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Radiation-Induced Defects in 4H- and 6H-SiC Epilayers Studied by Positron Annihilation and Deep-Level Transient Spectroscopy

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Abstract. Vacancy defects in high-quality 4*H* and 6*H* SiC epilayers induced by electron irradiation have been characterized using positron annihilation and deep level transient spectroscopy (DLTS). Vacancy defects were annealed in two steps below 700°C and above 1200°C irrespective to polytype. From the correlation between positron annihilation and DLTS data using the same wafers, it was confirmed that complexes including silicon vacancies are the origin of the $E_{1/2}$ levels in 6*H* SiC and the $Z_{1/2}$ level in 4*H* SiC.

Introduction

The understanding of fundamental properties of point defects in SiC is the key for device processing because the electronic characteristics of crystals are strongly altered by them. Recent studies show that particular defects detected by DLTS, such as the $E_{1/2}$ in 6*H* SiC and the $Z_{1/2}$ in 4*H* SiC are important in high temperature annealing process above 1000°C [1]. These defects exhibit so-called negative-*U* characteristics. It is proposed that these centers have a correlation with the photoluminescence D_1 centers [2]. Despite of the extensive studies, the microscopic origins of these defects are still unknown. In this study, we detected vacancy defects in 4*H* and 6*H* SiC epilayers induced by electron irradiation using positron annihilation and DLTS. From the correlation between positron annihilation and DLTS data through annealing, it was confirmed that defects responsible for the $E_{1/2}$ in 6*H* SiC and the $Z_{1/2}$ in 4*H* SiC involve silicon vacancies.

Experiment

Specimens are chemical-vapor-deposition grown *n*-type 4*H* and 6*H* SiC epilayers (5 μm thick) doped with nitrogen (N_D~$5\text{x}10^{15}$ cm^{-3}). These were irradiated with 2 MeV electrons with doses of $1\text{x}10^{15}$ and $3\text{x}10^{17}$ e^-/cm^2 for DLTS and positron annihilation measurements, respectively, at room temperature. Isochronal annealing was conducted from 100 to 1700°C for 30 minutes in vacuum or dry argon ambient. Positron annihilation (the Doppler broadening and lifetime) measurements were performed using slow positron beams (incident positron energy: E_+=0-40keV) at room temperature. After fabricating ohmic and Schottky contacts using Ni, DLTS measurements were carried out in the temperature range from 100 to 700K.

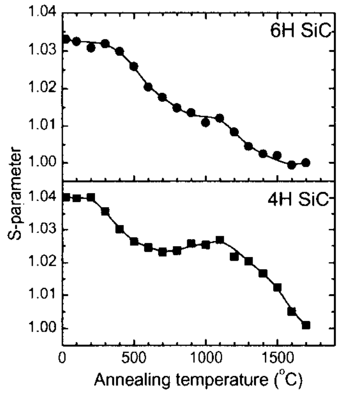


Fig. 1 Annealing behavior of S-parameters for the electron-irradiated 6H and 4H SiC specimens (dose: 3x10^{17}e$^-$/cm^2). Annealing time is 30 minutes.

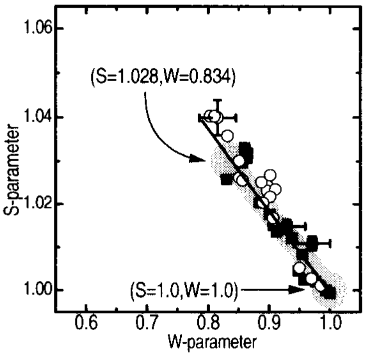


Fig. 2 S-W correlation plot from the start of annealing to the end for the 6H (■) and 4H (○) samples.

Results and Discussion

After the irradiation (dose: 3x10^{17} e$^-$/cm^2), the peak and tail intensities of the Doppler broadening spectra increased and decreased, respectively, in both 4H and 6H SiC samples. Average positron lifetime increased from 142 ps, which is in good agreement with bulk positron lifetime [3], to 190-200 ps as well. It was found that S parameter only weakly depends on incident positron energy up to 30 keV. The above results show that vacancy defects are spatially uniformly generated by electron irradiation.

