Characterization of strain field under the SiO₂/Si interface with using the phase-sensitive X-ray diffraction (PSXD) technique

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Modulation of the crystal truncation rod (CTR) scattering intensity caused by the Bragg reflection has been first reported by the calculations using Darwin’s theory extended to the three-wave case [1], and shown to be sensitive to atomic structures near crystal surfaces [2,3,4]. We proposed a new method to investigate strain fields near crystal surfaces by using the phenomenon [5]. We applied the method to measure small lattice distortion near surface of Si(001), which was oxidized at 700°C (wet oxidation).

The X-ray beam monochromatized by the double-crystal monochromator was further monochromatized by two Si(111) channel-cut crystals arranged in the (+ +) setting. We measured the intensity of the CTR scattering along the 50 rod under the excitation of the 004 Bragg reflection from Si(001) samples. The samples were cut on a flat plate placed on a high-precision goniometer. The measurements were carried out at some wavelengths around 1.24 Å. A result is shown in Fig. 1, where filled and open circles are the experimentally obtained intensities of the CTR scattering and the Bragg reflection, respectively. From the modulation profile we can obtain information on the small strain field near the SiO₂/Si interface.

References

Study on Dependence of Polarization states of Incident X-Rays and Structure Factors of Quasi-Forbidden Reflections on Tow-dimensional Goniometry in Silicon Three-Beam Simultaneous Reflection Cases

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The above equation (1) is the new n-beam X-ray dynamical theory one of the present author has derived based on the Takagi-Taupin equations [1,2]. It has already been reported that computer-simulated pinhole topographs based on (1) agree excellently with experimental pinhole topographs [2,3].

The new theory (1) can also simulate results of two-dimensional X-ray goniometry by using the terms of $\beta^0$ and $\beta^1$ which are angular deviations of incident X-rays from the strict n-beam reflection. Figure 1 shows experimental (left) and computer-simulated (right) two dimensional rocking curves in the vicinity of the three-beam reflection condition giving 733 and 353 Laue-Laue reflections simultaneously. The simulated and experimental profiles agreed well, which reveals the efficiency of (1) also for n-beam two-dimensional goniometry. Furthermore, from comparison between the experimental and computer-simulated rocking curves of 733 and 222 simultaneous reflection condition, the 222 structure factor was determined to be 2.495.

Fig. 1 Two-dimensional rocking curves in the vicinity of $733\text{ and } 353$ simultaneous reflection. The left- and right-column figures show experimental and computer-simulated profiles. (a), (b) and (c) show intensities of forward, 733 - and 353-reflected X-rays, respectively. $\phi$ and $\theta$ are rotation angles around $733\text{ and }353$ axes. Scan ranges of $\phi$ and $\theta$ were 23.85 and 8.0 seconds of arc. The sample was a $[110]$-oriented floating zone silicon crystal of 0.24 mm thickness. The incident X-rays were horizontal-linearly polarized.

References