PS–11.01.20 THE INTERFACIAL STRUCTURES OF THERMALLY OXIDIZED Si-SiO$_2$ SYSTEMS BY O$_2$ AND O IN RELATIVELY LOW TEMPERATURES.
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The interfacial structures of Si-SiO$_2$ systems have long been of great interest, because their electric properties such as fixed charge density and interface states are strongly structure dependent. There have been a lot of reports on the existence or nonexistence of the c-SiO$_2$ interlayer between a-SiO$_2$ and c-Si. The opposite results from different studies suggest that the formation of the c-SiO$_2$ interlayer might depend on the oxidation conditions, such as oxidizing temperature, atmosphere, and so on. If so, the interfacial structure should be closely related to the oxidation kinetics. In this report the interfacial structures of thermal oxide formed with different oxidizing species and temperatures are studied with variable incident angle ellipsometry and are discussed in relation to the oxdation mechanism. Comercial P-type (001)CZ-Si wafers were thermally oxidized with 100% dry O$_2$ in the temperature range of 700 ℃ to 1050 ℃ (hereafter dry O$_2$ oxidation) and with the afterglow of microwave plasma of 270 Pa dry O$_2$ in 450 ℃ to 800 ℃ (afterglow oxidation). The refractive indices of the assumed interlayers at the interface of these Si-SiO$_2$ systems analyzed by ellipsometry were 1.4~1.6 for the dry O$_2$ oxidation and 3.0~3.15 for the afterglow oxidation. It is quite probable that at the interface of the Si-SiO$_2$ systems there exist a c-SiO$_2$ interlayer in the dry O$_2$ oxidation and a mixed layer of a-SiO$_2$ and c-Si in the afterglow oxidation. This result is consistent with the structure model of a-SiO$_2$ deduced from the X-ray CTR scattering measurement by I.Takahashi, et al. (this congress, 11·02) and with the interstitial related oxidation model (T.Tamura, et al., Jpn. J. Appl. Phys., 1992, 32, pp.12-16) proposed to explain the external stress dependencies of afterglow oxidation curves (Fig.1), which opposes to and cannot be explained by the usual Deal-Grove oxidation model.
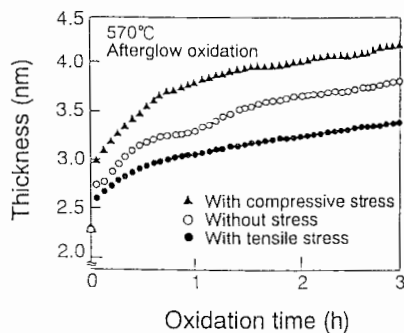
Fig.1 Effct of external srtess on the afterglow oxidation curves of (001) Si. The amount of stress is 100MPa.

PS–11.01.21 EVALUATION OF THE THEORIES OF CTR SCATTERING BY ABSOLUTE MEASUREMENT OF ITS INTENSITIES
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The validity of several theories with respect to the crystal truncation rod (CTR) scattering was assessed by comparing the intensity with that observed on an absolute scale, the intensity ratio to the incident X-ray beam, I_{obs}/I_0. Intensity of the CTR scattering from a Si(111) wafer was measured simultaneously with the thermal diffuse scattering (TDS) by using Imaging Plate (IP) detector. It enables us to convert the intensity of the CTR scattering onto the absolute scale because the intensity of the TDS can be estimated in terms of the elastic constants (C_{ij}) and the absorption coefficient of silicon. In fig.1 the intensities of the CTR scattering around 111 Bragg point observed on the absolute scale are indicated by the circles.

CTR scattering is a diffraction effect due to abrupt truncation of the periodicity of the lattice at the surface so that it comes from the Laue function of the Bragg scattering term along the line perpendicular to the surface. In general it can be written as

$$\Phi(K) \equiv \sum_{n=N_0}^{N_1-1} e^{iKna} = \frac{e^{iKN_0a}}{1-e^{iKa}} - \frac{e^{iKN_1a}}{1-e^{iKa}}, \qquad (1)$$

in which K and a are the scattering vector and the lattice constant perpendicular to the surface, respectively. N_0 and N_1 represent the height of the surface and the other end, which depend on the in-plane position, respectively. Assuming the other end is not clear (The specimen is much thicker than the coherent length of the incident beam.), the second term disappears when $\Phi(K)$ is summed up over the in-plane position, as K is not a reciprocal lattice vector. The intensity of CTR scattering is, therefore, proportional to $1/(1 - e^{iKa})$. Robinson [Phys. Rev. (1986) **B33**(6) 3830-3836], however, treated eq.(1) by averaging the fine oscillation of the numerator of the Laue function, $|\Phi(K)|^2$. Vlieg et al. [Surface Sci. (1989) **210** 301-321] ignored the second term by taking an absorption coefficient, μ, into the summation, $\sum e^{iKna}e^{-\mu na}$, where the exponential term with the absorption coefficient was tended to be one after the summation.

The calculations for an ideally flat surface based on these three treatments are shown by the dashed (Robinson) and solid (Vlieg et al. and our treatment) curve in fig.1. The calculation for the Vlieg et al. is the same as for our treatment. The calculation for Robinson is just two times as much as that for Vlieg et al. and our treatment. It is clear from fig.1 that the treatment by Vlieg et al. and our treatment is appropriate.

A difference between two treatments by Vlieg et al. and our treatment appears when K approaches a reciprocal lattice point. In the treatment by Vlieg et al. the intensity diverges to an infinite value. But in our treatment the intensity doesn't diverge because the second term doesn't disappear when K is equal to a reciprocal lattice vector even if the distribution of N_1 is random for the in-plane position. Therefore the intensity at a reciprocal lattice point is proportional to the $N^2(N = N_1 - N_0 + 1)$. This result is consistent with the usual kinematical theory.
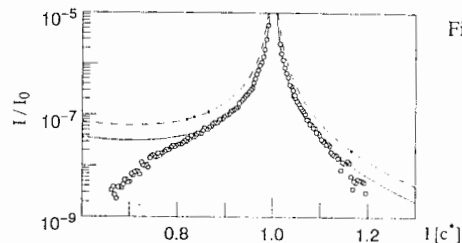

Fig.1