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Citation	Symposium R: Radiation Effects and Ion-Beam Processing of Materials, Boston, Massachusetts, USA, 1-5 December 2003, v. 792, p. 255-260
Issued Date	2003
URL	http://hdl.handle.net/10722/54218
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Mat. Res. Soc. Symp. Proc. Vol. 792 © 2004 Materials Research Society R3.19

Vacancies in electron irradiated 6H silicon carbide studied by positron annihilation spectroscopy

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ABSTRACT

Positron lifetime spectroscopy was employed to study the as-electron-irradiated (10 MeV, 1×10^{18} cm^{-2}) n-type 6H silicon carbide sample in the measuring temperature range of 15 K to 294 K. Isochronal annealing studies were also performed up to the temperature of 1373 K by carrying out the room temperature positron lifetime measurement. Negatively charged carbon vacancies and V_CV_{Si} divacancy were identified as the major vacancy type defects induced by the electron irradiation process. The concentration of the V_CV_{Si} divacancy was found to decrease dramatically after the 1973 K annealing.

INTRODUCTION

Silicon Carbide (SiC) is a wide band gap semiconductor having a high thermal conductivity, a high breakdown electric field, a high saturated drift velocity, a high thermal stability and an inert chemical reactivity. It can be used for fabricating high-temperature, high-frequency and high-power devices [1]. Electrical and optical defects were generally found in the as-grown SiC materials and they are also induced in ion implantation, electron and neutron irradiation processes [1]. Electron irradiation has been widely used to induce defects in semiconductors, and electron irradiation induced defects in 6H-SiC have also been investigated by various spectroscopies [2-21].

Positron lifetime spectroscopy has been used extensively as a non-destructive probe for vacancy type defects in semiconductors because of its selective sensitivity towards neutral and negatively-charged vacancies. Positron is possibly trapped in the potential well created by the missing atomic core of the vacancy. Positron annihilating from different states in the samples exhibits thier own characteristic lifetime in the lifetime spectrum [22]. Different vacancies can thus be identified by their characteristic positron lifetimes. In addition, defect information such as the concentration, the charge state, and the ionization energy can be extracted from the positron lifetime data.

In the present work, we have performed temperature dependent positron lifetime measurements on the as-irradiated 10 MeV electron-irradiated n-type 6H-SiC. Isochronal

annealing studies were also performed on the electron irradiated sample and the non-irradiated control sample by carrying out room temperature positron lifetime measurements.

EXPERIMENTAL

Samples with size of about 1×1 cm^2 were cut from the Lely-grown nitrogen-doped n-type 6H silicon carbide wafer (n=1.2×10^{18} cm^{-3}) purchased from the Cree Research Inc. The samples were irradiated with 10 MeV electrons with dosage of 1×10^{18} cm^{-2}. The sample was kept at temperature below 293 K during the irradiation process. The positron source used was 20 μCi ^{22}NaCl encapsulated with kapton foils. The source foil was sandwiched by the two pieces of samples, and the sample assembly was loaded into a 10 K Oxford closed cycle He fridge. Lifetime spectra were accumulated over the temperature range from 15 K to 294 K and each spectrum contained 4×10^6 counts. Each of the annealing steps was performed in forming gas atmosphere for a period of 30 minutes. The resolution of the fast-fast lifetime spectrometer was fwhm=245 ps.

RESULT AND ANALYSIS

The normalized positron lifetime spectrum is the summation of the exponential components originated from the corresponding annihilating sites, i.e.: [22]

$$S(t) = \sum_i I_i \exp(-t/\tau_i) \qquad (1)$$

where I_i and τ_i are the intensity and the characteristic lifetime of the i-th defect component respectively. The POSITRONFIT [23] program was used to decompose the lifetime spectra after subtracting the background and the source contributions. The average lifetime of the spectrum is given by: [22]

$$\tau_{ave} = \int tS(t)dt / \int S(t)dt = \sum I_i \tau_i \qquad (2)$$

The average positron lifetime of the as-irradiated sample as a function of the measuring temperature is shown in Figure 1. From the figure, the average lifetime decreases about 189 ps to 175 ps as the temperature

