Mesoscopic-Scale and Small Strain Field beneath SiO$_2$/Si Interface Revealed by a Multiple-Wave X-ray Diffraction Phenomenon — Depth of the Strain Field*

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Small strain field distributed over a mesoscopic-scale beneath SiO$_2$/Si interface was investigated by using intensity of CTR scattering modulated by a Bragg reflection, which is a multiple-wave X-ray diffraction phenomenon. Assuming that the depth-profile of the total displacement of the strained layer is expressed by an exponential function, we calculated the intensities of the CTR scattering and the Bragg reflection on the basis of the three-wave Darwin theory. The results showed that the modulation is sensitive to the total displacement of the atomic layers in the strained layer, while the curve of the Bragg reflection is sensitive to the depth of the strained layer. We compared the results of the numerical calculations with the experimental results of a Si(0 0 1) wafer covered with a thermal oxide layer, which was formed by wet oxidation process at 900 °C, and found that the total displacement in the strained layer is 0.132Å and the depth of the strain field is a few hundreds of nanometers.

Keywords: X-ray scattering, diffraction, and reflection; Surface structure, morphology, roughness, and topography; Surface stress; Silicon; Oxidation

I. INTRODUCTION

Strains in a crystal play important roles in hetero- crystals. Even small strains near crystal surfaces can affect not only electronic structures but also crystal growths on the surfaces (for example, Refs. [1–4]). X-ray diffraction is a powerful tool to investigate strain field distributed over a scale from atomic to more than one micrometer scale. Bragg reflection has been conventionally used to investigate relatively long-range strain field distributed over more than one micrometer [5]. Recently proposed extremely asymmetric Bragg reflection is one of promising techniques to investigate structures near crystal surfaces [6]. On the other hand, crystal-truncation-rod (CTR) scattering [7–10] has been applied to determine not only atomic structures but mesoscopic-scale (a few tens ~ hundreds of nanometers) strain fields near surfaces and interfaces. Recent progress in computational methods for retrieving phase of the CTR scattering have opened up a new window: these methods provide directly images of atomic structures [3, 4, 11–23] and strain fields [24–29] by the Fourier transformation of the scattering amplitude of the CTR scattering.

In a previous paper we have reported another approach to investigate strain fields near crystal surfaces using a multiple-wave X-ray diffraction phenomenon, which experimentally provides information on the phase of CTR scattering. The approach uses intensity of CTR scattering modulated by a Bragg reflection [30–36], and revealed that there is a small strain field distributed over a mesoscopic-scale beneath a SiO$_2$/Si interface [36], which is difficult to be found by the conventional X-ray diffraction measurements [37]. However, the depth of the strain field were not determined, although it has to be sufficiently less than the extinction depth of the Bragg reflection used and not a few atomic planes. In this paper we propose a method to determine the depth of the strain field by using the phenomenon. Assuming that the depth-profile of the total displacement of the strained layer is expressed by an exponential function, we calculated the intensities of the CTR scattering and the Bragg reflection on the basis of the three-wave Darwin theory. The results showed that the modulation is sensitive to the total displacement of the atomic layers in the strained layer, while the curve of the Bragg reflection is sensitive to the depth of the strained...
FIG. 1: Illustration of a model of mesoscopic-scale small strain field. A strained layer containing \( n \) atomic planes is formed on an ideal semi-infinite perfect crystal. The filled circles represent the positions of atoms or unit cells in bulk crystal, and the open circles represent those in the strained layer near the interface. The parameter \( D_j \) represents the sum of displacements under the \( j \)th atomic plane.

layer. We compared the results of the numerical calculations with the experimental results of a Si(0 0 1) wafer covered with a thermal oxide layer, which was formed by wet oxidation process at 900 °C, and found that the depth of the strain field is a few hundreds of nanometers.