Figure 1 shows the annealing behavior of the average S parameter at E_+=20-30 keV after electron irradiation. Here, S parameter is normalized to that of unirradiated sample. That is, S=1 corresponds to the unirradiated state. It is found that the S parameter decreases in two steps, i.e., until 600°C and above 1200°C in both polytypes. Thus, vacancy defects disappear in these temperature regions. Figure 2 shows the S-W plots through the course of annealing. Specific S and W parameters of fully annealed state (S=1, W=1) and silicon vacancies (S=1.028, W=0.834) [4] are also shown as gray circles. It is found that S-W data vary straightly between these states. This indicates that one type of vacancies, i.e., silicon vacancies, dominates the annealing process. The observed average positron lifetimes 190-200 ps in as-irradiated state supports that silicon vacancies are important positron trapping centers.

To obtain the further evidence that silicon vacancies are the major sources for positron trapping, we also carried out so-called coincidence Doppler broadening (CDB) measurement and analyzed core electron momentum distribution. Figure 3 shows the CDB spectra (ratio to unirradiated state) of 4H SiC after irradiation and subsequent annealing at 1000°C for 30 minutes. The horizontal axis is converted to momentum p_L instead of energy with the relation $\Delta E = cp_L/2$, where ΔE and c are the Doppler energy shift from 511 keV and light speed, respectively (ΔE=1 keV corresponds to p_L=3.91x10^{-3} m_0c). Firstly, we consider the spectrum shape itself. The observed momentum distribution $N(p_L)$is written by

$$N(p_L) = (1-f)N_B(p_L) + fN_V(p_L), \qquad (1)$$

where $N_B(p_L)$ and $N_V(p_L)$ are the momentum distributions of bulk and vacancies, respectively, and

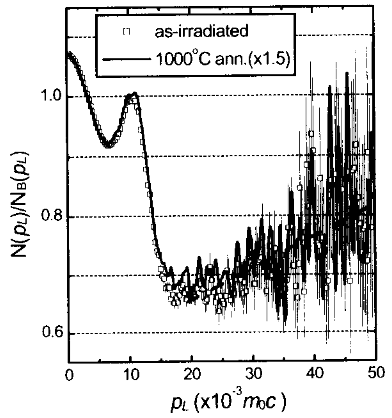


Fig. 3 CDB spectra (ratio to the unimplanted state) for the 4*H* SiC irradiated with 2 MeV electrons to a dose of 3x10^{17}e$^-$/cm^2 and subsequent annealing at 1000°C for 30 min.

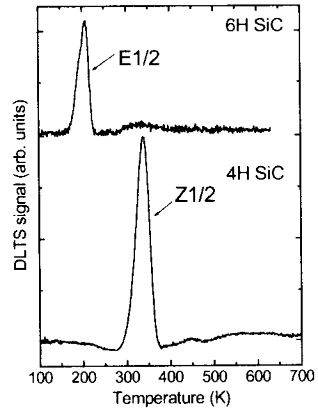


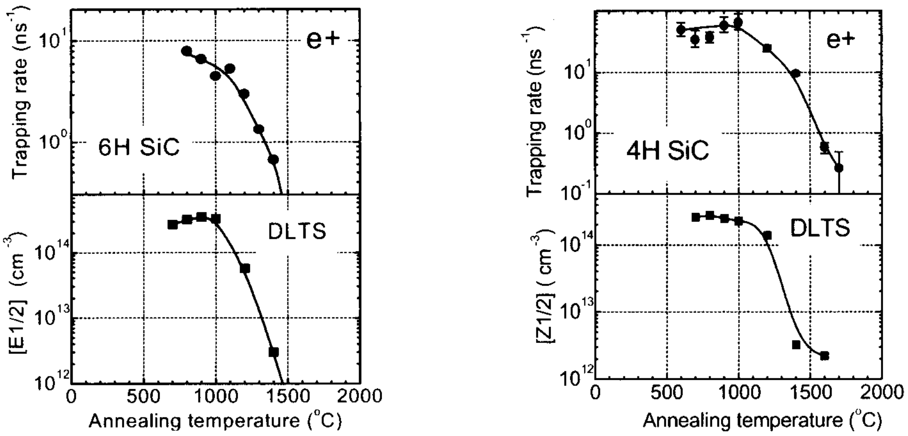
Fig. 4 DLTS spectra obtained after 2MeV electron irradiation at a dose of 1x10^{15}e$^-$/cm^2. and subsequent annealing at 1200°C. The rate windows are 8ms/16ms and 2ms/4ms for 6H and 4H specimens, respectively.

