Low Energy Electron Irradiation Induced Deep Level Defects in 6H-SiC: The Implication for the Microstructure of the Deep Levels E_1/E_2

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N-type 6H-SiC samples irradiated with electrons having energies of $E_e = 0.2$, 0.3, 0.5, and 1.7 were studied by deep level transient technique. No deep level was detected at below 0.2 MeV irradiation energy while for $E_e \geq 0.3$ MeV, deep levels $ED1$, E_1/E_2, and E_i appeared. By considering the minimum energy required to displace the C atom or the Si atom in the SiC lattice, it is concluded that generation of the deep levels E_1/E_2, as well as $ED1$ and E_i, involves the displacement of the C atom in the SiC lattice.

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Silicon carbide (SiC) is a promising wide band gap material for fabricating high-temperature, high-power, and high-frequency electronic devices [1]. Deep level defects induced by ion implantation or particle irradiation have been extensively studied because of their great influence on the materials' electrical and optical properties. A general classification for ion implanted or particle irradiated n-type 6H-SiC includes levels $ED1$ ($\sim E_C$-0.27 eV), E_i ($\sim E_C$-0.51 eV), E_1/E_2 ($\sim E_C$-0.34/0.44 eV, with the name of Z_1/Z_2 for 4H-SiC), and Z_1/Z_2 ($\sim E_C$-0.58/0.72 eV, with the name of E_1/E_2 for 4H-SiC) [2–9]. Information involving the microstructures of these deep levels is controversial and incomplete. The E_1/E_2 doublet is not only the most dominant but also appears to be the most thermal stable in electron irradiated n-type 6H-SiC. The microstructure responsible for this level has been attributed to $V_C V_{Si}$ [5], V_{Si} complex [8], V_C related defect [6,9], and N_i-C_i complex [10].

All previous deep level transient spectroscopy (DLTS) studies on electron irradiated 6H-SiC materials usually involved high energy electron irradiations (>MeV). Such investigations induce defect types originating from both C and Si atoms displacement and thus provide no basis for discriminating between primary vacancy defects originating on either sublattice. Since the C atom has a significantly smaller mass than that of Si atom (Si/C = 2.33), the maximum energy transferred from the electron to the C atoms in the SiC lattice during elastic collision is larger than that of the Si atom. This implies the value of the minimum electron energy for creating the defect V_C, originating from displacing a C atom, would be lower than that for creating the defect V_{Si}. This idea has been nicely demonstrated recently by Rempel *et al.* [11]. Using both positron lifetime and coincident Doppler broadening techniques, it was shown that for low electron irradiation energy 0.5 MeV $> E_e >$ 0.3 MeV, only V_C was generated, while at higher energy ($E_e > 0.5$ MeV), V_{Si} could also be detected [11]. The precise values of threshold electron irradiation energies for displacement of either the C or the Si atoms are difficult to estimate since they depend to some extent on the conduction type, the growth techniques, or the relative orientation of crystallographic planes of the sample to the incident electron direction and on sample temperature. Nevertheless, the approximate values given above can provide helpful information in defect microstructure determinations.

The aim of the present experiment has been to study the irradiation energy dependence of the different electron irradiation induced deep levels in n-type 6H-SiC. Deep level defects in n-type 6H-SiC have been produced by irradiating with electron energies of 0.2, 0.3, 0.5, and 1.7 MeV and these have been investigated by DLTS technique combined with annealing experiments.

The starting epi n-type 6H-SiC materials used in this experiment were purchased from CREE Research Inc. The 5-μm-thick nitrogen doped (0001) oriented epitaxial layer with $n = 1 \times 10^{16}$ cm^{-3} was grown on the n^+-type 6H-SiC substrate ($n = 8 \times 10^{17}$ cm^{-3}). The detailed procedures for fabricating the Ohmic and the Schottky contacts can be found in Ref. [9]. The samples were irradiated with electrons energies of 0.2, 0.3, 0.5, and 1.7 MeV (dosage 10^{15} cm^{-2}). Isochronal annealing of the irradiated samples was carried out in a nitrogen atmosphere at temperatures between 100 and 1200 °C for 30 min. DLTS measurements were carried out by applying a reverse bias of $V_r = -8$ V, with a forward filling pulse of $V_p = 8$ V. The energy levels and the capture cross sections were obtained from the Arrhenius plot of the emission rate, and the concentrations were determined from the peak heights of the normalized DLTS spectra [12]. We have also performed photoluminescence (PL) at 10 K to reinforce the results of our interpretation. The excitation light source used in the PL measurement is the 325 nm line of a 30 mW HeCd laser. The luminescence was

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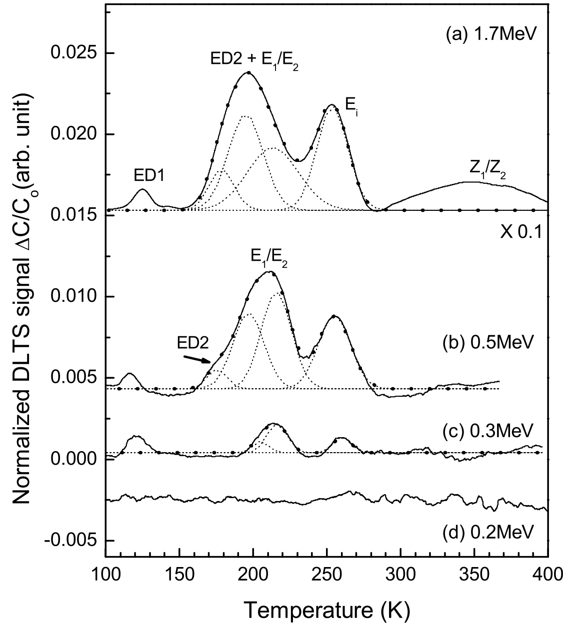

FIG. 1. Normalized experimental (solid lines) DLTS spectra for *n*-type 6*H*-SiC irradiated with electron having energies of 1.7 MeV (*a*), 0.5 MeV (*b*), 0.3 MeV (*c*), and 0.2 MeV (*d*), respectively. A rate window of 6.82 ms was used in the measurements. The dotted cures are the modeled curves of fitting the E_1/E_2 peaks with two or three Gaussians as described in the text.

detected by a liquid nitrogen cooled Ge detector after passing through a Spex 500 M monochrometer.

