Ordered structure in the internal thermal oxide layer of SIMOX wafers

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Introduction

The silicon-on-insulator (SOI) wafer, composed of a top Si layer, a buried oxide (BOX) layer and a Si substrate, has an ideal structure for complementary metal oxide semiconductor (CMOS) devices. A separation-by-implanted-oxygen (SIMOX) wafer, fabricated by O⁺ ion implantation and subsequent high-temperature annealing, is one of the most promising SOI wafers, because of its brief fabrication process and uniform thickness of the top Si and BOX layers.

When a SIMOX wafer was investigated by X-ray diffraction, diffraction streaks perpendicular to the wafer surface were observed at the middle of the reciprocal lattice points of Si, such as $0.5 \ 0.5 \ L \ (0.6 < L < 1.6)$ and $1.5 \ 0.5 \ L \ (0.4 < L < 1.4)$, where diffraction from bulk Si is forbidden. Based on these results, the ordered oxide was estimated to have an epitaxial relation of 2×2 with (001) Si, using surface structure notation, but poor periodicity perpendicular to the interfaces [1].

SIMOX wafers fabricated by O^+ ion implantation at doses of ~2×10¹⁸ and ~4×10¹⁷ cm⁻² are commonly called high-dose and low-dose SIMOX wafers, respectively. The low-dose SIMOX process is followed by an internalthermal-oxidation (ITOX) process, since the reduction of the ion dose leads to a decrease in the integrity of the BOX layer. In the ITOX process, the wafer is oxidized at about 1350°C in an oxidizing environment, so that the BOX layer increases in thickness at the interface between the top Si layer and the BOX layer. The additional BOX layer is called an ITOX layer

In this paper, we show the results of X-ray diffraction experiments for the ordered SiO_2 in the ITOX layers of the ITOX SIMOX wafers.

Experimental

X-ray diffraction experiments were performed using four circle diffractometers installed on BL-4C at the Photon Factory (PF), KEK, Tsukuba. The intensity distributions of the streaks were measured under a symmetric condition, in which the incident and outgoing angles to the wafer surface are equal to each other. Each intensity distribution represents the series of the integrated intensities obtained by rotating the samples at each measurement point, and the background intensities were subtracted. The wavelength was chosen to be 0.1542 nm.

Results

The intensity distributions of the 1.0 1.0 L (0.2<L<1.5) streaks for the low-dose and ITOX SIMOX wafers were observed. The intensities of the ITOX SIMOX wafer are higher than those for the low-dose SIMOX wafer in the range of L<0.7, while the intensities are roughly the same in the range of L>1.3. The intensities of these streaks depend on the roughness of three interfaces: the top surface, the buried interface of the top Si layer, and the interface between the BOX layer and the substrate. The interface roughness reduces the intensity of the streaks symmetrically with respect to the Bragg point. It is therefore apparent that the interface roughness is not the origin of the intensity differences between the wafers for L<0.7, since the intensities are the same in the range of L>1.3. The intensity of the streaks for L<0.7 also depends on the ordered SiO₂ with 2×2 symmetry in the BOX layer. However, this is not the reason in the present case because the intensity distributions of other streaks at the middle of reciprocal lattice points of Si are the same for the low-dose and ITOX SIMOX wafers, indicating that the amount and quality of the ordered SiO₂ of 2×2 symmetry in these wafers are similar to each other.

We therefore conclude that the ITOX layer has a structure similar to that of a thermal oxide layer on Si(001) substrates, which is due to a memory effect during the oxidation process [2]. In diffraction patterns from the thermal oxide layers on Si(001) substrates, an extra peak is observed at 1 1 ~0.45 in reciprocal space which is located just on the crystal truncation rod (CTR) scattering from the substrate. Based on these results, we have proposed a pseudo-cristobalite structure for the ordered SiO₂ in the thermal oxide layer. It may be assumed that the ITOX layer has basically the same atomic arrangement as that of the thermal oxide layer.

References

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