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# Inhomogeneous strain in thin silicon films analyzed by grazing incidence x-ray diffraction

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High-quality thin silicon overlayers (SOLs) in silicon-on-insulator (SOI) wafers have attracted a lot of interest in recent years. To obtain a thin SOL less than 50-nm thick, thermal oxidation of a SOL with a thickness of several hundred namometers on SOI wafers is usually employed. The thickness of the SOL on the SOI wafers decreases during the thermal oxidation as the oxide thickness increases, resulting in a kind of $SiO_2$/Si(<50 nm)/ $SiO_2$ sandwiched structure on the Si wafer.

It is well known that strain in SOI wafers mainly originates from the difference in the specific volume between the Si and $SiO_2$ at the $SiO_2$/Si interface. The existence of strain, however, will usually induce defects, such as lattice distortion, finite domain size, and dislocations, at the interface and inside the SOL. Accordingly, evaluating the strain and related lattice distortion in a SOL becomes important as the SOL thickness deceases below 50 nm.

In this work, we characterized the lattice strain and strain distribution in a 47-nm and 5-nm-thick SOL in separation by implantation of oxygen (SIMOX) wafers using the grazing incidence X-ray diffraction (GIXD) near the critical angle of total reflection in the beamline BL24XU of SPring-8 (Fig. 1).

The GIXD experiments were performed using the z-axis goniometer of the beamline. The 0.124 nm x-ray wavelength was used at incident angle $\alpha$ varying from 0.01° to 0.4°.

Figure 2 shows GIXD curves of the SIMOX wafer at different grazing angles and fitting curves calculated by kinematical theory on the basis of a two-layer-strained model. Figure 1 shows the (220) Bragg diffraction curves collected from the 47-nm-thick SOL at different grazing angles from 0.01° to 0.2°. The strong peak at the center ($\theta$=0°) is from bulk Si(220). Additional oscillating subpeaks (denoted as $0^{th}$, $1^{st}$, $2^{nd}$ in Fig. 2) appear at the lower and higher sides of the Si(220) reflection, they are clearly observed for the grazing angles between 0.01° and 0.1°. However, with increasing grazing angle, the peaks merge and become unclear at the shoulder of the main peak. This suggests that they originate from the surface region of the sample. In addition, it can be seen that the oscillating peaks are asymmetric with respect to the center of the Si(220) peak. The asymmetric feature also becomes clear with decreasing the grazing angle from 0.1 to 0.01°. These findings indicate that the origin of the peak oscillation is independent of the strong peak related to the Si(220) reflection, suggesting the existence of finite domains at the SOL surface. From the curve fittings to the experimental results, we found that the 47-nm thick SOL in SIMOX has ～500-nm-wide surface domains that are less strained than the bulk of the SOL on the order of $10^{-4}$. A simple schematic of the model is illustrated in Fig. 3.

To assess the thermal stability of the SOL, we annealed the sample at 1000℃ and measured GIXD at the grazing angle of 0.01°. Figure 4 shows the GIXD curves obtained during the anneal at 1000℃ and at room temperature (RT) after the anneal. At 1000℃, the additional peaks completely disappear at the shoulder of the Si(220), which makes the peak symmetric with respect to $\theta$=0°. After the anneal (i.e. at room temperature, as seen in Fig. 3, it is evident that the main peak becomes sharper while there are no additional peaks at the shoulder of the main peak. During annealing, the degree of strain becomes smaller than the detection limit of our apparatus, while the domains at the surface increase in size from 490 to 2000 nm. These results clearly show that the post-annealing treatment is effective in improving the spatial inhomogeneous strain distribution in the SOL.

Additionally, we characterized an ultrathin (5-nm-thick) SOL sandwitched by $SiO_2$. Figure 4 shows Bragg profiles obtained from the SOL at $\alpha$=0.02° and $\alpha$=0.12°. The Bragg peak positions at $\alpha$=0.02° and at $\alpha$=0.12° are different, suggesting the origins are different. The peak at $\alpha$=0.02° mainly originates from the ultrathin SOL (See the inset in Fig. 5) and that at $\alpha$=0.12° is from the Si substrate. The different angle of the peaks clearly indicates that the ultrathin SOL is tensile strained on the order of $10^{-4}$ in plane with respect to the Si substrate. In addition, in Fig. 5, there are none of the subpeaks that were observed for the 47-nm-thick SOL. The ultrathin Si film covered with thermal silicon oxides is homogeneously tensile strained in contrast to the case of the 47-nm-thick film without the top thermal silicon oxides.

