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Stresses Relaxation Mechanism in the Si-SiO_2 System and its Influence on the Interface Properties

Daniel Kropman [α], Tõnu Laas [σ], Viktor Seeman [ρ] & Artur Medvids [ω]

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I. Introduction

It is known that internal mechanical stresses due to the differences in the thermal expansion coefficient between films and substrates and lattices mismatch appear in the Si-SiO_2 system during the process of its formation and that point defects generation and redistribution reduce partially the surface strain. However, no investigation of this process on the atomic scale has been carried out so far. The purpose of the present work is to investigate the strain relaxation mechanism in the Si-SiO_2 system by means of EPR, IR absorption spectroscopy, scanning electron microscopy (SEM) and samples bending measurements.

II. Experimental

Si n-type with 15 Ω·cm resistivity and (111) orientation was used. The oxides were thermally grown in dry oxygen at 1100-1200 °C. The SiO_2 film thickness varied from 0.2 μm to about 0,5 μm. The density of point defects was varied by varying the cooling rate of the samples (3 of 25 °C/s). The EPR spectra were taken at 115 K by an X-band ESR 231 spectrometer. To evaluate the influence of the defects structure on the stresses in SiO_2, the measurements of SiO_2 IR absorption spectra were carried out. The strain in the Si-SiO_2 system were investigated by means of SEM and samples bending measurements. Laser irradiation (λ=520nm, 10mW/cm^2) were performed after oxidation.

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III. Results and Discussion

It has been found that samples bending increases or decreases simultaneously with EPR signal intensity depending on the oxidation temperature, oxidation time and cooling rate.(Fig.1) It may be due to the relaxation of stresses by the strain accompanied by the point defects gettering and by creation of point defects by the stresses. It has been found that in case of a lower oxidation temperature (1100^{0}C) the deflection of the samples decreases with an increase of the EPR signal intensity (E`centres in SiO_2 and vacancy complexes in Si) while at a higher oxidation temperature (1200^{0}C) the deflection of the samples and EPR signal intensity increase simultaneously[1,2]. The revealed differences in the strain dependence on the point defects density (type) at different oxidation temperature allow to suggest that relaxation mechanism of the internal mechanical stresses (IMS) is different. During oxidation at 1100^{0}C oxygen diffuses through the oxide to the interface where oxidation happens which is associated with a volume expansion. Part of the volume is released by injection of Si self-interstitials into the Si. At 1200^{0}C diffusion of Si from the interface into the oxide occurs and the oxidation reaction happens in the oxide. This process is associated with vacancy injection into the Si. The decrease of the deflection with an increase of the vacancies type point defects EPR signal intensity indicates that self-interstitial Si atoms injection are responsible for the stresses in the samples oxidized at 1100^{0}C. This oxidation kinetics model is in agreement with point defects generation kinetics in the Si-SiO_2 system proposed in [3] and confirmed experimentally [4]. It has been suggested that the incorporation of the ionic charge into the oxide cause repulsive forces expanding the silicon wafer [5]. This allows one to explain this simultaneous increase of the E` centers EPR signal intensity and deflection in samples oxidized at 1200$^0$C. E`centers cause repulsive forces expanding the Si wafer and giving rise for the deflection in Si-SiO_2 structure.

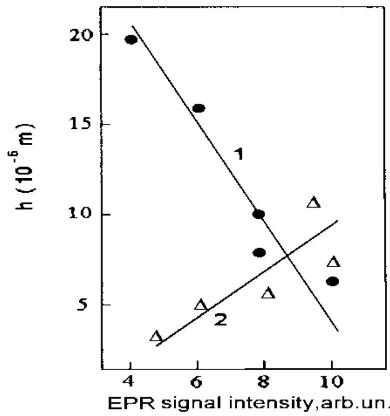

Fig. 1: Relation between the deflection of samples and EPR signal of Pa centers for the samples oxidized at 1100 (1) and 1200^{o}C (2)

At an appropriate choose of the oxidation temperature tensile stresses in Si and compressive stresses in SiO$_2$ can be equal and canceled out.To find thise temperature oxidation at 1120,1130 and 1140^0 C were performed. With an increase of the oxidation temperature the thickness of the oxide layer decreases.This can be explained by the increase of tensile stresses in Si and decrease of compressive stresses in SiO$_2$. Absent of defects on crossection of samples prepared at oxidation temperature 1130^{0}C (Fig.4) confirm this assumption.

