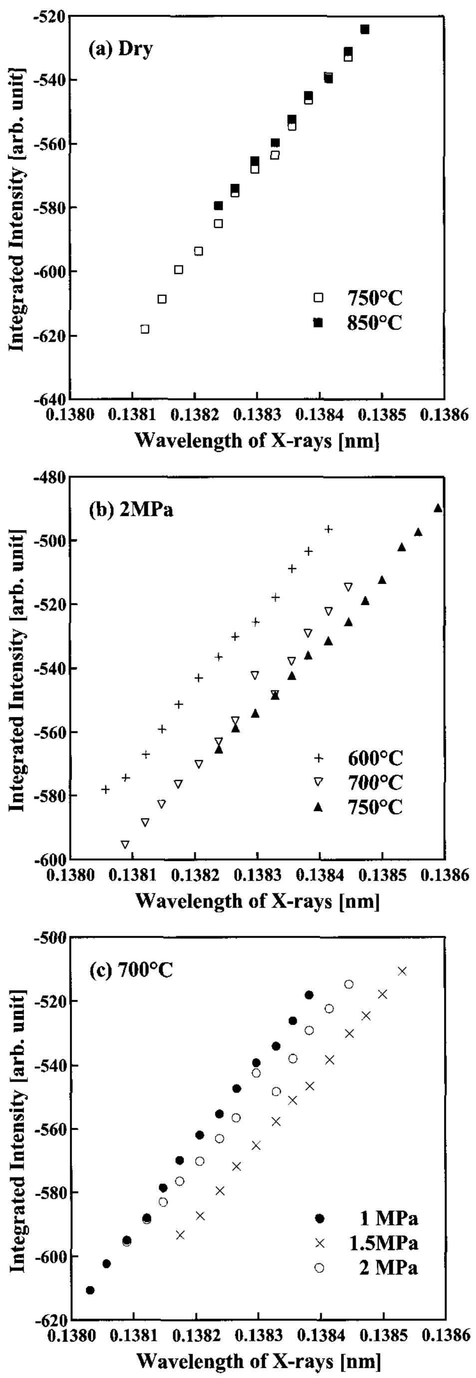

Fig. 4 Dependence of the experimental integrated logarithmic intensities on the X-ray wavelength. Comparison of (a) dry oxidation, (b) temperature of high pressure oxidation and (b) pressure of high pressure oxidation.

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	243000			
750	257000			213000
700		260000	221000	232000
650				234000
600		268000		

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