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Defects in as-grown Si probed by positron annihilation

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Positron lifetime and Doppler broadening experiments were performed on Czochralski-grown Si wafers which exhibit oxidation-induced stacking faults (OSF). A monoenergetic positron beam was also used to measure the diffusion length of positrons in the wafer. From the measurements, it was found that the value of the diffusion length of positrons decreased at the region where OSF was observed. It was also found that the line shape parameter S decreased and the lifetime of positrons increased at the region of OSF. These results can be attributed to the annihilation of positrons trapped by vacancy-oxygen complexes. These defects are considered to be associated with nuclei of stacking faults.

1. INTRODUCTION

It is well known that a ring-shaped region with a high density of oxidation-induced stacking faults (R-OSF) could be observed after thermal treatments of Czochralski (Cz)-grown Si wafers [1]. The density of stacking faults inside R-OSF is higher than that outside by orders of magnitude. Shinoyama *et al.* [2] reported that a diameter of R-OSF depends on the pulling rate of Si crystals. Since the performance of gate oxides used in metal/oxide/semiconductors is known to depend on the pulling rate of Si crystals [2], the nature of R-OSF has attracted interest. Because a periphery of R-OSF is very sharp, it might be possible that some kind of fast diffusing native point defects or impurities participate to develop R-OSF [3]. The formation mechanism of R-OSF, however, has open questions.

The positron annihilation technique is now established as one of the best method for the investigation of defects in materials [4]. This technique enables us to detect defects such as monovacancies or vacancy-clusters with very high sensitivity. A positron implanted into the specimen eventually annihilates with an electron producing 511-keV γ rays. Since a positron is positively charged, it is repelled from ion cores by a Coulomb interaction. Thus, if a specimen contains vacancy-type defects, there is a finite probability of positrons being trapped in these regions. The lifetime of positrons in materials reflects the density of electrons in the places where the positron annihilates. Due to a reduced electron density in vacancy-type defects, the lifetime of positrons trapped by such defects increases. Thus, measurements of lifetime of positrons provide information of vacancy-type defects. The relationship between the lifetime of positrons and the species of defects is well established for metals and semiconductors [4, 5].

The motion of the positron-electron pair causes a Doppler shift in the energy of the annihilation photons. Since the momentum distribution of electrons in defects is different from that in the bulk, one can also detect defects through measurements of Doppler broadening profiles of the annihilation radiation. The change in the Doppler broadening spectrum is characterized by the line shape parameter S, which is the ratio of counts in the central region of the spectrum to the total count [4].

By using the positron annihilation technique, Dannefaer *et al.* [5] reported a systematic study of vacancy-type defects in Si specimens. They also reported that positrons can be trapped by interstitial oxygen clusters and the lifetime of positrons trapped by such defects is shorter than that of positrons annihilated in the bulk in Cz-Si specimens. In the present paper, we report the application of the positron annihilation technique to the study of native defects in as-grown Cz-Si wafers which exhibit R-OSF

2. EXPERIMENTAL

The specimens used in the present experiment were Cz-Si wafers vertically sliced from an ingot (p-type, 10 Ωcm). The oxygen concentration of the specimens was measured by an infrared (IR) absorption band at 1107 cm^{-1} using Fourier transform IR spectrometer. The obtained oxygen concentration was $9\sim10\times10^{17}$ atoms/cm^3. In order to measure the distribution of R-OSF, the wafer sliced from the same ingot was annealed at 1100 °C for 80 min in a stream ambient.

The positron lifetime spectra were obtained by the fast-fast system with BaF_2 scintillators attached to XP2020Q (Philips) photomultiplier tubes. The full width at half maximum (FWHM) of the time resolution curve was about 200 ps. Each lifetime spectrum contained 4×10^6 counts. The positron source was 8×10^5 Bq of $^{22}NaCl$ deposited on kapton foils. The obtained lifetime spectra were analyzed by using PATFIT88 [6].

Doppler broadening profiles of the annihilation radiation were obtained using an intrinsic Ge detector with FWHM of 1.2 keV at 512 keV γ-line of ^{106}Ru. A total of 4×10^7 counts was recorded for each spectrum. The obtained spectrum was characterized by the S parameter, where the central region of the spectrum was defined from ~510.5 keV to ~511.5 keV.

