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Strain Evaluation at the Si/SiO_2 Interface Using ER Method

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A surface strain measurement technique for the Si/SiO_2 interface called "Electro-reflectance"(ER) method is proposed. The ER method is demonstrated to be more powerful than any other conventional methods, such as Raman scattering measurement. The surface strain is theoretically evaluated from a pseudopotential band structure calculation including spin-orbit interaction.

1 INTRODUCTION

It has been well recognized that during thermal oxidation of silicon, a strain generates at the Si/SiO_2 interface due to the expansion in the volume of SiO_2. The strain significantly is considered to affect long term device degradation as well as fabrication yield of MOS LSIs as the size is miniaturized. Therefore, the need of a technique measuring the surface strain has increased in recent years. This paper demonstrates that the "Electro-reflectance"(ER) method is a very powerful technique to measure the surface strain, which decays within only several hundred angstroms from the Si/SiO_2 interface, compared with other conventional methods such as Raman scattering measurement. In the photon energy range used in this study, the effective penetration depth of probe light is only 40Å~300Å [1] which is suitable for the surface strain measurement. The ER method [2] uses the modulation electric field to change the dielectric properties at the surface region and investigates optical transitions at critical-points in electronic band structure. The strain is evaluated through the energy shifts of optical transitions because lattice distortion due to a strain changes energy band structures of silicon. The energy shift of peaks due to strain is evaluated from the pseudopotential calculation including spin-orbit interaction [3].

2 EXPERIMENT

We used 670μm-thick p-type(100)silicon wafers subjected to different annealing processes after growing 100Å of SiO_2 at 800°C in dry O_2/HCl atmosphere. RTN (Rapid Thermal Nitridation) and RTO (Rapid Thermal Oxidation) were also carried out for annealing processes in our experiments. RTN and RTO processes, thermal annealing in NH_3 and dry oxygen atmospheres for short time, provide high integrity SiO_2 layer and also relax the Si/SiO_2 interface strain. After the thermal processes, the samples were cut into small rectangular chips of 1.0×1.0-cm size and the backside oxides of the chips were etched off in HF-acid solution. A semitransparent gold film (~200Å) is deposited on the front oxide by vacuum evaporating technique. The modulation voltage is applied to the front semitransparent electrode.

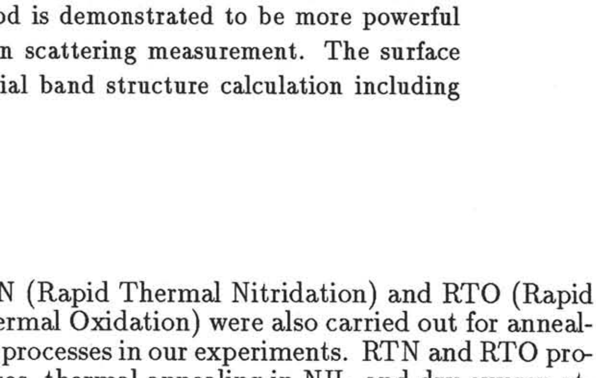

Fig. 1 Block diagram for electro-reflectance measurement

Figure 1 shows a block diagram of the measurement set-up used in this study. In the experiment, we used a 500 W Xe arc lamp for a light source and a 50 cm single monochromator with a 1200 lines/mm grating blazed at 300nm. The monochromatic light through the monochromator was focused on the sample. The surface potential at the reflecting surface was modulated by a 322 Hz square-wave ac voltage with dc offset applied to the semitransparent electrode. The maximum applied voltage was kept lower than 5 V to avoid the oxide breakdown. The reflected light from the sample with a low incident angle was focussed onto the photomultiplier tube (PMT). The signals from the PMT are amplified by a lock-in-amplifier tuned to the modulation frequency. An electric servo mechanism on the high-voltage power supply of the PMT (divided power supply) is used to maintain a constant DC voltage across the load resistance of the PMT, allowing us to obtain the ratio $\Delta R/R$ directly. The digitized data are recorded by a personal computer. All the experiments were carried out at the room temperature.

