STRAIN FIELD UNDER THE SiO_2/Si(001) INTERFACE REVEALED BY PHASE-SENSITIVE X-RAY DIFFRACTION TECHNIQUE

Strain near an interface affects its electronic structure, but such a strain is still not completely understood even in the case of SiO_2/Si, which has been applied to electronic devices since the 1960s. We have developed a new powerful technique, the phase-sensitive X-ray diffraction (PSXD) technique, for characterizing strain fields near crystal surfaces, and applied it to a Si(001) wafer whose surface is covered with a thermal oxide layer [1]. It was revealed that there is a small strain field extending over a mesoscopic-range depth up to several hundreds nm under the SiO_2/Si interface and having a static fluctuation in the lateral direction.

The PSXD technique is an application of a phenomenon, that is, the modulation of the intensity of crystal-truncation-rod (CTR) scattering under an excitation of a Bragg reflection [1-5], which is an interaction between the CTR scattering, satisfying the two-dimensional diffraction condition, and the Bragg reflection, satisfying the three-dimensional diffraction condition. An example of the phenomenon in the case of using the Si(001) wafer is shown in Fig. 1, where the intensity of 50 rod CTR scattering is modulated by the excitation of 004 Bragg reflection. The experiment was carried out at beamline **BL09XU**. The experimental setup is shown in Fig. 2 (a). The arrangement was set to be particularly sensitive to strain fields extending over a mesoscopic-range depth (that is, Δl in Fig. 2 (b) was set to be very small).

In Fig. 1 the solid and open circles represent the experimentally obtained intensities corresponding to the 50 rod CTR scattering and the 004 Bragg reflection. The horizontal axis is the deviation of incident angle from the 004 Bragg angle. The broken line (green) is the best-fit curve of the experimentally obtained intensity of Bragg reflection.

We showed that the modulation profile can be characterized by two parameters: the phase shift, which represents the dip or peak position of the modulation profile, and the visibility. The solid line (red) in Fig. 1 is the best-fit curve calculated for the modulation profile, where the phase shift and the visibility are fixed at $-2\pi \times (0.117 \pm 0.001)$ and 0.521 ± 0.002, respectively. Both the experimentally obtained values were different from those of an ideal perfect crystal (0 and 0.711, respectively), which is shown by the dotted line (blue) in Fig. 1.

Figure 3 shows an illustration of the strain field under the SiO_2/Si(001) interface, which can explain the experimentally obtained modulation profile. The phase

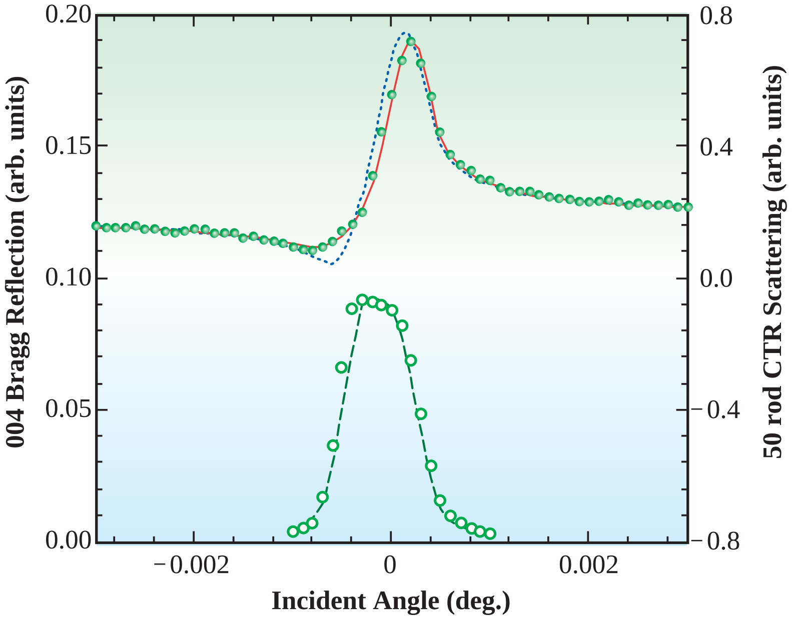

Fig. 1. Example of modulation of intensity of CTR scattering in the case of a Si(001) wafer covered with a thermal oxide layer. The intensity of 50 rod CTR scattering is modulated by the excitation of 004 Bragg reflection.

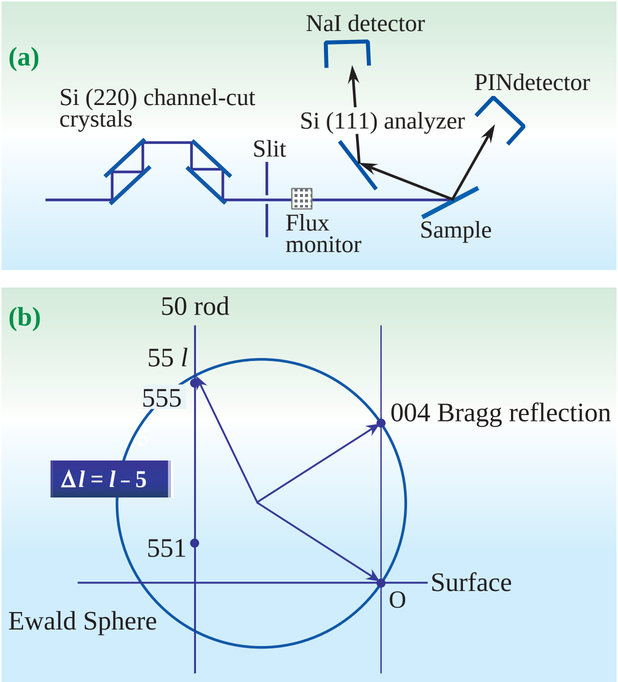

Fig. 2. **(a)** Side view of experiment setup. **(b)** Illustration of diffraction condition of experiment in reciprocal space.

shift can be simply interpreted as the sum of displacements of atomic planes under the interface projected onto the direction perpendicular to the 004 plane (–0.16 Å in Fig. 3). On the other hand, the experimentally obtained visibility indicates that the total displacement has a static fluctuation in the direction parallel to the interface. The visibility was interpreted as a static fluctuation of at least ±0.13 Å in the lateral direction. The features revealed by the PSXD technique are expected to provide a new aspect for understanding the mechanism of Si surface oxidation.

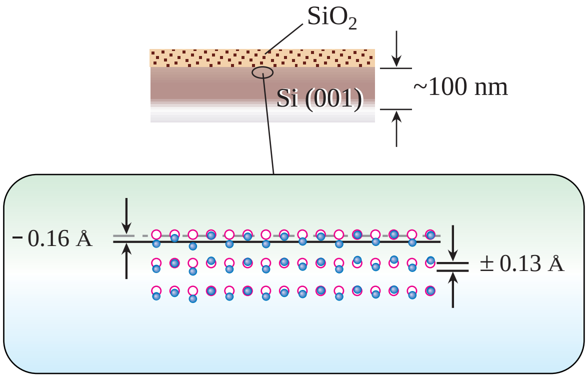

Fig. 3. Illustration of strain field under SiO_2/Si(001) interface, which can explain the experimentally obtained modulation profile. The open circles represent the sites of atoms or unit cells in a bulk crystal, and the solid circles represent the positions of atoms in the strained layer near the interface.

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