Application of positron annihilation technique to front and backend processes for modern LSI devices

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Abstract. Developments of the semiconductor industry depend on ability to decrease the size of integrated circuits. Significant efforts to introduce new materials and their fabrication processes have been made in order to achieve such trends. However, one faces difficulties in the control of materials properties caused by atomic scale disorder. In the present paper, we used monoenergetic positrons to characterize ultra shallow junction formed on Si substrates and materials buried in LSI circuit structures. It was shown that the positron annihilation technique is a powerful characterization tool for modern Si-technology related materials.

1. Introduction
Developments of the semiconductor industry depend on the ability to decrease the size of integrated circuits [1]. This is often expressed by Moore’s Law, and this tendency has resulted in the significant improvements in cost per function, microprocessor throughput, long operating time with batteries, etc. Significant efforts to introduce new materials and their fabrication processes have been made in order to achieve such trends. However, one faces the difficulties in the control of materials properties caused by atomic scale disorder. Positron annihilation has been successfully used to detect defects in Si-technology related materials [2,3]. In the present paper, we used monoenergetic positrons to characterize ultra shallow junction formed on Si substrates [4] and materials buried in LSI circuit structures [5].

Plasma immersion ion implantation has attracted attention for fabricating ultrashallow junctions and conformal doping of the sidewall of fin field-effect transistors, where it is necessary to suppress the short-channel effect and increase the device drive current [1]. Ion bombardment, however, causes the introduction of a large number of defects into the subsurface region. Thus, knowledge about the behavior of defects during annealing processes is crucial. The signal propagation delay and resultant power consumption and crosstalk can be suppressed by integration using low dielectric permittivity (low-\(k\)) materials and Cu interconnects. The characteristics of those materials are important factors determining the circuit properties, but the patterning and metallization processes could introduce damage and degrade device performance. In the present work, we show that the monoenergetic positrons can characterize the materials buried in the circuits without beam-focusing on integrated device structures.

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2. Experiment

The samples investigated were n-type Si wafers doped with B using a B2H6/He plasma mixture up to a dose of 1×10^{15} \text{cm}^{-2} \text{cm}^{-2} [4]. After the doping, the wafers were annealed by spike rapid thermal annealing (spike RTA) at 1075 °C. The depth profiles of the B concentration were measured by secondary ion mass spectroscopy (SIMS). Before the measurements, step-by-step etching was performed.

The Cu/low-k structure was fabricated using the conventional device process [5]. Chemical vapor deposition was used to deposit 800-nm SiO2 and 250-nm SiOCH films on Si substrates. After the trench formation, the Cu damascene structure was fabricated with Cu thickness of 350 nm. The schematic view of the sample is shown in Fig. 1. The k value and density for SiOCH were 2.7 and 1.26 g/cm³, respectively. A similar pattern structure with SiO2 films was also fabricated.

3. Results and discussion

3.1. Vacancy-Boron Complexes in Plasma Immersion Ion-Implanted Si

Figure 2 shows the \( S \) values of the plasma B-implanted samples before and after RTA as a function of incident positron energy \( E \). For the annealed sample, the measurements were made after step-by-step etching (the etching depth was 4 nm). For the as-doped sample, the \( S \) value at low \( E \) was larger than that for the unimplanted sample, suggesting the trapping of positrons by vacancy-type defects. For the annealed sample, the \( S \) value in the subsurface region (0-5 keV) was smaller than the characteristic \( S \) value obtained for the defect-free Si. The solid curves are fits to the experimental data, and the derived depth distributions of the \( S \) value are shown in an inset of figure 2. For the annealed sample, the region with the small \( S \) value is similar to the region of high B concentration, suggesting that the observed decrease in the \( S \) value could correlate with doped B atoms. Figure 3 shows the \( S-E \) curves for B-implanted Si and 6H-SiC before and after annealing (conventional ion-implantation). In this figure, the \( S \) value was normalized to that for the defect-free samples. For Si, the ion energy and dose were 10 keV and 1×10^{13} \text{cm}^{-2}, respectively. For 6H-SiC, five fold implantation was used to form a box profile to a depth of 450 nm; the B concentration in the box profile was (1-2)×10^{18} \text{cm}^{-2}. The annealing was performed for 30 min at 1000°C for Si and at 1400°C for 6H-SiC. For the annealed samples, the \( S \) values in the damaged region were smaller than 1.00 except near the surface. Thus, the results shown in figures 2 and 3 are considered to be typical one for B-implanted Si and SiC. It has been suggested that the vacancy-oxygen pairs or oxygen precipitates in Si may play a certain role in the decrease in the \( S \) value [6-9]. However, the effect of oxygen in 6H-SiC on the \( S \) value is unlikely to be large because its defect-free \( S \) value is small (0.458), which is mainly due to carbon in the matrix [8].