The monoenergetic positron beam line installed at the University of Tsukuba was used in order to measure the diffusion length of positrons [7]. Doppler broadening profiles of the annihilation radiation were measured by an intrinsic Ge detector as a function of incident positron energy. For a homogeneous specimen, the measured S parameter as a function of incident positron energy E, $S(E)$, is expressed as a superposition of S corresponding to the annihilation at the surface, S_s, and that in the bulk, S_b, as follows:

$$S(E)=S_S F_S(E) + S_S[1 - F_S(E)], \tag{1}$$

where $F_s(E)$ is the fraction of positrons annihilating at the surface. $F_s(E)$ is given by

$$F_S(E)=\int_0^\infty P(x,E)\exp(-x/L_d)\,dx, \tag{2}$$

where $P(x,E)$ is the implantation profile of positrons [8] and L_d is the diffusion length of positrons, respectively. L_d depends on the net escape rate of positrons from the freely diffusing state, κ_{eff}, and the diffusion constant of positrons, D_+, through the relation $L_d=(D_+/\kappa_{eff})^{1/2}$. κ_{eff} can be connected both to the annihilation rate from the free state, λ_f, and to the concentration of defects, C_d, by the relation $\kappa_{eff}=\lambda_f+\mu_d C_d$, where μ_d is the specific positron trapping rate of the defect.

3. RESULTS AND DISCUSSION

Figure 1 shows the S parameter as a function of incident positron energy for the Cz-Si specimen, where the beam position is indicated by "1" in

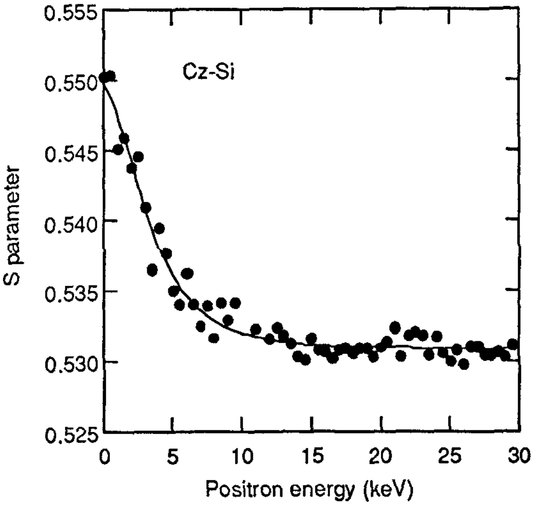
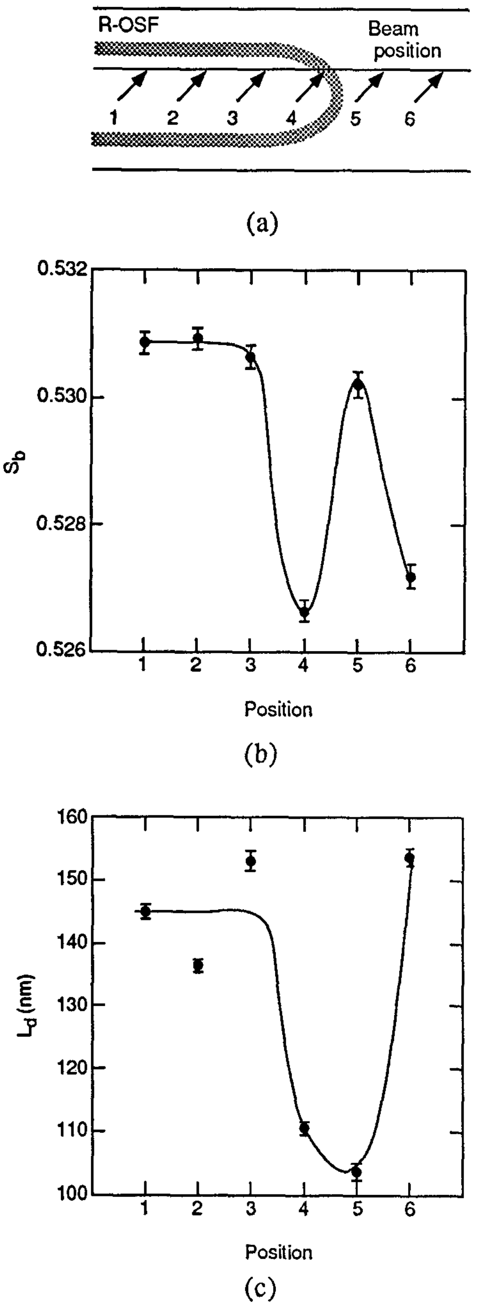


Figure 1. The line shape parameter S as a function of incident positron energy for the Cz-Si specimen.