To evaluate the strain dependence on the SiO$_2$ film thickness the EPR signal and IR absorbtion at 1100 cm^{-1} line-width were measured (2). EPR signal dependence on the oxidation time reveal one or two maximum depending on the cooling rate. In fast-cooled samples there exist a interdependence between EPR signal and IR absorption line-width at 1100cm^{-1}($\Delta\nu$). In slowly cooled samples the increase of the EPR signal is accompanied by the decrease of $\Delta\nu$ that indicated stress dependence on SiO$_2$ film thickness.In samples with SiO$_2$ thicness >0.4 μm point defects density decreasing in Si is accompanied by $\Delta\nu$ increase.This may be explained by O inclussion formation in Si.In samples with SiO$_2$ film thickness ~ 0,2 and ~ 0,4 μm absent of cooling rate influence on point defects density and $\Delta\nu$ allow to suggest IMS absent.

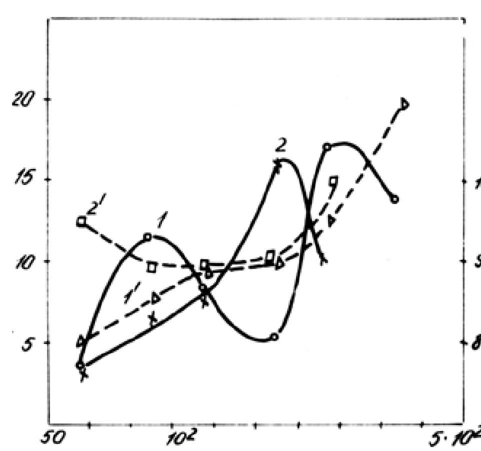

Fig. 2: Dependence of the EPR signal (1, 2) and the line-width of SiO$_2$ IR absorption at 1100 cm-1 (1', 2') on the oxidation time, cooling rate 25 (1, 1') and 3^{o}Cs (2, 2')

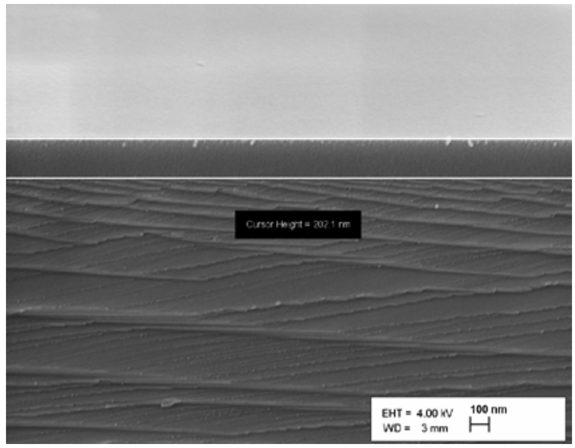

Fig. 3: Si-SiO2 cross-section micrograph, oxidation temperature 1120oC.