Figure 4 shows the \( S-W \) relationships for the B-implanted samples. The \( S-W \) values obtained using the projector augmented-wave (PAW) method are also shown [4], where calculations were made for the annihilation of positrons in the delocalized state and in vacancy-type defects such as the divacancy \( (V_2) \), its complex with B atoms \( (V_{(\text{B}_n)2}) \) \((n=0, 2, 4, \text{ and } 6)\), and clusters such as icosahedral B \( (V_5B_{12}) \). The value calculated for defect-free Si is located below and to the right of the value for the undoped sample. This difference might be due to several causes such as the limitations of the first-principles calculations applied to Doppler broadening spectra. The \( S-W \) value of \( V_2B_2 \) is close to that for as-doped Si, suggests that the major defect species detected by positrons are the complexes between \( V_2 \) and B atoms. The relation between the calculated \( S-W \) values for \( V_2B_{12} \) and defect-free Si was similar to that between the values for the unimplanted and annealed samples. Thus, the decrease in the \( S \) value
for the annealed sample can be attributed to the trapping of positrons by B clusters such as B\textsubscript{12}. The presence of B\textsubscript{12} for the present sample was confirmed by measuring soft-x-ray-excited B 1\textsc{s} photoelectron spectra [4]. From the calculation, positrons were found to mainly exist outside the cluster and annihilate in the distorted Si matrix around it (figure 5). Because of the negative charges of B\textsubscript{12} [10], positrons can be weakly captured by the cluster and annihilate in the distorted matrix around the cluster. This trapping mechanism is also likely to be valid for B-implanted 6H-SiC. The results discussed above suggest the possibility of the trapping of positrons by B clusters in Si. The stress introduced by B\textsubscript{12} could attract interstitial oxygen to the clusters and drive to form boron oxides. Thus, the residual oxygen or oxygen incorporated in Si could couple with B clusters and form complexes such as boron suboxides (B\textsubscript{2}O).

**Figure 2.** (colour online) $S$–$E$ curves for plasma immersion B-implanted Si before and after spike RTA.

**Figure 3.** (colour online) $S$–$E$ curves for B-implanted Si and 6H-SiC before and after annealing.

**Figure 4.** (colour online) $S$–$W$ relationships for B-implanted Si. The values calculated by the PAW method for defect-free Si and various defects were also shown.

**Figure 5.** (colour online) Atomic configuration for V\textsubscript{2}B\textsubscript{12} (a) and the positron density distribution around the defects (b).

### 3.2. Characterization of low-$k$/Cu damascene structures

Figure 6 shows $S$ values of the samples with SiOCH and SiO\textsubscript{2} interlayers. The increase in the $S$ value at $E\approx1$ keV is due to the annihilation of positrons in SiCN. The $S$ value started to decrease with increasing $E$ because of the annihilation of positrons in SiO\textsubscript{2} and Cu. The increase in the $S$ value at $E = 2$-10 keV was due to the self-annihilation of $p$-Ps in SiOCH. The $S$ value above $E = 10$ keV was mainly attributable to the annihilation of positrons in Si ($S = 0.534$) and the valley at $E = 10$ keV was
due to the positron annihilation in Cu (0.412). Although the locations of SiOCH and Cu in the cross-sectional view are the same, their contributions to the $S$–$E$ curve appear at different energies. This is because of the difference in their densities and a resultant difference in the corresponding mean implantation depths of positrons. The $S$ values for SiOCH were smaller for the samples with the 0.54-μm pattern than those for the samples with the 2.16-μm pattern. A similar decrease in the $S$ value was also observed for the samples with a SiO$_2$ interlayer. The change in those parameters suggests suppression of the Ps formation in SiOCH and SiO$_2$, and a decrease in the pore size caused by scaling. The probability density function (PDF) of the annihilation rate was shown in figure 7. Three annihilation modes with different positron lifetimes were observed. For the SiOCH-based samples, the shortest, middle, and the long-lived components can be attributed to i) the annihilation of positrons and $p$-Ps, ii) the pick of annihilation of $o$-Ps and iii) the annihilation of $o$-Ps in pores. The mean lifetimes of $o$-Ps trapped by pores were determined to be 7.0 ns and 8.2 ns for the samples with pitch patterns of 0.54 and 2.16 μm, respectively. Using the relationship between the Ps lifetime and pore diameter [11], the mean pore diameters were estimated to be 1.1 and 1.2 nm, suggesting the shrinkage of pore sizes by the scaling. In conclusion, we have shown that the positron annihilation technique is a useful tool for determining point defect behavior in ultra-shallow junctions formed on Si substrates. It was also shown that positron annihilation parameters can be used to trace the variation of pore sizes during the Cu/low-$k$ damascene processes.

References

[1] International Technology Roadmap for Semiconductors 2009 (San Jose: Semiconductor Industry Association)
[2] Schultz P J and Lynn K G 1998 Rev. Mod. Phys. 60 701
[3] Krause-Rehberg R and Leipner H S 1999 Positron Annihilation in Semiconductors Solid-State Sciences, Vol. 127 (Springer: Berlin)
[4] Uedono A, Tsutsui K, Ishibashi S, Watanabe H, Kubota S, Nakagawa Y, Mizuno B, Hattori T and Iwai H 2010 Jpn. J. Appl. Phys. 49 051301
[5] Uedono A, Inoue N, Hayashi Y, Eguchi K, Nakamura T, Hirose Y, Yoshimaru M, Oshima N, Ohdaira T and Suzuki R 2009 Jpn. J. Appl. Phys. 48 120222
[6] Dannefaer S and Kerr D 1986 J. Appl. Phys. 60 1313
[7] Uedono A, Ujihira Y, Ikari A, Haga H and Yoda O 1993 Hyperfine Interactions 79 615
[8] Uedono A, Tanigawa S, Sugiyama J and Ogasawara M 1989 Jpn. J. Appl. Phys. 28 1293
[9] Eichler S, Gebauer J, Börner F, Polity A, Krause-Rehberg R, Wendler E, Weber B, Wesch W and Börner H 1997 Phys. Rev. B 56 1393
[10] Yamauchi J, Aoki N and Mizushima I 1997 Phys. Rev. B 55 R10245
[11] Dull T L, Frieze W E, Gidley D W, Sun J N and Yee A Y 2001 J. Phys. Chem. B 105 4657