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Investigation of Amorphization in Si Induced by Ion Implantation

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Amorphization and structural relaxation in Si-implanted Si have been studied using slow positrons and Raman spectroscopy. The S parameter in the defect region decreases slightly with the annealing temperature. However, no significant change of S parameter was observed with 200°C and 450°C isothermal annealing. One interesting point is that S parameter holds lower value in the amorphized region, but such a behavior cannot observed by the W parameter. The change of TO peak half width in the Raman spectra (480 cm^{-1}) was found to correlate with the change of S parameter. The defect configuration is expected to alter during isothermal annealing.

1. INTRODUCTION

Ion implantation is a increasingly important technology for fabrication of doped layers in semiconductor micro-electronic devices as devices sizes are decreased. The temperature dependence of ion-beam-induced amorphization has been generally considered to be due to competition between defect accumulation in an energetic collision cascade and out-diffusion of the defects from the cascade,[1] however, the amorphization mechanism is still controversial and not yet fully understood.[2] Furthermore, the completely understanding of recovery of defects and the recrystallizations of amorphized Si by subsequent heat treatments is urgently required.

In this presentation, we have investigated the defect in amorphized Si prepared by Si self-implantation, using a slow positron beam and Raman spectroscopy.

2. EXPERIMENTAL

The substrates used in this study were optically flat 6 ~ 8 Ω·cm *p*-type Si (100) wafers. ^{30}Si ions were implanted at energies of 100 keV and 150 keV in doses from 10^{14} to 5×10^{15} ions/cm^2 at room temperature. Isothermal annealing were performed in the furnace at 200°C and 450°C under nitrogen gas flow for 150-keV Si implanted specimens with a dose of 5×10^{14} cm^{-2}. The annealing time was set from 30 min to 180 min by a increasing step of 30 min for 200°C isothermal annealing, and from 10 min to 60 min by a step of 10 min for 450°C isothermal annealing. The thickness of amorphized layers were 180 nm for 100-keV Si-implanted specimen and 200 nm for 150-keV Si-implanted specimens, as determined by Rutherford backscattering spectrometry (RBS) and by transmission electron microscopy (TEM), respectively. Structural relaxation of a-Si layer was observed by using Raman scattering spectroscopy. 488 nm Ar ion laser was used as a light source with the diameter of illumination 0.1 mm on the specimen surface and a total power of 120 mW.[3] Measurements were repeated three times for each specimens with small displacements of the laser irradiation point. The TO peak in the Raman spectra (480 cm^{-1}) was observed in the following experiments with a accuracy of ≈ 2 cm^{-1}.

The Doppler broadened spectra of annihilation radiations were measured using a slow positron beam line constructed at University of Tsukuba. The Doppler broadened spectra were characterized by the line shape S and W parameter.

3. RESULTS AND DISCUSSION

Figure 1 shows the S parameter as a function of incident positron energy, i.e., the S(E) response, for Si-implanted specimens with energy of 100 keV and doses of 1.0×10^{14} ~ 1.0×10^{15} cm^{-2}. The data are displaced upwards by 0.01 for clarity. The solid lines indicated the fitting of positron diffusion model to the experimental data. However, no significant change was observed in S(E) response within the implantation doses though the RBS results indicate the increasing of damage with the implantation dose.[4]

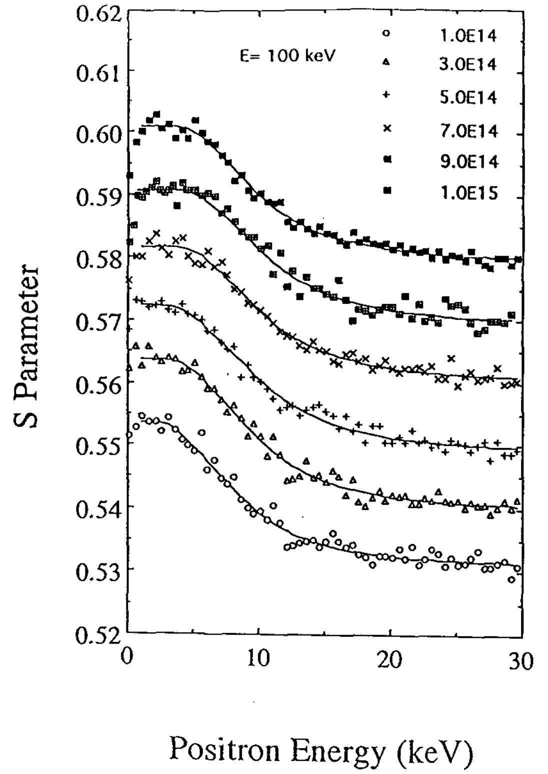

Figure 1. S(E) response for Si-implanted specimens with energy of 100 keV and doses of $1.0 \times 10^{14} \sim 1.0 \times 10^{15}$ cm^{-2}. The solid lines indicate the fitting of positron diffusion model to the experimental data. The data are displaced upwards by 0.01 for clarity.

