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UV Raman study of cleavage effects on stress distribution in Si STI structure

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1. Introduction

Stress control in Si transistors is one of the key issues to improve device performance since the stress in the device areas strongly affects the electronic properties. Therefore it is important to measure the local stress distribution in Si device structures. Raman spectroscopy is a powerful technique to measure the local stress in Si [1-6]. To estimate the stress in the channel region under the gate electrode, however, we should make measurements on cleaved cross sections of device structures. Thus, it is important to estimate how the local stress of device structure is altered by the cleavage.

In this work, we have studied the cleavage effects using Raman spectroscopy measurements and finite element method (FEM) simulations.

2. Experimental

The sample STI structure used in the present work is illustrated in Fig.1. Polarized Raman measurements were performed using an UV confocal Raman microscope (Nanofinder 30, Tokyo Instruments) equipped with an Olympus 1.3 numerical aperture (×100) oil immersion micro-objective lens with *xx* (both the polarization directions of excitation and detection light are *x*) and *xy* configurations (the polarization direction of excitation light is *x*, that of the detection light is *y*). The excitation wavelength was 364 nm. The diameter of the probed area is about 130 nm. The peak positions of the measured spectra were determined by Lorentz curve fittings.

3. Results and Discussion

The spatial variation of the Raman spectra was measured along the AA' line at the trench bottom on the (001) surface with the *xx* polarization configuration. The point A' is at the edge of the cleaved surface (Fig.1). In Fig.2, the stress induced Raman shift, $\Delta\omega=\omega-\omega_0$ (ω_0 =520.5cm^{-1}, the Raman shift of unstressed Si), is plotted as a function of the probe position. As seen, the stress induced Raman shifts change from negative to positive values near the edge, which means the tensile stress becomes compressive stress near the edge.

We made FEM simulations to calculate the stress distribution at the trench bottom. In the simulations, the STI structure is supposed to be stress-free at 1000ºC, and is cooled to 25ºC, where the stress arises due to the thermal expansion mismatch between Si and SiO_2. The elastic constants used in the simulation were taken from Refs.1 and 4. The variation of the calculated stress tensors, σ_{xx}, σ_{yy}, and σ_{zz}, along the line AA' are shown in Fig.3. The simulation result shows that an abrupt change from tensile to compressive stresses occurs near the surface, which is caused by bending of the upper part of the cleaved surface toward the front (Fig.4). We also calculate the Raman shift using the simulated stress values by solving the secular equation in Ref.3. As seen in Fig.2, the result is consistent with the measured Raman shift data.

Next, we measured the spatial variation of the Raman shift along the BB' line on the (1-10) cross section, with the *xx* and *xy* polarization configurations. We observed that the Raman shift for the *xy* configuration is larger than that for the *xx* configuration. Figure 5 shows the ratio of the stress induced Raman shift with the *xy* configuration to that with the *xx* configuration, $\Delta\omega_{xy}/\Delta\omega_{xx}$, plotted as a function of the probe position. As seen, the ratio near the top of the Si stripe is about 1.25, while it is about 2.0 under the stripe bottom.

Using the calculation with the elastic constants and the phonon deformation potentials of Si, $\Delta\omega_{xy}/\Delta\omega_{xx}$ is estimated to be 1.25 under the uniaxial [110] stress, and to be 2.0 under the uniaxial [001] stress [6]. This means that the uniaxial [110] stress at the top of the Si stripe of the STI sample turns into the uniaxial [001] stress below the Si stripe bottom. We calculate the σ_{xx} and σ_{yy} from the measured Raman shifts, $\Delta\omega_{xy}$ and $\Delta\omega_{xx}$, assuming that the other stress components such as shear components are negligibly small on the line BB'. The result is shown in Fig.6. The compressive [110] stress decreases as the probing point moving down from B to B', while the compressive [001] stress increases below the Si stripe bottom.

The spatial variation of σ_{xx}, σ_{yy}, and σ_{zz} along the line BB' calculated with the FEM simulation is shown in Fig.7(a), and that along the line CC' is also shown in (b), where the line CC' is 4 μm inside from the surface (Fig.1). On the surface, σ_{yy} is compressive and is consistent with the measurement. Inside the sample, however, σ_{yy} is calculated to be tensile as seen in Fig.7 (b). Thus, the observed compressive [001] stress is caused by the cleavage effect: bending of the upper part of the cleaved surface toward the front.

4. Conclusions

We have investigated the cleavage effects on local stress distribution of the Si STI structure using the high spatial resolution confocal Raman spectroscopy and the FEM simulations. We observed that the change in stress distribution and even in direction occurred near the cross section. We confirmed by the FEM simulations that this is due to the cleavage effects.

