Materials Science Forum
ISSN: 1662-9752, Vols. 264-268, pp 611-614
doi:10.4028/www.scientific.net/MSF.264-268.611

Online: 1998-02-01

Characterization of Defects in Electron Irradiated 6H-SiC by Positron Lifetime and Electron Spin Resonance

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Keywords: Electron Irradiation, Vacancies, Defects, Positron Lifetime, ESR

Abstract. Defects in 6H-SiC produced by 3 MeV electron irradiation were studied using positron lifetime and electron spin resonance (ESR) with annealing experiment. From the positron lifetime measurements, vacancy-type defects were found to be generated by irradiation. Three ESR signals were observed. Comparing with the positron lifetime data, the ESR centers were related to vacancy defects. Structural models and annealing kinetics are discussed for defects produced by irradiation.

Introduction

Silicon carbide (SiC) holds great potential for high-frequency and high-power electronic devices which is functional in extreme conditions, such as radiation environment and high temperature. In the fabrication process of SiC devices using ion implantation, the control of defects as well as impurities is indispensable [1]. Thus, it is important to clarify the properties of point defects in SiC from both fundamental and industrial view points. In this research, we attempted to characterize vacancy defects in 6H-SiC irradiated with 3 MeV electrons using positron lifetime and electron spin resonance (ESR) measurements.

Experiment

Specimens were cut from a modified-Lely-grown 6H-SiC wafer doped with nitrogen (net doping concentration~6×10^{17} cm^{-3}). They were irradiated with 3 MeV electrons up to a fluence of 1.0×10^{18} e^-/cm^2 at 60℃. Isochronal annealing was performed in the temperature range between 100 and 1500℃ for 5 minutes in a dry argon atmosphere. Positron lifetime was measured at room temperature. After subtracting the source and background components, lifetime spectrum L(t) was decomposed to two components (bulk and defect) using a computer program of PATFIT-88 [2]: $L(t)=(I_1/\tau_1)\exp(-t/\tau_1)+(I_2/\tau_2)\exp(-t/\tau_2)$, where I_i (i=1,2) are the intensities ($I_1+I_2=1$) and τ_i are the lifetimes. If the two-state trapping model, where positrons are assumed to annihilate through bulk state and trapped state at defects, is a good approximation, the above lifetimes are given by $\tau_1=1/(\tau_B^{-1}+\kappa)$ and $\tau_2=\tau_V$, where τ_B is the positron lifetime in the bulk state, τ_V the positron lifetime at vacancy defects, and κ the positron trapping rate due to the defects $\kappa=(I_2/I_1)(1/\tau_B-1/\tau_2)$. The bulk lifetime was determined to be $\tau_B=138\pm2$ ps from the measurements of unirradiated p-type 6H-SiC. The validity of the analysis based on the trapping model can be checked by the difference between the lifetime τ_1 determined by the fitting procedure and that expected from the trapping model. The trapping rate is proportional to the concentration of defects. Electron spin resonance measurements were performed from 4 K to 296 K with an X-band (9GHz) microwave incident on a TE_{110} cylindrical cavity using a JEOL JES-TE300.

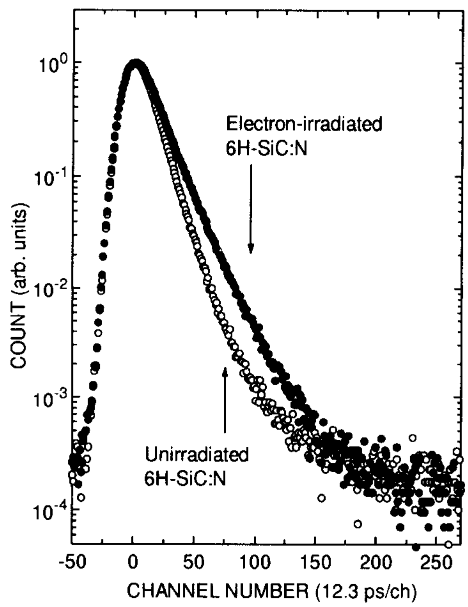

Fig. 1 Positron lifetime spectra before and after 3 MeV electron irradiation recorded at 296 K.