II. NUMERICAL CALCULATIONS

We calculated simultaneously the intensities of the CTR scattering and the Bragg reflection on the basis of three-wave Darwin theory [30]. As shown in Fig. 1, we considered a strained layer containing \( n \) atomic planes on an semi-infinite perfect crystal. We assumed that the depth-profile of the displacement \( D_j \) defined in Fig. 1 is expressed by an exponential function \( (D(z) = \exp(z/h)) \). The assumption of the exponential decay should be natural because the strain induced by the SiO\(_2\)/Si interface approaches to zero in a deep region. Note that almost the same result is obtained for a given total displacement \( D_n \) if \( D_j \) slowly varies in the strained layer and \( D_n \) is sufficiently smaller than the lattice spacing of the Bragg reflection used [36, 38].

We calculated the intensities of 0 0 4 Bragg reflection and 5 0 rod CTR scattering for a Si(0 0 1) crystal, as illustrated in Fig. 2. Figures 3 and 4 are results of the numerical calculations (Fig. 3: the 0 0 4 Bragg reflection; Fig. 4: the 5 0 rod CTR scattering). Here the wavelength was fixed at 1.24432 Å, for which the extinction depth of the Bragg reflection is 1.8 µm. You can see that the curves in Fig. 3 are slightly asymmetric except for the curve for a perfect crystal. The sign of the asymmetry is determined by the sign of the strain: if the sign of the strain is minus, the intensity on the high glancing angle side is larger than that on the low glancing angle side. For a given \( D_n \), the asymmetry of the curve increases with increasing \( h \) (see curves for \( D_n = 0.1d_{004} \)). On the other hand the intensity of the CTR scattering modulated by the Bragg reflection is sensitive to the strain field. The dip (or peak) positions of the modulation profiles reflect the total displacement \( D_n \); in fact, if \( D_n \) is given, the dip position of the modulation profile is almost the same even when \( h \) is close to the extinction depth of the Bragg reflection (see the curve for \( h = 2000d_{001} \)). Hence the total displacement \( D_n \) can be determined from the modulation profile, while the depth \( h \) of the strain field should be determined from the slight deviation of the rocking curve of the Bragg reflection from that of a perfect crystal.

III. EXPERIMENT AND RESULTS

The experiment for the Si(0 0 1) wafer covered with a wet-thermal oxide layer was performed at BL09XU in SPring-8, where a high-brilliance horizontally polarized X-ray beam from the undulator is available [39]. The premonochromatized SR beam was shaped by slits into a size of 1 mm (vertical) \( \times \) 1 mm (horizontal), and then highly monochromatized by using two Si channel-cut crystals arranged in the (+ +) geometry. The wavelength of X-rays and the experimental condition were the same as the above calculation. The sample was put on a very
The fact that the former curve fits to the experimental data were close to the rocking curves confirming that the depth of the strain field is about a few hundreds of nanometers. In fig. 6 we show two modulation profiles calculated for $h = 250d_{001}$ and $500d_{001}$. The fact that the former curve fits to the experimental data better than the latter indicates that the depth of the strain field is closer to $h = 250d_{001}$ than $500d_{001}$. Although a sophisticated simultaneous-fitting algorithm should be required, we showed that using both the rocking curve of a Bragg reflection and the intensity of the CTR scattering modulated by the Bragg reflection provides a powerful way to investigate mesoscopic-scale strain fields near crystal surfaces.

**IV. CONCLUSION**

Depth of small strain field distributed over a mesoscopic-scale beneath SiO$_2$/Si interface was determined by using both intensities of a Bragg reflection and CTR scattering modulated by the Bragg reflection. Assuming that the depth-profile of the total displacement of the strained layer is expressed by an exponential function, we calculated the intensities of the CTR scattering and the Bragg reflection on the basis of the three-wave Darwin theory. The results showed that the modulation is sensitive to the total displacement of the atomic layers in the strained layer, while the curve of the Bragg reflection is sensitive to the depth of the strained layer. We compared the results of the numerical calculations with the experimental results of a Si(0 0 1) wafer covered with a thermal oxide layer, which was formed by wet oxidation process at 900 °C, and found that the total displacement in the strained layer is −0.132Å and the depth of the strain field is a few hundreds of nanometers.
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