f the fraction of positron annihilation at vacancies. Thus, the ratio spectrum is given by

$$N(p_L)/N_B(p_L) = f[N_V(p_L)/N_B(p_L) - 1] + 1. \tag{2}$$

The second term of the right hand side gives just an offset. The spectrum shape is determined by the term in the bracket of the right hand side. The spectrum shape thus depends on the electron momentum distribution at vacancies. If the type of vacancies does not change due to annealing, the spectrum shape is conserved although intensity changes because of the change of the fraction *f*. As seen in Fig. 3, the shape of the spectrum is maintained before and after annealing although intensity itself becomes weaker due to annealing. This suggests that the dominant defect species does not change during annealing. This conclusion is also consistent with what expected from the *S*-*W* plot in Fig. 2. The valence electron component is important at p_L<15x10^{-3} m_0c. On the other hand, the core electron momentum component emerges at p_L>20x10^{-3} m_0c. Here, we focus on the latter. It is theoretically shown that the CDB spectrum of core electron annihilation region show different characteristics for carbon and silicon vacancies [5]. That is, the intensity of the ratio spectrum decreases and increases with increasing momentum at p_L>20x10^{-3} m_0c when carbon and silicon vacancies, respectively, are the main positron trapping centers. This is explained as the preferential annihilation of positrons with nearest neighbor silicon and carbon core electrons in carbon and silicon vacancies, respectively. The intensities of the CDB spectra in Fig. 3 apparently increase at p_L>20x10^{-3} m_0c, i.e., carbon core electron characteristics, suggesting that silicon vacancies are responsible for positron annihilation centers. Similar result was obtained for 6*H* SiC [6]. Since isolated silicon vacancies are mobile below 1000°C, the first annealing stage (<600°C) in Fig. 1 can be attributed to the disappearance of isolated silicon vacancies and the other types of vacancies. The higher annealing stage should be interpreted in terms of complexes including silicon vacancies, which have higher thermal stability than isolated silicon vacancies.

From the DLTS measurements [7], a series of deep levels are found to be introduced in the upper half of the band gap. From Fig. 4, it is seen that one major peak is observed either in 6*H*



(a) (b)

Fig. 5 Comparison between the positron trapping rate related to silicon vacancies and the concentrations of (a) $E_{1/2}$ levels in 6*H* and (b) $Z_{1/2}$ levels in 4H specimens.

SiC or 4*H* SiC due to post irradiation annealing. In the case of the 6*H* SiC, the energy level and capture cross section related to this peak are determined to be E_C-0.37±0.01 eV and ~1×10^{-15} cm^2, respectively. As well, for 4*H* SiC, these are E_C-0.69±0.01 eV and 8×10^{-16} cm^2, respectively. These levels are assigned to the $E_{1/2}$ level in 6*H* SiC and the $Z_{1/2}$ level in 4*H* SiC, which are thought to have the same atomic arrangement. Since only these levels are observed at above 1000°C, we compare the annealing behavior of these levels and vacancy defects detected by positron annihilation. The positron trapping rate which is proportional to the concentration of vacancy defects was calculated by $\kappa=\tau_B^{-1}(S-1)/(S_V-S)$, where τ_B is the positron bulk lifetime and S_V the specific S parameter for vacancy defects. Here we assumed S_V=1.028 for silicon vacancies. As shown in Figs. 5(a) and (b), the positron trapping rate of vacancy defects and the concentration of the corresponding DLTS centers decreases in the similar way during the annealing between 1000 and 1500°C. This allows us to conclude that the $E_{1/2}$ and $Z_{1/2}$ levels in 6*H* and 4*H* SiC, respectively, are related to complexes including silicon vacancies.

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