Acknowledgements

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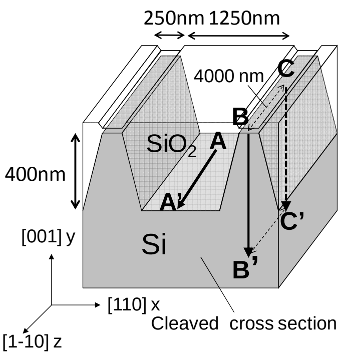

Fig.1 The schematic illustration of the Si STI structure used in the present work.

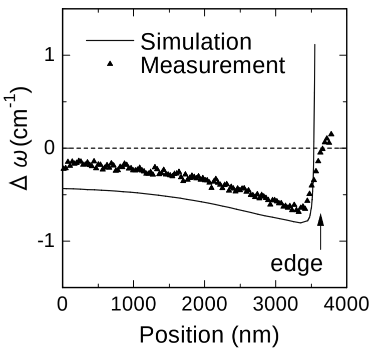

Fig.2 The spatial variation of the stress induced Raman shift along the line AA' (▲), and that of the simulation result (solid line).

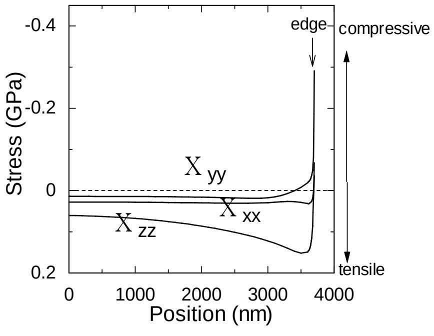

Fig.3 The spatial variation of σ_{xx}, σ_{yy}, and σ_{zz} along the line AA' calculated with the FEM simulation.

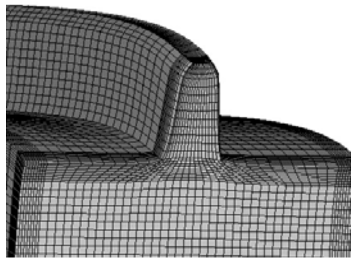

Fig.4 The STI structure after cooling down calculated with the FEM simulation. The displacement of the mesh points in the Si is exaggerated. The meshes in the SiO_2 are omitted in the figure.

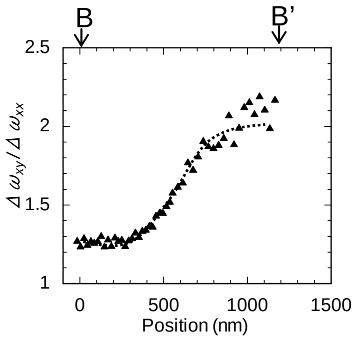

Fig.5 The ratio of the stress induced Raman shift with the *xy* configuration to that with the *xx* configuration along the line BB' on the cross section.

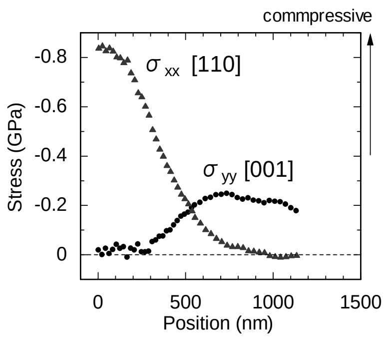

Fig.6 σ_{xx} and σ_{yy} from the measured Raman shifts, $\Delta\omega_{xy}$ and $\Delta\omega_{xx}$ along the line BB'.

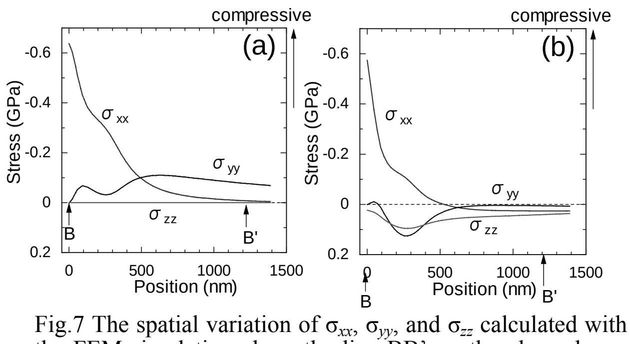

Fig.7 The spatial variation of σ_{xx}, σ_{yy}, and σ_{zz} calculated with the FEM simulation along the line BB' on the cleaved surface (a) and the line CC'4μm inside Si stripe from the surface (b).