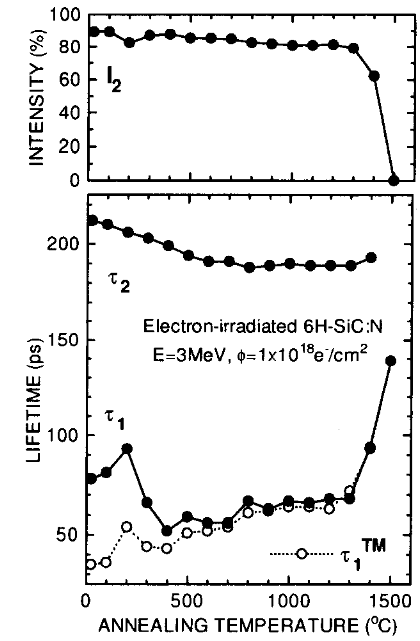

Fig.2 Positron lifetimes and intensity as a function of annealing temperature.

Results and Discussion

Figure 1 shows positron lifetime spectra obtained before and after electron irradiation. The positron lifetime prolongs after irradiation. This prolonged positron lifetime just shows the production of vacancies due to irradiation. Figure 2 shows the annealing behavior of positron lifetimes τ_1 and τ_2 and intensity I_2. The lifetime τ_2 is about 210 ps for the as-irradiated state and decreases toward ~190 ps upon annealing. Theoretical lifetimes of positrons localized at a carbon vacancy, a silicon vacancy and a divacancy were calculated to be 153 ps, 183-194 ps and 214 ps, respectively, by Brauer et al [5,6]. The second lifetime τ_2 is close to the theoretical lifetimes of positrons trapped at divacancies below 500 ℃ and at silicon vacancies above 500 ℃. Thus, the second lifetime is considered as a weighted average between the lifetimes for divacancies and silicon vacancies. The intensity I_2 responsible for the second component reaches the detection limit at 1500 ℃. This shows that all the vacancy defects acting as positron trapping centers disappear at this temperature. The first lifetime τ_1 considerably deviates from that expected from the trapping model (τ_1^{TM}) below 500 ℃. This is explained as the presence of carbon vacancies which trap positrons [7]. That is, since the theoretical positron lifetime at a carbon vacancy (153 ps) is quite close to the bulk lifetime (~140 ps), the carbon vacancy component can not be resolved from the bulk one. It is found from the obtained positron lifetimes that defects related to carbon vacancies, silicon vacancies and divacancies are formed in 6H-SiC by irradiation.

Figure 3 shows typical ESR spectra obtained at 100K for the irradiated specimen. The ESR signals termed NA, NB and NC are observed. The number and intensity ratio of ESR lines and the g-value (2.0030) of the NA signal are similar to those for single-negative silicon vacancies (V_{Si}^-) with S=3/2 found in irradiated 3C-SiC[3,4]. It is therefore suggested that the NA signal originates from isolated silicon vacancies in 6H-SiC. The angular dependences of the NB and NC signals are well-described by the spin Hamiltonian βSgH+SDS with an effective spin S=1. The g

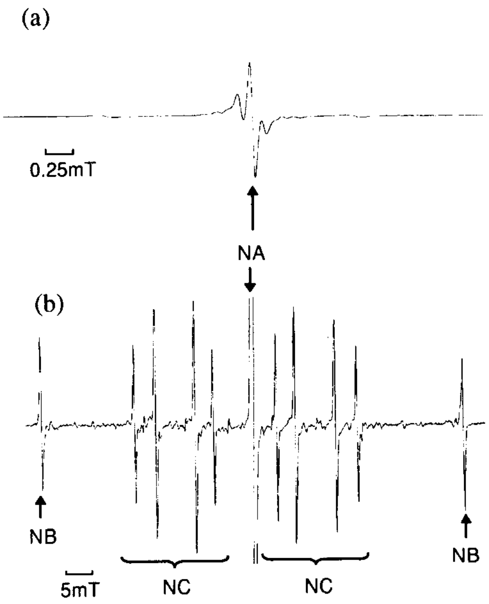

Fig. 3 ESR spectra observed at 100K after 3 MeV electron irradiation at 1x10^{18} e$^-$/cm^2. The angle between the magnetic field and the c-axis was (a) 0° and (b) 5°.

and D tensors for the NB center are found to have an axial symmetry along the c-axis, i.e., $g_{//}$=2.0054, $g_{\perp}$=2.0087 and |D|=3.95x10^{-2} cm^{-1}. These results indicate that two electron spins interacting each other are aligned along the c-axis in the NB center. Assuming that the fine structure is mainly caused by the magnetic dipole-dipole interaction, the average distance of two electron spins is estimated to be 4.04 Å. The NB signal is thought to arise from pairs of point defects combined along the c-axis, such as vacancy-interstitial pairs. As for the NC center, a g-value is estimated to be 2.013. The principal axis of D-tensor for the NC signal is on the three equivalent {11-20} planes and deviates 45° from the c-axis. Splitting lines overlap to each other and hence eight lines are observed as shown in Fig.3(b). The magnitude of D is determined to be |D|=5.51x10^{-2} cm^{-1}. The average distance of the electron spins is estimated to be 3.62 Å. Since this value is approximately twice as long as the Si-C bond length (1.89 Å), divacancies are considered as a possible structure of the NC center.

