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Rapid Research Note

Positron Annihilation Due to Silicon Vacancies in 3C and 6H SiC Epitaxial Layers Induced by 1 MeV Electron Irradiation

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Positron annihilation spectroscopy is extensively used to study vacancy-type defects in semiconductors [1]. To characterize defects in SiC by this technique, it is necessary to know annihilation parameters for various kinds of vacancies, e.g., silicon and carbon vacancies, divacancies and so on. The lifetime of positrons trapped at isolated silicon vacancies in 3C SiC was determined to be ≈190 ps previously [2] from the direct comparison of annealing behavior of positron lifetime and electron spin resonance (ESR) $T1$ signal, which is related to isolated silicon vacancies [3, 4]. Although the Doppler broadening S parameter is also reported for silicon vacancies in the previous studies [5, 6], this should be further confirmed. In addition, W parameter is important when identifying vacancies by the Doppler broadening measurements [1]. We note that silicon vacancies are annealed in two stages at approximately 200 and 700 °C [3]. This fact can be used as a decisive proof in other experiments if observed signals are originating from silicon vacancies or others [2, 7]. In this work, we performed the Doppler broadening measurements for 3C and 6H SiC epitaxial layers after 1 MeV electron irradiation. We found a typical two-step recovery of isolated silicon vacancies for S parameter. Based on this result, the specific S and W parameters for isolated silicon vacancies are evaluated.

The samples used in this study were cut from chemical-vapor-deposition-grown n-type 3C and 6H SiC epilayers with a net carrier density of 5×10^{15} to 1×10^{16} cm^{-3} at room temperature. The 3C epilayer was produced at JAERI, while the 6H epilayer was purchased from Cree Research Inc. These were subjected to 1 MeV electron irradiation with a dose of 6×10^{17} e$^-$/cm^2 at 40 °C. Isochronal annealing was carried out in the temperature range from 100 to 900 °C for 5 min in vacuum. The Doppler broadening of annihilation radiation (511 keV) was measured with a positron beam at 20–30 keV using a single Ge detector with an energy resolution of 1.2 keV. The signal to noise ratio was approximately 7×10^3. The S and W parameters were determined in the high energy part of the Doppler spectra to avoid the effect of the Compton scattering. For the S parameter, the energy window was taken at 511.0–511.8 keV. Since the contribution from the valence electron annihilation to the Doppler broadening vanishes above 516 keV [8] in the case of SiC, the energy window for the W parameter was selected at 516.0–522.0 keV. The as-grown layers showed unique S and W parameters, i.e., $S = 0.435–0.437$ and $W = 0.0032–0.0033$, which were characterized as S and W parameters in the perfect region (S_B and W_B) from the compremental study with the positron lifetime [9]. All S and W parameters were normalized to S_B and W_B, respectively.

After electron irradiation, the S parameter was found to increase suggesting the generation of vacancy-type defects. Annealing characteristics of S parameters for the 3C and 6H epilayers are displayed in Fig. 1a and b, respectively. The S parameter for both epilayers decrease at 200 and 700 °C. This is the common annealing feature of isolated silicon vacancies in 3C SiC detected by ESR [3, 4], photoluminescence [7] and positron lifetime [2] measurements after 1 MeV electron

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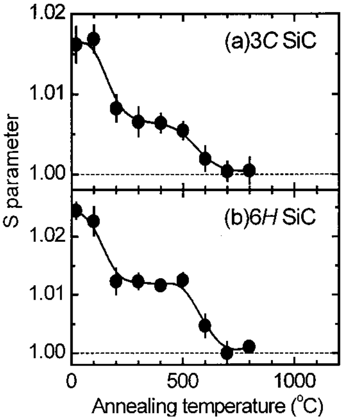

Fig. 1. S parameters for the 3C and 6H epilayers after 1 MeV electron irradiation. The horizontal broken lines are the level of as-grown state