3 RESULTS and DISCUSSION

Fig. 2 shows the measured ER spectra for the samples subjected to different annealing processes after the oxidation and for a reference bare silicon (sample(a)) wafer. Except for the reference silicon shown on the top of Fig. 2, the process conditions for the samples used are described as follows: silicon wafers were thermally annealed in NH_3 followed by dry oxygen atmospheres at different temperatures, 900°C 1 min.(sample(c)), 1000°C 1 min.(sample(d)), 1200°C 1 min.(sample(e)), after the oxidation.

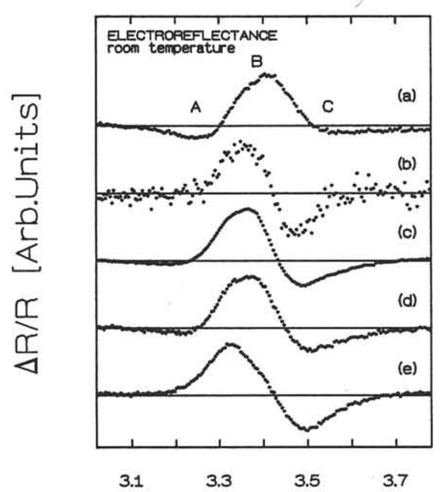

Fig. 2 Experimental electro-reflectance spectra at room temperature. The samples from the top: bare Si(a), oxidized Si(b) at 800°C, in O_2/HCl atmosphere, wafers annealed by RTN and then RTO each at 900°C,1min.(c), 1000°C,1min.(d), 1200°C,1min.(e) after the same oxidation. The oxide thickness is 100Å.

The disappearance of low energy peak A , the growth of high energy side dip C after the oxidation and the shifting of main peak B are caused by the interface strain due to expansion in the volume of SiO_2 film during thermal oxidation: biaxial tensile strain generates along the Si/SiO_2 interface, while compressive strain in the direction of the oxide growth. The strain generated during thermal oxidation is referred as intrinsic strain. Fig. 3 shows the main ER peak energies for the samples shown as peak B in Fig. 2. The peak energy of ER spectra originates from optical transitions along the < 111 > equivalent directions in the Brillouin zone as shown in Fig. 4 by solid arrow. Large red shift of the peak for the samples(b) and (e) were thought to be caused by remain-

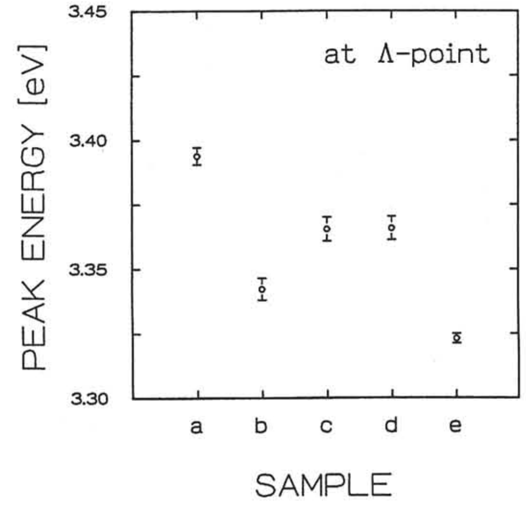

Fig. 3 Peak energy shifts of the samples(peak B) caused by the surface strain during oxidation except for sample(e).

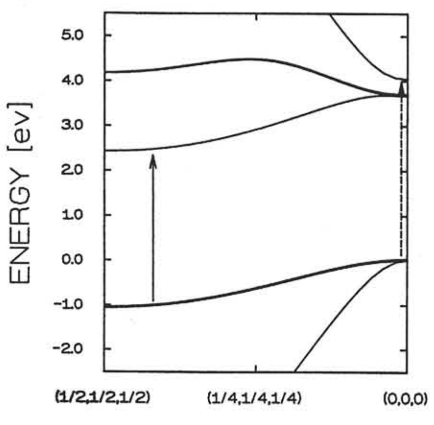

Fig. 4 Band structure of Si calculated by pseudopotential including the spin-orbit interaction. The optical transition observed in this experiment shown by solid and dashed arrows.

ing large surface strain. Smaller red shift of the peak for sample(c) and sample(d) was explained by the relaxation of intrinsic interface strain after annealed at 900°C and 1000°C because the intrinsic surface strain relaxes quite rapidly at high temperature annealing: The relaxation time at 1000°C is reported to be only 12 min.[4]. Relaxation characteristics of thermal oxide allow us to expect that the surface strain decreases with increasing annealing temperature. This is not the case for the sample annealed at 1200°C which exhibits large surface strain. The large surface strain originates from the formation of oxi-nitride layer during high temperature annealing in NH_3 gas.

