# Interfacial Structure between Oxynitrated Amorphous $SiO_2$ film and Si(100)

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## Introduction

The continuous scaling down of silicon-based devices requires ultrathin oxides with high reliability. This trend has claimed us to obtain precise information on the interfacial structure of $SiO_2$ thin films on Si(100). X-ray diffraction has been a reliable tool for determining interface structures non-destructively. We have studied several interfacial structures by utilizing X-ray crystal truncation rod (CTR) scattering and X-ray reflectivity. Most striking results of our research on the interfacial structure of $SiO_2$-Si(100) may be summarized as follows [1,2,3,4]. (1) A crystalline phase exists in thermally grown $SiO_2$ films on Si(100). (2) The crystalline should be microcrystals and they epitaxially (coherently) grow with respect to the Si(100). (3) Probability of finding the crystallites is high at the interface (less than 10%) and decays with increasing the distance from the interface. (4) If we assume that the microcrystals is an $SiO_2$-type, a plausible structure can be chosen, which is called a pseudo beta-cristobalite (Fig.4 in [1]). In the present study, ultrathin(< 2.5nm) oxynitrated films on Si(100) are investigated, since the implantation of nitrogen atoms in the oxide layer is expected to be one of the promising methods to control the electrical properties of the interface.

## Experimental

X-ray diffraction measurements were performed at BL4C and BL17A using the four-circle diffractometers with Si(111) analyzers. We measured several samples annealed in $NO+N_2$ ambient. Variation of the (111) CTR intensity which depends on the density of N-atoms was observed (Fig. 1). It clearly indicates that the oxynitridation process does produce a structural transformation at the interface.

## Results and Discussion

A quantitative analysis based on the kinematical diffraction theory was carried out so as to obtain the parameters characterizing the interfacial structure. Up to now, several important features have been clarified: the Si atoms located at the interface are relaxed and pulled to the bulk; The mean displacement of the interfacial Si atoms increases with increasing the concentration of N-atoms; Interfacial roughness may also increase with increasing the N-atoms at the interface. We are now expecting that many important electrical properties which depend on the oxynitridation process can be explained by the change of the structural parameters revealed by the present study. In order to confirm our results, other CTR intensities have been collected, and the analyses are now in progress.

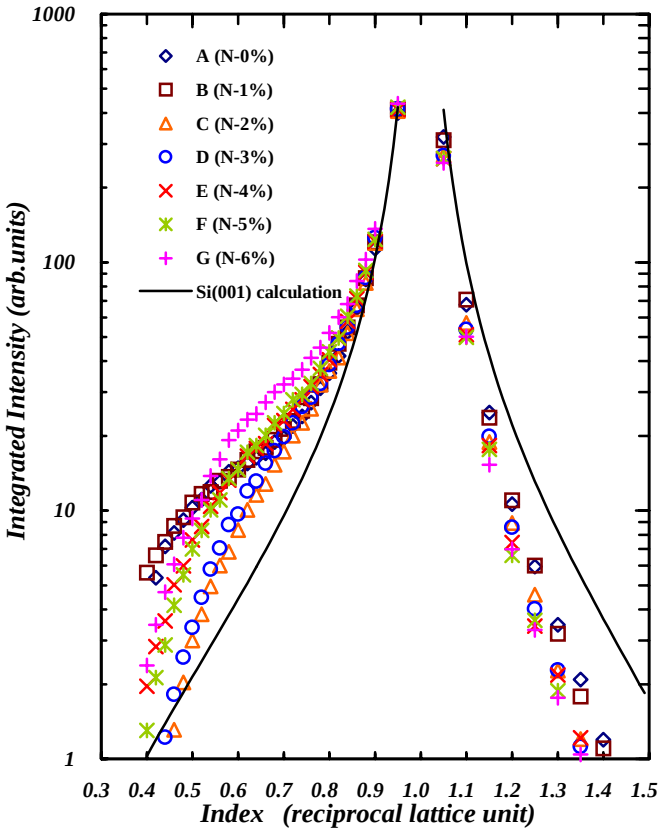


FIG.1. Integrated intensity of (11l)CTR scattering. A systematic deviation from the CTR of ideal interface is seen.

## References

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