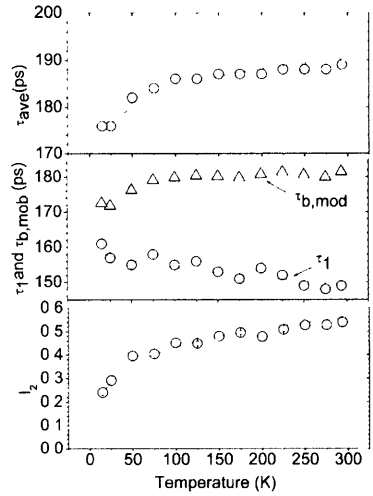

Figure 1 The average lifetime and the fitted lifetime parameters as a function of the temperature for the 10 MeV 1×$10^{18}$$cm^{-2}$ as-electron-irradiated n-type 6H-SiC sample.

decreases from 294 K to 15 K. All the spectra are well represented by the two component model. The lifetime of the long lifetime component (i.e. the defect component) τ_2 was found to be constant at 223 ps irrespective of the measuring temperatures. The fitting results of τ_1 and I_2 as a function of the temperature are also shown in Figure 1. The 223 ps characteristic lifetime is close to that of the V_CV_{Si} observed in previous studies [17,19,20] and is thus attributed to this defect.

In order to check the validity of the single defect simple trapping model (i.e. only the 223 ps defect exists and no positron detrapping occurs), the modelled bulk lifetime was calculated by: [22]

$$\tau_{b,\mathrm{mod}} = \left(I_1\lambda_1 + I_2\lambda_2\right)^{-1} \tag{3}$$

and the results were shown in Figure 1. The modelled bulk lifetime increases with temperature from about 170 ps to 180 ps. These values are much larger than the generally accepted value (~140 ps - 150 ps) and thus the simple trapping model is not valid for describing the present data.

The increase of the average lifetime, the increase of I_2 and the decrease of τ_1 with increasing temperature is a reflection of less positron trapping into the V_CV_{Si} site at low temperatures. The existences of positron shallow trap or negatively charged carbon vacancy can also lead to such observation. A positron shallow trap is a non-open volume negatively charged centre (for example, ionized acceptor impurity) that forms hydrogen-like binded state with a positron. As the electronic environment of the positron shallow trapped state is very similar to that of the Bloch state, the lifetime of the positron in the positron shallow trapped state is indistinguishable from that of the delocalized positron. As the binding energy of this Ryhberg state is usually several tens of meV (as compared to ~1 eV for vacancy type defect), positron detrapping is possible at room temperature. This implies these shallow traps compete with vacancy type defects and they become the significant positron trapping centre at low temperatures. We have attempted to fit the present data with the positron shallow trap model shown in reference [18], but we could not obtain good fit with physically compatible parameters.

Positron trapping rate into the vacancy is given by: [22] $\kappa = \mu C$, where μ and C are the specific trapping coefficient and the concentration of the vacancies. For neutral vacancies, μ is independent of the temperature, and for negatively-charged vacancy, it follows: [22] $\mu \sim T^{-1/2}$. V_C has a characteristic lifetime of ~160 ps [19,21], which is close to the fitted τ_1 (as shown in Figure 1) and is thus inseparable from the τ_1 component if it exists. As the presence of the concentrations of negatively-charged V_C would decrease the positron trapping rate into the divacancy at low temperatures and thus this would be a possible explanation for the temperature dependence of τ_{ave}, τ_1 and I_2 as shown in Figure 1. In order to model this physical process, the trapping and the annihilation of positrons in different states can be modelled as:

$$\begin{aligned}
\frac{dn_b}{dt} &= -\lambda_b n_b - \kappa_{V_CV_{Si}} n_{V_CV_{Si}} - \kappa_{V_C} n_{V_C} \\
\frac{dn_{V_C}}{dt} &= \kappa_{V_C} - \lambda_{V_C} n_{V_C} \\
\frac{dn_{V_CV_{Si}}}{dt} &= \kappa_{V_CV_{Si}} - \lambda_{V_CV_{Si}} n_{V_CV_{Si}}
\end{aligned} \tag{4}$$

where n_i is the normalized density, $\tau_i = 1/\lambda_i$ is the characteristic lifetime and κ_i is the trapping rate of the state i. The solution of equation (4) yields a positron lifetime spectrum having three components, where :

$$\begin{aligned}
\lambda_1 &= \lambda_b + \kappa_{V_C} + \kappa_{V_C V_{Si}} \\
\lambda_2 &= 1/\tau_{V_C} \\
\lambda_3 &= 1/\tau_{V_C V_{Si}} \\
I_1 &= 1 - I_2 - I_3 \\
I_2 &= \kappa_{V_C} /(\lambda_b - \lambda_2 + \kappa_{V_C} + \kappa_{V_C V_{Si}}) \\
I_3 &= \kappa_{V_C V_{Si}} /(\lambda_b - \lambda_3 + \kappa_{V_C} + \kappa_{V_C V_{Si}})
\end{aligned} \qquad (5)$$