In order to evaluate the surface strain near the Si/SiO_2 interface, we calculated electronic band structure by using the pseudopotential method by taking into account of the spin-orbit interaction under the biaxial strain condition. The ratio of the strains along the x, y and z directions used in this study are 1, 1 and −0.772, respectively where xy plane is the plane along the Si/SiO_2 interface, and z axis is the direction of oxide growth. Fig. 5 shows the optical transition energy as a function of surface strain. The calculated transition energy linearly decreases with the strain at the interface. Comparison between the experimental(Fig. 3) and the calculated results(Fig. 5) allows us to evaluate the surface strain along the plane of the interface as follows: 0.22 % for sample(b), 0.13 % for sample(c), 0.13 % for sample(d), 0.29 % for sample(e), for which the stresses of the plane direction are calculated to be 3.3, 1.9, 1.9, 4.3×10^9dym/cm^2, respectively, by using the stress-strain relation[5]. Comparing the stresses obtained in our experiment with another paper's[6], our values are slightly smaller because of the difference in the thickness of Si substrate.

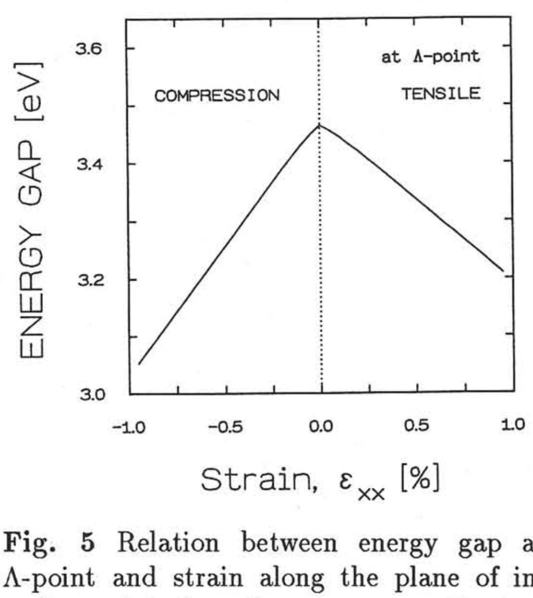

Fig. 5 Relation between energy gap at Λ-point and strain along the plane of interface. (−) sign of strain means the tensile strain while (+) means the compressive strain.

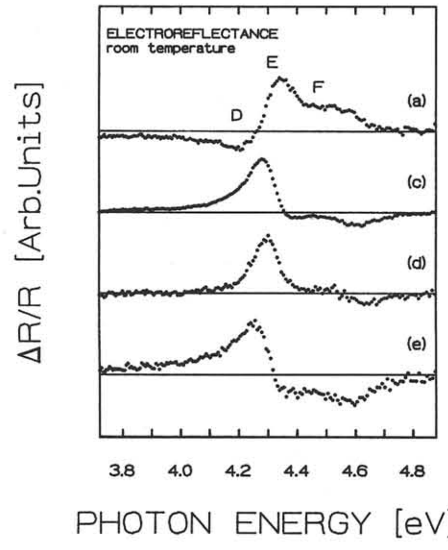

Fig. 6 Experimental electro-reflectance spectra at room temperature in the high photon energy range for the samples(a), (c), (d)and(e).

The existence of surface strain is further confirmed by investigating the optical transitions to the upper band at Γ-point existing in the photon energy range of 3.7 ∼ 4.9 eV as shown in Fig. 6. The relaxation of surface strain can be explained from the spectral shape: the disappearance of low energy dip D, the decrease of high energy peak F and also the red shift of peak E allow us to evaluate the strain.

4 CONCLUSIONS

By using electro-reflectance method, we investigated the surface strain at the Si/SiO_2 interface for samples annealed in different ambients. Taking into account the attractive features described above, ER method has been found to be a simple and powerful method to evaluate the surface strain within several hundred angstroms from the Si/SiO_2 interface.

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