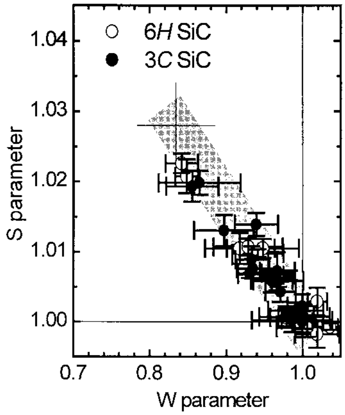

Fig. 2. S versus W plots through the annealing experiments shown in Fig. 1. The cross represents the $S-W$ position for the isolated silicon vacancies (see text)

irradiation. It is also reported that the optically detected magnetic resonance (ODMR) signals related to isolated silicon vancacies in 3C and 6H epilayers vanish after 700 °C annealing [10, 11]. If one type of vacancies acts as positron trapping centers, S and W parameters are given by $S = (1 - f)\, S_B + fS_V$ and $W = (1 - f)\, W_B + fW_V$, where S_V (W_V) are S (W) parameters for vacancies, and f is the fraction of positrons trapped by the vacancies. These equations suggest that the correlation between S and W parameters should be straight in between (S_B, W_B) and (S_V, W_V) on the $S-W$ plane when only the fraction f changes. In fact, Fig. 2 shows the $S-W$ data are more or less on one straight line from the as-irradiated state to the fully annealed state.

Although carbon vacancies and divacancies are thought to capure positrons, these defects have only minor effects. The concentration of divacancies is probably fairly low as compared to that of silicon vacancies since the average primary knock-on atom energy (50–60 eV for 1 MeV electron irradiation of SiC) is somewhat small to cause cascade damage. It is known that silicon vacancies are in single negative charge state [3, 4], while carbon vacancies are expected to be in neutral charge state since they are not detected by ESR in n-type 3C SiC like present case. The specific positron trapping rate for single negative silicon vacancies in SiC is reported to be greater than 1×10^{16} s^{-1} [2, 5, 6], while that for neutral vacancies is on the order of 10^{14} s^{-1} [1]. Thus, positrons may be preferentially trapped by negatively charged silicon vacancies. Furthermore, Dannefaer et al. reported that the S parameter for carbon vacancies may be close to that for bulk, i.e., $\approx$1 [12]. This is explained as the weak localization of positron wavefunction at carbon vacancies and resultant insufficient suppression of the core annihilation rate. Therefore, even if carbon vacancies trap positrons this effect on the Doppler parameters may be significantly small.

Thus, it is concluded that isolated silicon vacancies are the main positron trapping centers after 1 MeV electron irradiation. The trapping fraction f is given by $f = \mu C_V/(\lambda_B + \mu C_V)$, where μ is the specific trapping rate due to the vacancies, C_V the concentration of the vacancies and λ_B the annihilation rate of positrons from bulk state (= 7.14 ns^{-1}) [2]. The concentration of silicon vacancies is evaluated to be $\approx 1.0 \times 10^{16}$ cm^{-3} from the production rate (1.7×10^{-2} cm^{-1}, [5]). Taking the specific trapping rate for negatively charged silicon vacancies to be 1.1×10^{-6} cm^3/s from Refs. [5, 6], S_V and W_V are determined to be 1.028 ± 0.003 and 0.834 ± 0.005, respectively. The magnitude of S_V coincides with the previous value (1.031 ± 0.003) [5, 6] within the experimental uncertainties. Considering the theoretical calculations that the core annihilation rate for silicon vacancies is approximately half of that for bulk [8], the above W_V for silicon vacancies seems to be somewhat overestimated. This might be due to the measurements using the single detector. For the detailed comparison with theories, a higher S/N ratio may be necessary. An additional care should be taken when referring the above W_V since this quantity is sensitive to the selection of the energy window and energy resolution of the detector. The above arguments are restricted to 3C SiC. Nevertheless, the Doppler parameters obtained for 3C SiC may also be applicable for 6H SiC because positron annihilation parameters are insensitive to inequivalent lattice sites in hexagonal SiC as well as polytype [13].

In summary, a two-step recovery of the *S* parameter, which is identified as the annealing of isolated silicon vacancies, was found for both 3C and 6H SiC epilayers after 1 MeV electron irradiation. The specific *S* and *W* parameters for isolated silicon vacancies in 3C SiC have been determined. These parameters will be utilized and examined in further research of defects in SiC.

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