Atomic Displacement at the Gate Oxide / Si Interface Evaluated by X-ray CTR Scattering

Driven by the demand for higher electric performances as assessed in the International Technology Roadmap of Semiconductor (ITRS), complementary metal oxide semiconductor (CMOS) devices have been scaled down continuously. As a result, the thickness of SiO_2-based gate oxide is approaching atomic dimensions and the requirement of the electric properties for the gate oxide is becoming increasingly severe. As shown in Fig. 1, a typical thickness of gate oxides for 90-nm-node CMOS transistors is 1.1 nm, which corresponds to only four SiO_2 molecular layers. For the achievement of CMOS devices with such ultrathin SiO_2, nitrogen must be incorporated into the gate oxide to suppress boron penetration from the polycrystalline-Si gate into the underlying channel region, and to decrease gate leakage current. Controlling the depth profile of nitrogen in the gate oxide is a key issue since an excessive amount of nitrogen at the gate oxide/Si interface generates fixed charge and an interface level, which lead to the degradation of the electric properties and reliability of the gate oxide. To fabricate the CMOS devices with high electric performance and high reliability, the evaluation techniques for the gate-oxide/Si interface structure with nitrogen incorporation in an atomic scale has been desired but have not been realized.

Crystal truncation rod (CTR) scattering is a surface X-ray diffraction which is particularly sensitive to the structure of surfaces and thin films [1-3]. CTR scattering is a continuous scattering perpendicular to the surface because the Laue condition is relaxed to a non-integer Miller index in the vertical direction due to the abrupt termination of the crystal periodicity at the surface. The intensity of CTR scattering contains information on the structure of the surface atoms through the interference with the scattering amplitude from the substrate. In this work, we developed an evaluation technique of the interface atom displacement (IAD), expressed by δc, using CTR scattering, which is sensitive to the interfacial atom structure, particularly for nitrogen distribution. IAD is defined as the vertical displacement of the topmost Si atoms from the expected position for crystalline Si at the interface.

Based on the calculation of kinematical diffraction for the interface model with IAD, we found that δc introduces asymmetry of the CTR peak profile. By measuring the asymmetry, we can evaluate δc from the measured CTR profiles. We developed an analytical program, which can be used to evaluate δc based on the optimization of the measured CTR profile using the IAD model.

Since the intensity of CTR scattering is very weak compared to the bulk diffraction peak, high flux X-rays are required for the measurement. We carried out the CTR measurement using the newly installed four-circle diffractometer at the undulator beamline **BL16XU**. In the experiment, the X-ray wavelength of 0.116 nm was selected using a double-crystal monochromator. For the detection of X-rays diffracted from samples, an Si (111) analyzing crystal was used to improve the angular resolution. We measured theSi (11L) CTR scattering for the gate oxides formed on the Si(100) substrate by the rocking measurement

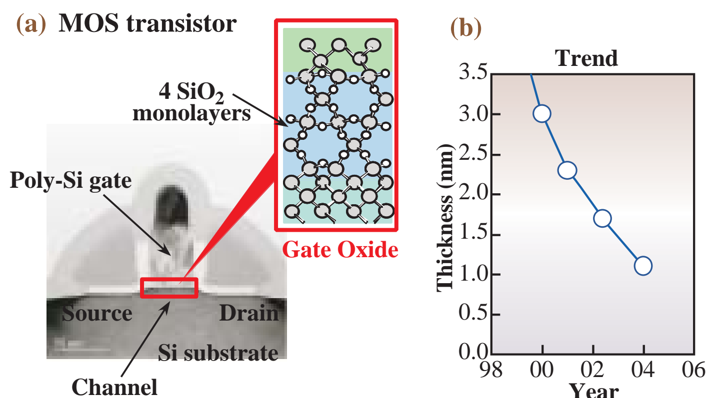

Fig. 1. TEM image of MOS transistor **(a)** and trend of gate oxide thickness **(b)**. The gate oxide has become thinner year by year. In 2004, the thickness of the gate oxide for the 90 nm technology node reached 1.1 nm.

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By applying the analytical program, we successfully reproduced the measured data, as shown by the solid lines in Fig. 2. As a result, δc was As a result, δc was determined with the accuracy of 0.0005 nm. The obtained δc for samples A and B were –0.013 nm and +0.010 nm, respectively, as shown in Fig. 3. A positive value of δc means the displacement of interface Si atoms toward the gate oxide and the negative value means displacement toward the Si substrate. For the SiO_2 sample without nitridation, δc is usually close to zero. After evaluating δc for the various nitridation samples, we found that δc distributed between –0.03 nm and +0.03 nm is strongly correlated with the nitridation procedure and like temperature and time. By evaluating δc from the measured CTR profile, we could readily observe the slight difference in the nitrogen contribution at the interface.

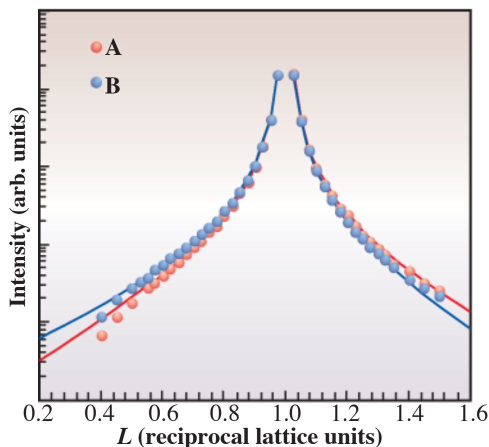

Fig. 2. The experimental results of the Si(11L) CTR scattering intensity for the gate oxides processed under two different nitridation conditions. These two profiles show the different peak asymmetries that are reproduced well by using the IAD model, as shown by the solid lines.

The electric measurements have been performed for the corresponding gate structures and gate leakage current and carrier mobility were found to have a close relation to δc. These results may be due to the fact that δc is related to the nitrogen distribution and the chemical bonding at the interface that sensitively reflects the electric performance.

In summary, atomic displacement at the SiO_2/Si interface has been successfully evaluated by applying the IAD model to the CTR scattering data, and its close relation with the electric properties was observed. This new technique provides a parameter, δc, that sensitively reflects the nitrogen distribution at the gate oxide/Si interface and that can be used to determine the optimum nitridation condition of a gate oxide with superior electric properties.

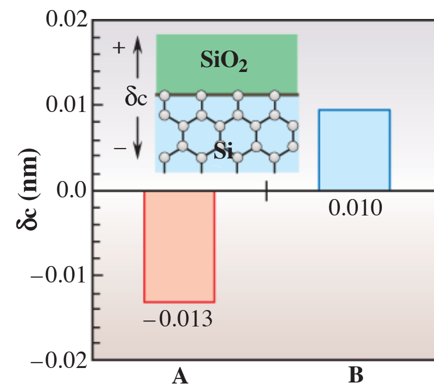

Fig. 3. Displacement of interfacial atom, δc, obtained from the analysis. In sample A, δc has negative value, but in sample B, δc has a positive value, which reflects that the difference in the interface structure corresponds to the different nitridation conditions.

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