Figure 4 shows the annealing behavior of positron trapping rates for the second lifetime component (κ_2: silicon vacancies + divacancies) and for the mixed component including the first lifetime (κ_1: carbon vacancies) and the ESR signal intensities. The trapping rate κ_2 decreases at 200, 400 and 800℃ and finally disappears at 1500℃. Considering the decrease in the lifetime τ_2 at 200℃, the decrease in the trapping rate at 200℃ is caused by the disappearance of not only silicon vacancies but also divacancies. The drastic decrease in the trapping rate κ_2 at 200℃ is similar to those of the NA and NC signal intensities. Thus, the positron data supports that these ESR signals are arising from vacancy defects, i.e., the NA and NC centers can be ascribed to silicon vacancies and divacancies, respectively. It seems to be somewhat strange that silicon vacancies and divacancies disappear at such low temperatures, since isolated silicon vacancies start to move at around 750℃ [3,4]. Probably, this peculiarity may be due to the recombination with interstitials. Considering the fact that the trapping rate κ_1 (carbon vacancies) increases at around 200℃, it is probable that divacancies recombine with silicon interstitials to form carbon vacancies. By 500℃ annealing, the trapping rate κ_2 decreases and the lifetime τ_2 reaches the theoretical lifetime at a silicon vacancy. This shows the disappearance of defects related to divacancies and thereafter defects related to silicon vacancies become predominant. Defects related to carbon vacancies are also annealed out up to 500℃. Since no annealing stages at 400℃ are observed for the ESR signals, the defects which disappear at 400℃ is different from those disappearing at 200℃. The decrease in the trapping rate κ_2 at 800℃ shows that defects related to silicon vacancies disappear. The decrease in the trapping rate well agree with that in the NB signal intensity. As mentioned above, the NB signal may originate from some pair of point defects with the c-axis symmetry. The positron result suggests that one of the constituent of the paired defect is a silicon vacancy. Even after annealing at 800℃, defects related to silicon vacancies still remains and they ultimately diminish up to 1500℃. Probably, the residual defects above 800℃ is arising from complexes between silicon vacancies and impurities and they break-up at around 1400℃.

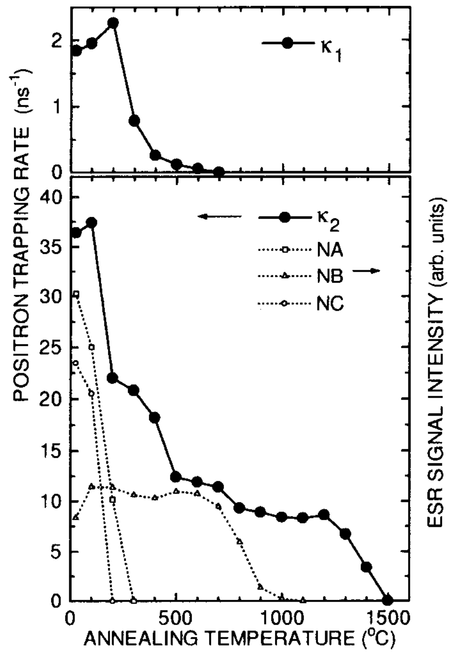

Fig.4 Positron trapping rates κ_1 (carbon vacancies) and κ_2 (silicon vacancies+ divacancies) and the ESR signal intensities as a function of annealing temperature.

Summary

In this research, we carried out positron lifetime and ESR measurements for 3MeV electron irradiated 6H-SiC with annealing experiment. From the positron data, we confirmed that defects related to carbon vacancies, silicon vacancies and divacancies were generated due to irradiation. Positron trapping rate responsible for silicon vacancies and divacancies decreased by annealing at 200, 400, 800 and 1400℃. Three major ESR signals (NA, NB and NC) were observed after irradiation. The NA and NC centers were annealed at 200℃ and the NB at 800℃. From the comparison with positron lifetime data, the observed ESR centers are related to vacancy defects. It is proposed that the NA and NC centers are related to silicon vacancies and divacancies, respectively. The NB center consists of two point defects aligned along the c-axis and one of the constituent is the silicon vacancy.

Acknowledgment

We thank H. Sunaga and H. Takizawa for their help in electron irradiation.

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10.4028/www.scientific.net/MSF.264-268

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