The data have been modeled using a variation of an analysis successfully used in the previous investigation of Si.[5–7] The implantation profile P(x, E) of positrons may be described by a Makhovian profile[8]

$$P(x,E) = -\frac{d}{dx}[\exp(-\frac{x}{x_0})^m], \qquad (1)$$

$$x_0 = \bar{x}/\Gamma(1+1/m), \qquad (2)$$

where m is selected as 1.9 and $\bar{x}$ is the mean penetration depth of positrons, which is expressed as $\bar{x} = (40/\rho)E^{1.6}$. The Doppler response S(E) is found by summing the integral of P(x, E) and weighting by the characteristic S value for different depth of specimen. Thus, the energy-dependent Doppler response S(E) can be defined as

$$S(E) = S_s F_s(E) + S_d F_d(E) + S_b F_b(E), \qquad (3)$$

where S_s, S_d and S_b indicate the characteristic values of S parameter for the annihilation at surface, in the damaged region and in the defect-free substrate, respectively.

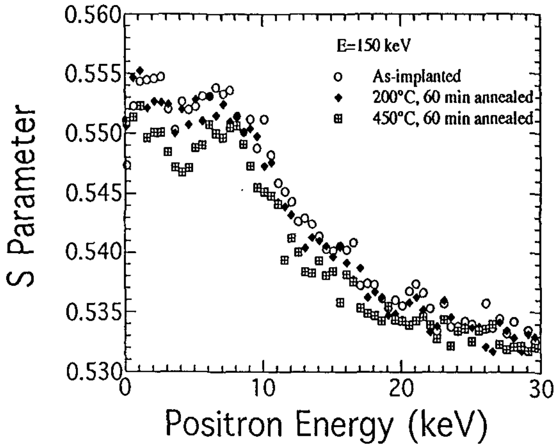

Figure 2. S(E) response for isothermally annealed specimens and for as-implanted one. Only two data for annealed specimens are included for clarity of the graph.

The values of damaged depth were estimated to be around 500 nm, larger than the thickness of amorphized region obtained by RBS measurement. Since the values of S_d/S_b, which are about 1.043, are larger than those for divacancies, the main defect species can be identified as vacancy clusters.

The 150 keV Si-implanted specimen with dose of 5×10^{15} cm^{-2} were isothermally annealed at

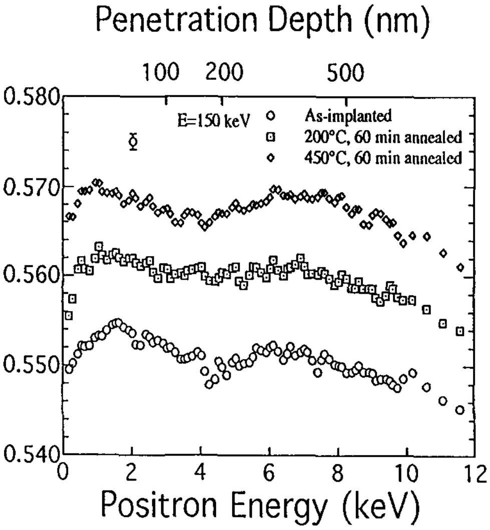

Figure 3. S(E) response for isothermally annealed specimens and for as-implanted one measured in detail. Data are displaced upwards for clarity.

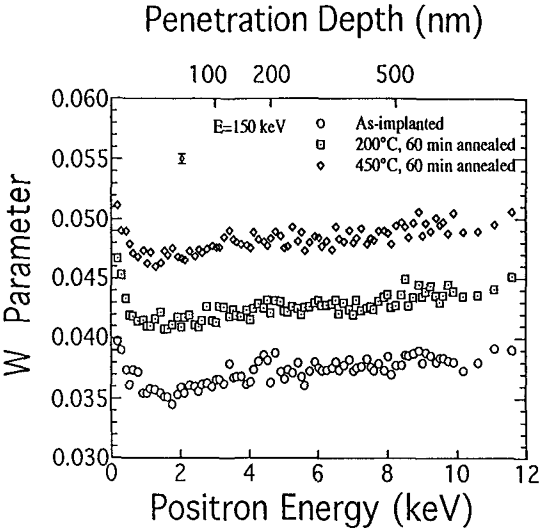

Figure 4. W parameter for isothermally annealed specimens and for as-implanted one measured in detail. Data are displaced upwards for clarity.