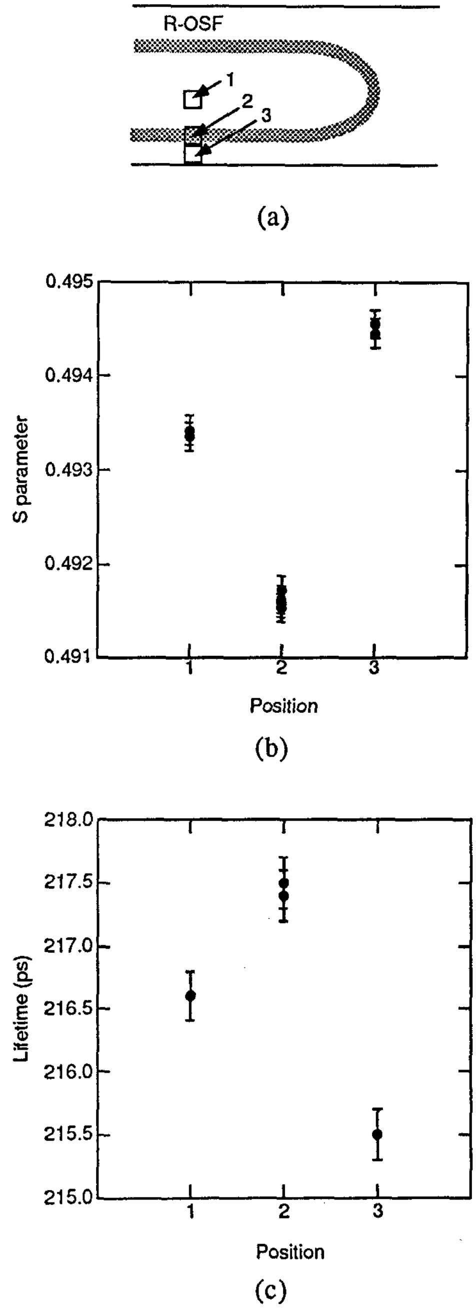


(a)

(b)

(c)

Figure 2. (a) The position of the monoenergetic positron beam in the Cz-Si wafer. The region of R-OSF is shown by a hatch. (b) The characteristic value of *S* for the positron annihilation in the bulk Si at each position. (c) the diffusion length of positrons at each position.



(a)

(b)

(c)

Figure 3. (a) The position of the specimens in the Cz-Si wafer. (b) The *S* parameter for each specimen. These values were obtained by the conventional positron annihilation experiments, (c) The lifetime of positrons for each specimen.

Fig. 2 (a). In Fig. 1, the result of the fitting to eq. (1) is shown by a solid curve. The *S*-*E* relationships at different beam positrons were also measured. The obtained values of S_b and L_d are summarized in Figs. 2 (b) and (c). From these figures, it can be seen that the value of S_b and that of L_d decreased at the region where R-OSF was observed. The observed short diffusion length of positrons means the trapping or the scattering of positrons by defects.

In order to know the annihilation characteristics of positrons at the region of R-OSF in more detail, lifetime spectra were measured for the specimens sliced from the same ingot. The position of the specimen was shown in Fig. 3 (a). From Fig. 3 (b), the value of *S* was found to decrease at the region of R-OSF (position 2). This result is in good agreement with that obtained by the monoenergetic positron beam. From Fig. 3 (c), it was found that the value of lifetime increased at the region of R-OSF.

Uedono *et al.* [9] reported that the characteristic value of *S* for a complex of a monovacancy and two oxygen atoms (VO_2) was found to be smaller than the characteristic value of *S* for the bulk, S_{Si}, while that of *S* for *VO* is larger than S_{Si}. The positrons trapped by such complexes have the probability of annihilation with electrons of oxygen atoms. Because of a broad momentum distribution of electrons of oxygen atoms, the characteristic value of *S* for vacancy-oxygen complexes is considered to decrease with increasing number of oxygen atoms coupled with vacancy-type defects. Therefore, the observed decrease of *S* and the increase of lifetime can be attributed to the annihilation of positrons trapped by vacancy-oxygen complexes.

4. CONCLUSIONS

We have presented the study of native defects in the Cz-Si wafers which exhibit R-OSF. From the results obtained by using the monoenergetic positron beam, the values of the *S* parameter and that of the diffusion length of positrons were found to decrease at the region of R-OSF. The similar behavior of *S* was also observed by the conventional positron annihilation experiments. The lifetime of positrons was found to increase at the region of R-OSF. These results suggest that the concentration of vacancy-oxygen complexes at the region of R-OSF is higher than that at inside or outside of R-OSF. Thus, these defects are considered to associate with nuclei of stacking faults. This investigation shows the potential of the positron annihilation technique for native defects in as-grown Cz-Si wafers.

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