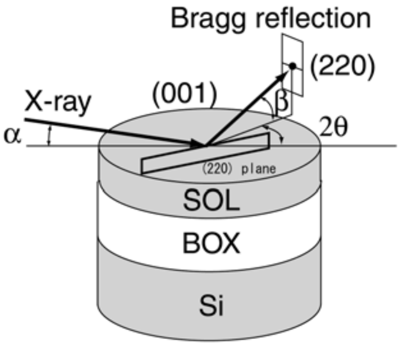


Figure 1: A schematic diagram of grazing incident X-ray diffraction from the SIMOX wafer. After etching a wafer in HF dilute solution, the wafer was oxidized at 1200℃ in a 0.2% $O_2$/Ar mixture to form a silicon oxide layer on top of the SOL. Then, the thermal oxide on the SOL was removed in a HF bath.

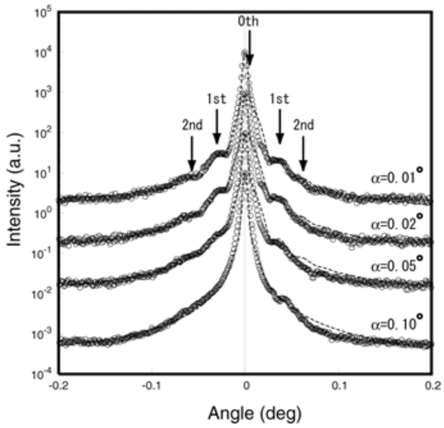


Figure 2: Si(220) Bragg diffraction curves at different incident angles. Additional subpeaks indicate the presence of strained surface domains. The dotted lines are theoretical fitting curves.

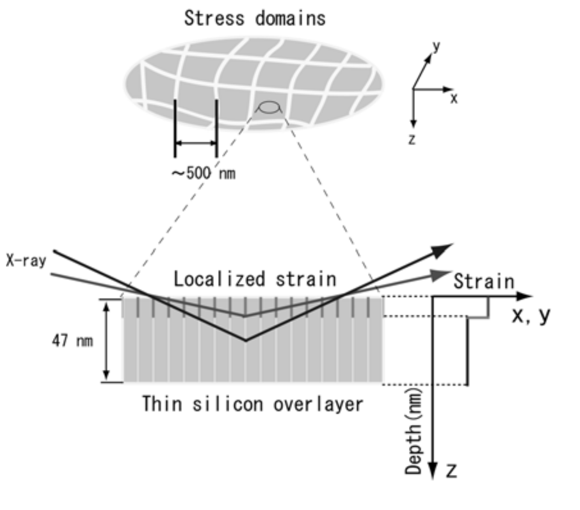


Figure 3: Schematic model of strain distribution in the 47-nm-thick silicon overlayers.

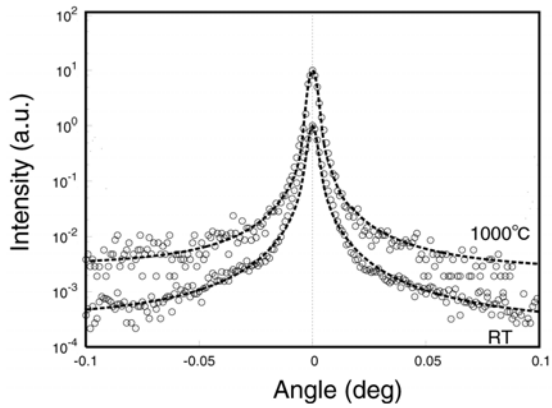


Figure 4: Si(220) Bragg diffraction curves obtained from the 47-nm-thick SOL in SIMOX wafer at different temperatures. The broken lines are the kinematical calculations.

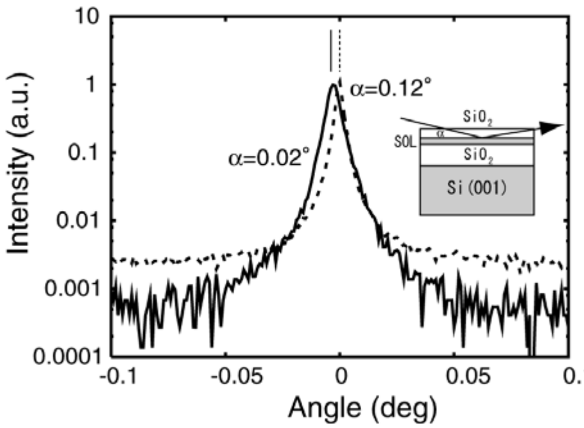


Figure 5: Si(220) Bragg diffraction curves from the $SiO_2$(30-nm-thick)/Si(5-nm-thick)/$SiO_2$(125-nm-thick)/Si substrate at different incident angles. The dotted and solid lines are obtained for $\alpha$ =0.02° and $\alpha$ =0.12° . Inset shows the schematic diagram of GIXD from the ultrathin silicon overlayer.