200°C and 450°C, respectively. The S parameters for isothermally annealed specimens are shown in Fig. 2. The S(E) for as-implanted specimen is also included. The S parameter in the damaged region decreased with the annealing time slightly, implying the recovery of defects in the damaged region. However, no further significant variation of S parameter was observed when the annealing time increased. The interest point is that the S parameter holds the lower value around 200 nm from the surface. The remeasured S(E) responses corresponding to Fig. 2 are shown in Fig. 3 in detail. Data are also upwards shifted for clarity in Fig. 3. The decreases of S parameter around 200 nm from surface within statistical deviation are also found in other post-annealed specimens. However, such a manner of S parameter could not be recognized by the W parameter as shown in Fig 4. The reason why S and W parameter show different manners remains elusive.

Figure 5 shows a typical example of Raman spectra of a-Si (formed by 150 keV, 5×10^{15} cm^{-2} Si$^+$ implantation) after furnace annealing for 360 min at 450°C. The TO peak half width decreased and the peak position shifted towards higher wavenumber after thermal treatment. At the same time the LA peak located at wavenumber 300 cm^{-1} became slightly stronger. The decrease of the TO peak half width can be attributed to the reduction of the bond angle deviation which describes the structural relaxation. Beeman *et al.*[9] proposed the following linear relationship between the TO peak full width of the half maximum Γ (cm^{-1}) and bond angle deviation $\Delta\theta$ (degree) in a-Si,

$$\Gamma/2 = 7.5 + 3\Delta\theta. \qquad (4)$$

Figure 6 show the a-Si TO peak half width $\Gamma/2$ of Si-implanted Si as a function of time of isothermal annealing at 200°C and 450°C. The bond angle deviation, $\Delta\theta$, generally decreased with annealing but detailed observation of $\Delta\theta$ shows a small increase after the initial decrease. The behavior is similar to the observation in the relaxation process of a-Si:H.[10] Make a comparison between the results of Raman spectra and the results of positron annihilation, one can find that the decrease of $\Delta\theta$ corresponds to the decrease of S parameter. The defect configuration is expected to alter during isothermal annealing. It is worthwhile to investigate the recovery and recrystallization of amorphized Si in aspect of structural

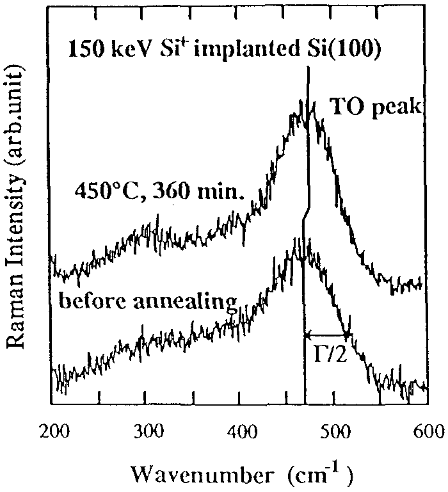

Figure 5. Typical Raman spectra from Si (100) specimens implanted with 5×10^{15} cm^{-2} Si$^+$ before and after annealing.

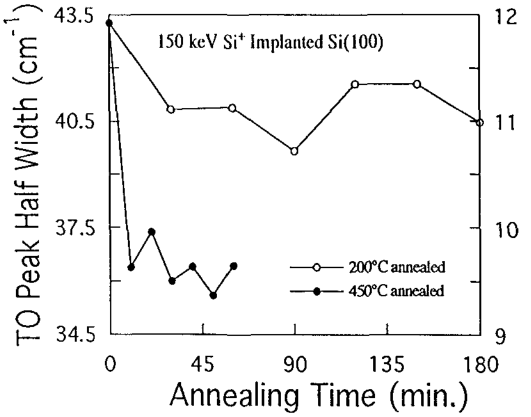

Figure 6. Changes in Γ/2 and $\Delta\theta$ during isothermal annealing at 200°C and 450° with different annealing times.

relaxation. The detailed studies, including cross-sectional TEM measurement are in progress now.

4. SUMMARY

The S parameter in the defect region decreases slightly with the annealing temperature. However, no significant change of S parameter was observed with 200°C and 450°C isothermal annealing. One interesting point is that S parameter holds lower value in the amorphized region, but such a behavior cannot observed by the W parameter. The change of TO peak half width in the Raman spectra (480 cm^{-1}) was found to correlate with the change of S parameter. The defect configuration is expected to alter during isothermal annealing.

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