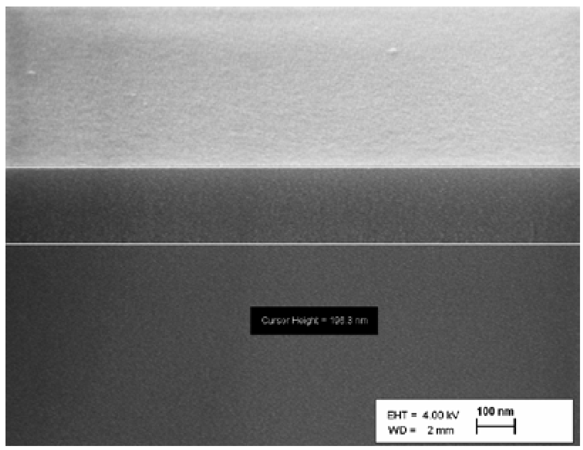

Fig.4: Si-SiO$_2$ cross-section micrograph, oxidation temperature 1130°C

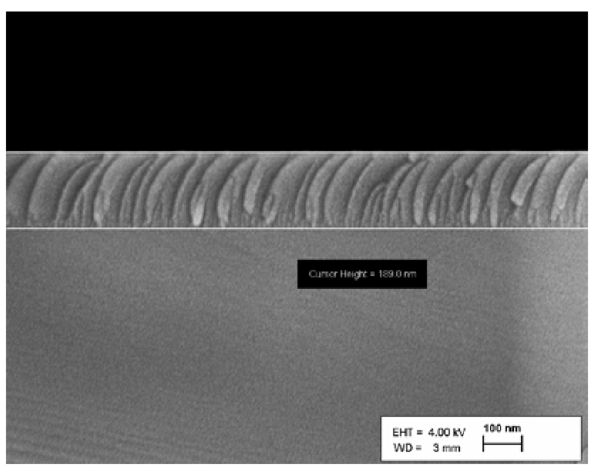

Fig. 5: Si-SiO$_2$ cross-section micrograph, oxidation temperature 1140°C

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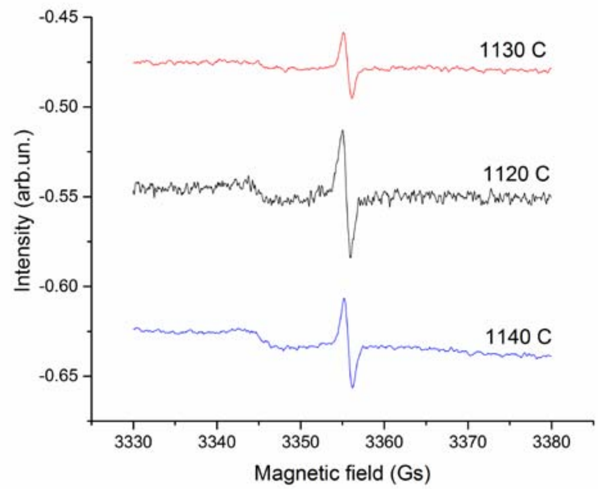

Fig. 6: EPR spectra of Si(n)-SiO_2 sample obtained at different oxidation temperatures

In Fig.6 EPR spectra of samples obtained at different oxidation temperature is shown.

It can be seen, that in n-type silicon samples obtained at 1130^0 C both centers (vacancies complexes and unsaturated bonds) EPR signal intensity is lower than in samples obtained at 1120 and 1140^0C. This confirm lower IMS at these oxidation temperature.

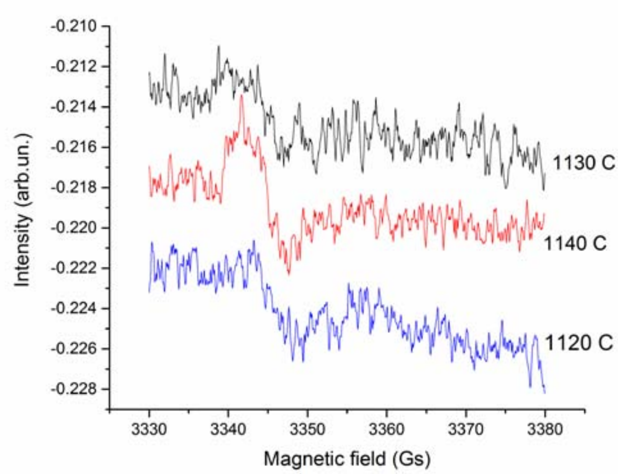

Fig. 7: EPR spectra of Si(p)-SiO_2 sample obtained at different oxidation temperatures

It can be seen that the oxidation temperature influence on generation of defects in p-type samples is lower than in case of n-type Si samples. The influence of oxidation temperature on vacancies is absent,and the influence on unsaturated bonds is the same as for n-type Si samples. Differences between n-type and p-type Si can be due to the different stresses in n- and p-type Si samples.Different deflection in Si(p)-SiO_2 and Si(n)-SiO_2 confirm thise assumption.

IV. Conclusion

The obtained results confirm that there exists an interdependence between the stresses created in the Si-SiO_2 structure and point defects in Si and SiO_2. It has been shown that at oxidation temperature 1130^0C performed Si-SiO_2 structures IMS canceled out. It has been established that the dependence of the EPR signal intensity from vacancy type defects on the oxidation time is non-monotonous and is accompanied by a non-monotonous change of the IMS. In samples with SiO_2 film thickness 0.2-0.4 μm IMS at the Si-SiO_2 interface dissapear. It was observed that dependence of EPR signal of Si(n)-SiO_2 and Si(p)-SiO_2 samples obtained at different oxidation temperatures was different. It can be concluded that this is related to different mechanical stresses in the n-type and p-type Si-SiO_2 samples.

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