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Strain relaxation mechanism in the Si-SiO_2 system and its influence on the interface properties

D. Kropman [a,*], E. Mellikov [a], A. Öpik [a], K. Lott [a], O. Volobueva [a], T. Kärner [b], I. Heinmaa [c], T. Laas [d], A. Medvid [e]

[a] Tallinn University of Technology, 5 Ehitajate tee, 12618 Mustamae, Tallinn, Estonia
[b] Tartu University, Estonia
[c] Institute of Chemical Physics and Biophysics, Estonia
[d] Tallinn University, Estonia
[e] Riga Technical University, Latvia

A B S T R A C T

The results of the investigation of stresses relaxation by strain by means of EPR spectra, IR absorption spectra, SEM and samples deflection are presented. It has been shown that stresses relaxation mechanism depended on the oxidation condition: temperature, cooling rate, oxide thickness. In the Si-SiO_2-Si_3N_4 system the stresses relaxation by the strain occur due to the opposite sign of the thermal expansion coefficient of SiO_2 and Si_3N_4 on Si. Laser irradiation allows to modify the system stresses.

1. 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.

2. 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 ($\lambda = 520$ nm, 10 MW/cm^2) were performed after oxidation before Al evaporation.

3. 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 [1]. It has been found that in case of a lower oxidation temperature (1100 °C) the deflection of the samples decreases with an increase of the P_a centers EPR signal intensity (E′ centers in SiO_2 and vacancy complexes in Si) while at a higher oxidation temperature (1200 °C) the deflection of the samples and EPR signal intensity increase simultaneously [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 °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 °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

* Corresponding author.
E-mail address: daniel.kropman@mail.ee (D. Kropman).

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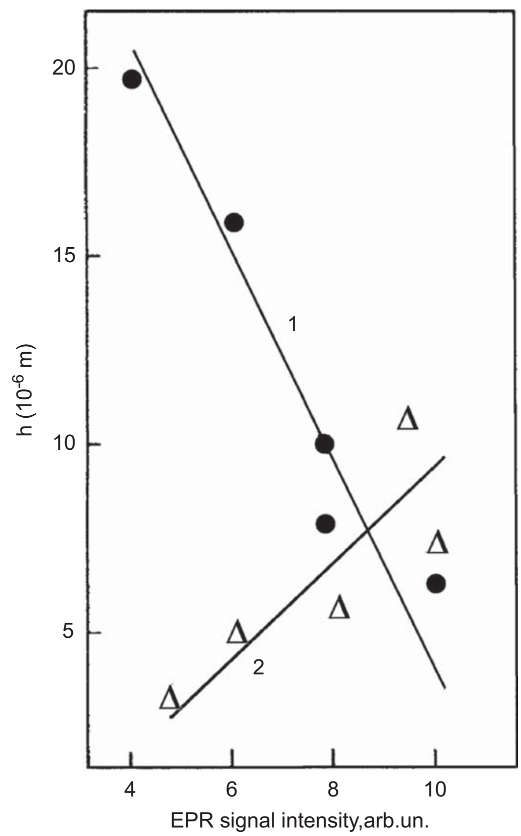

Fig. 1. Relation between the deflection of samples and EPR signal of P_a centers for the samples oxidized at 1100 °C (1) and 1200 °C (2).

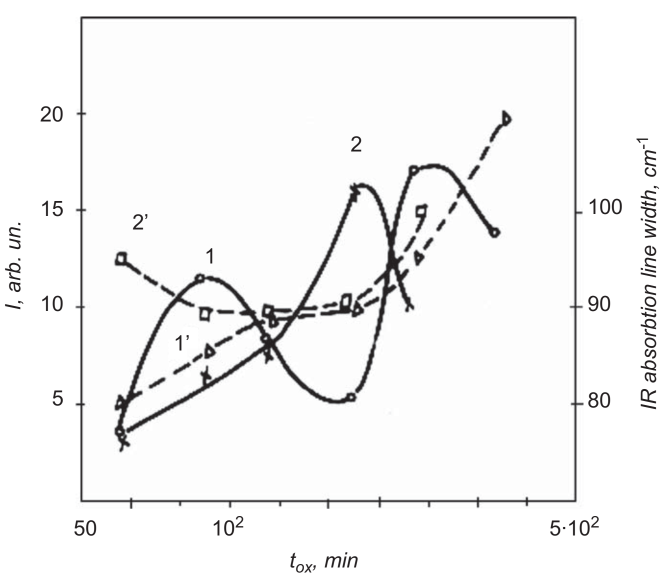

Fig. 2. Dependence of the EPR signal (1, 2) and the line-width of SiO_2 IR absorption at 1100 cm^{-1} (1′, 2′) on the oxidation time, cooling rate 25 (1, 1′) and 3 °C/s (2, 2′).