As $\tau_{V_C} \sim \tau_1$, the first two components cannot be separated and thus the two-component model well describes the spectrum:

$$\begin{aligned}
\tau_{1,\exp} &= \left(\frac{I_1}{I_1 + I_2}\right)\lambda_1^{-1} + \left(\frac{I_2}{I_1 + I_2}\right)\lambda_2^{-1} \\
I_{1,\exp} &= I_1 + I_2 \\
\tau_{2,\exp} &= \lambda_3^{-1} \\
I_{2,\exp} &= I_3
\end{aligned} \qquad (6)$$

where $\tau_{i,exp}$ and $I_{i,exp}$ are the fitted lifetime and the intensity of the i-th component. The data in Figure 1 were fitted with this model and simultaneous good fits were obtained for τ_{ave}, $\tau_{1,exp}$, and $I_{2,exp}$ (as shown by the solid lines in figure 1) with parameters given by: $\tau_b = 148ps$, $\tau_{V_C} = 160ps$, $\tau_{V_C V_{Si}} = 223ps$, $\kappa_{V_C}(T = 300K) = 1.8\times10^{10} s^{-1}$ and $\kappa_{V_C V_{Si}} = 2.5\times10^{10} s^{-1}$. Although the specific trapping coefficients of V_C and $V_C V_{Si}$ in 6H-SiC have not been reported, the defect concentrations can be estimated using the values of neutral V_2 in Si (8×10^{14} s^{-1}) [24] and the negative monovacancies in diamond (3.8×10^{15} s^{-1}) [25]. With these values, the negative charged V_C defect and the $V_C V_{Si}$ divacancy were found to be 8×10^{17} cm^{-3} and 5×10^{18} cm^{-3} respectively.

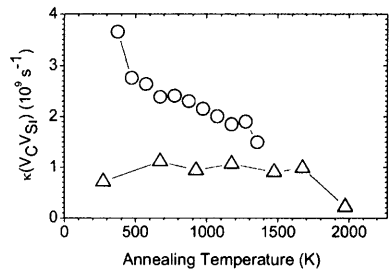

Figure 2. The positron trapping rates of the $V_C V_{Si}$ divacancy as a function of the annealing temperatures. The data of the 10 MeV irradiated sample and the non-irradiated sample are represented by the circle and the triangle.

In order to investigate the annealing behaviour of the $V_C V_{Si}$ divacancy, we have preformed isochronal annealing studies on the electron-irradiated (annealing temperature up to 1373 K), as well as the non-irradiated n-type 6H-SiC samples (up to 1973 K). The results of the

non-irradiated sample with the annealing temperature range up to 1673 K have been presented in reference [17], and in the present study, we have extended the annealing temperature up to 1973 K on the same sample used in reference [17]. The V_CV_{Si} divacancy was identified in the non-irradiated and also the electron-irradiated samples. The trapping rates into the V_CV_{Si} divacancy of the electron irradiated and the non-irradiated samples were calculated and are shown in Figure 2, respectively. It was found that the trapping rate of the V_CV_{Si} divacancy increases from $\sim 1\times10^9$ s^{-1} to 4×10^9 s^{-1} after the electron irradiation. Moreover, the concentration of the V_CV_{Si} divacancy decreases dramatically after the 1973 K.

CONCULSION

Positron lifetime annihilation spectroscopy has been used to study the vacancy defects in the 10-MeV electron irradiated n-type 6H-SiC. Negatively charged V_C and V_CV_{Si} divacancy are the major vacancy type defects identified. Moreover, annealing studies show that the concentration of the V_CV_{Si} divacancy drops significantly after the 1973 K annealing.

ACKNOWLEDGEMENT

This study was supported financially by the Research Grant Council, HKSAR, China [project no. 7085/01P] and the Committee of Research and Conference Grant, The University of Hong Kong, China

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