responsible for the stresses in the samples oxidized at 1100 °C. This oxidation kinetics model is in agreement with point defects generation kinetics in the Si-SiO_2 system proposed in Ref. [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 °C. E′ centers cause repulsive forces expanding the Si wafer and giving rise for the deflection in Si-SiO_2 structure. EPR signal dependence on the oxidation time reveal one or two maximum depending on the cooling rate (Fig. 2). In fast-cooled samples there exist an interdependence between EPR signal and IR absorption line-width at 1100 cm^{-1} (Fig. 2). In slowly cooled samples the decrease of the EPR signal and increase of the IR absorption line-width occur simultaneously. After Si_3N_4 deposition samples bending change sign and instead the tensile stresses, compressive stresses appear at the interface. This can occur due to diminishing of the internal mechanical stresses as a result of the opposite sign of thermal expansion coefficient of SiO_2 and Si_3N_4 on Si. To check this assumption, the Si-SiO_2 and Si-SiO_2-Si_3N_4 structures cross-section micro-photos, obtained by high-resolution scanning electron microscopy were made (Figs. 3 and 4). It can be seen that after Si_3N_4 deposition the thickness of the SiO_2 films decreases (Figs. 3 and 4) and after subsequent laser irradiation the thickness of the SiO_2 film increases (Fig. 5). Simultaneous with oxides thickness increasing after Si-SiO_2-Si_3N_4 structures laser irradiation increases the samples bending that indicated higher compressive stress in SiO_2. It has been revealed that Si-SiO_2 structure laser irradiation is accompanied by E′ centers EPR signal diminishing.

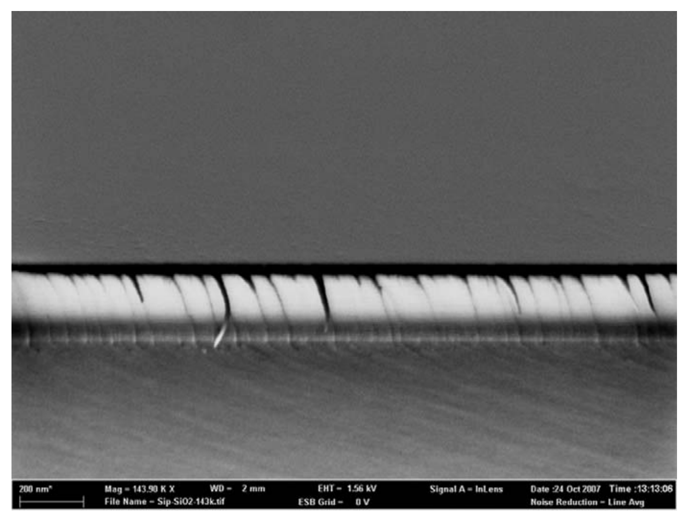

Fig. 3. Si- SiO_2 structure cross-section microphoto. SiO_2 thickness 200 nm.

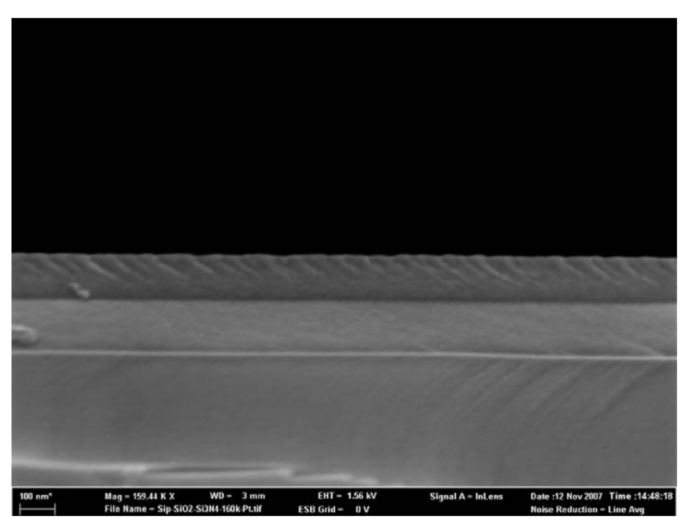

Fig. 4. Si-SiO_2-Si_3N_4 cross-section microphoto. Si_3N_4 thickness 100 nm. SiO_2 thickness diminished (150 nm).

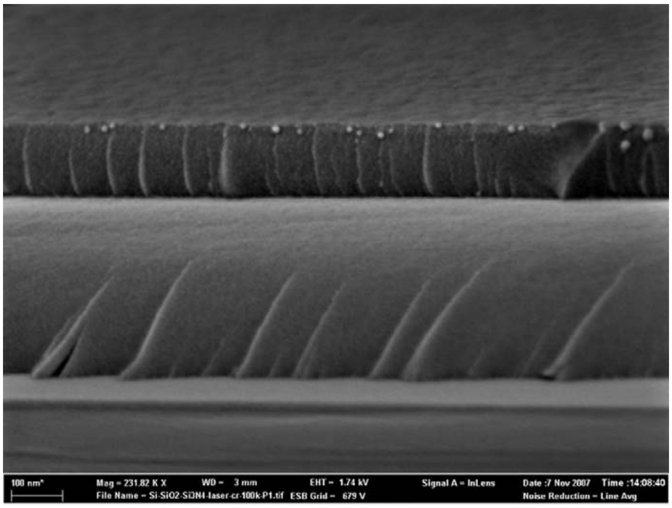

Fig. 5. $Si\text{-}SiO_2\text{-}Si_3N_4$ cross-section microphoto after laser irradiation. SiO_2 thickness 300 nm and Si_3N_4 thickness 150 nm.

4. Conclusion

The obtained results confirm that there exists an interdependence between the stresses created and relaxation in the $Si\text{-}SiO_2$ structure and the point defects in Si and SiO_2. 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 the $Si\text{-}SiO_2\text{-}Si_3N_4$ system the stress relaxation by strain occurs due to the opposite sign of the thermal expansion coefficient of SiO_2 and Si_3N_4 on Si. Laser irradiation allows to modify the stresses. Instead of the tensile stresses, compressive stresses appears in SiO_2 after laser irradiation. This is accompanied by E' centers EPR signals diminishing.

Acknowledgements

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