Figure 1 shows typical DLTS spectra of the electron irradiated samples (dosage of 5×10^{15} cm^{-2}) with $E_e =$ 0.2 MeV to 1.7 MeV. It is seen that peaks at 120, 200, and 260 K (previously reported as ED1 [5], E_1/E_2 [2–9], and E_i [4,6,9]) are clearly seen only for the samples irradiated with electrons having energies $E_e \geq 0.3$ MeV. No signal is found in the as-grown and the 0.2 MeV irradiated samples (with DLTS measurement detect limiting $\sim 10^{12}$ cm^{-3}). Moreover, the peak at about $T = 360$ K (Z_1/Z_2 in the 6*H*-SiC material [2–9]) was clearly observed in the 1.7 MeV electron irradiated samples, but was absent for the samples irradiated with low energy electrons. This Z_1/Z_2 defect pair is usually related to the isolated $V_{\rm Si}$ [13]. Providing the irradiation energy is larger than the corresponding threshold energy, the intensities of all these peaks is observed to increase with electron dosage, indicating that these deep levels are all induced by the electron irradiation process.

It is interesting to note that for the E_1/E_2 peak at about 200 K, a shoulder is observed at the low temperature side of the peak for the 0.5 MeV spectrum but this shoulder is not noticeable for the 0.3 MeV spectrum. For the case of 1.7 MeV, it is as if the peak position shifts to the low temperature direction. It is plausibly to associate this shoulder with another peak having ionization energy and capture cross section very close to those of the E_1/E_2. This observation of a peak located on the low temperature of E_1/E_2 was also observed by Gong *et al.* [5] who labeled it *ED*2. The composite ($E_1/E_2 + ED2$) peak data was fitted by superposition of Gaussians. The fitted curves are shown as dotted lines in Fig. 1. It was found that for the 0.3 MeV irradiated spectrum that a two-Gaussians fit was adequate while for those irradiated energies $E_e \geq 0.5$ MeV, a three-Gaussians model was needed. This implies ED2 is only created with electron energy $E_e \geq 0.5$ MeV. The ionization energies, capture cross sections, and concentrations of all these deep level defects (*ED*1, *ED*2, E_1/E_2, E_i, and Z_1/Z_2) are shown in Table I. These results are very close to the previously observed values lending strong confirmation that these defects are indeed the *ED*1, *ED*2, E_1/E_2, E_i, and Z_1/Z_2 levels as seen by other workers [2–9]

DLTS measurements were also performed on the 0.3 and the 1.7 MeV irradiated samples annealed at different temperatures. For both samples, E_1/E_2 do not entirely anneal after the 1200 °C annealing. In contrast, levels *ED*1, *ED*2, and E_i disappear after a relatively low annealing temperature of 300 °C. It is also noted that 300 °C annealing also effectively removes the shoulder of the E_1/E_2 peaks in the 1.7 MeV spectrum thus making the spectral shape almost identical to that of the 0.3 MeV spectrum.

The maximum energy transferred from an electron energy E to the atomic nucleus $E_{e,\max}$ is given by [14] $E_{e,\max} = 2E(E + 2m_ec^2)/(Mc^2)$, M, and m_e being the atomic mass and electron mass, respectively. As the C atom is lighter than the Si atom, for a given electron energy, more energy is transferred to the C atom in comparison to that of the Si atom. This implies the minimum electron irradiation energy required for displacing the C atom $E_{\min}$(C) is less than that for the Si atom $E_{\min}$(Si) in the SiC lattice because their threshold displacement

TABLE I. The ionization energy ΔE, capture cross sections σ, and concentrations N_t of the observed deep level defects induced by the electron irradiation process (dosage of 5×10^{15} cm^{-2}).

Deep levels	Ionization energies ΔE(eV)	Capture cross sections σ(cm^2)	Defect concentrations N_t(cm^{-3}))
*ED*1	0.23 eV	$\sim 10^{-15}$	$\sim 3 \times 10^{13}$ (0.3 MeV)
*ED*2	0.32 eV	$\sim 10^{-14}$	$\sim 1 \times 10^{14}$ (1.7 MeV)
E_1/E_2	0.36/0.44 eV	$\sim 10^{-14}/10^{-15}$	$\sim 6 \times 10^{13}$ (0.3 MeV)
E_i	0.50 eV	$\sim 10^{-14}$	$\sim 4 \times 10^{13}$ (0.3 MeV)
Z_1/Z_2	0.62/0.72 eV	$\sim 10^{-16}/10^{-17}$	$\sim 3 \times 10^{14}$ (1.7 MeV)

energy T_d is essentially identical and equal to ~40 eV [15]. Threshold displacement energies of $E_{\min}$(C) ~ 0.2 MeV and $E_{\min}$(Si) ~ 0.4 MeV are calculated. These values are supported by the positron annihilation study of Rempel *et al.* [11] who found (i) no evidence of vacancy formation with $E_e = 0.23$ MeV, (ii) evidence for V_C with $E_e = 0.3$ MeV, and (iii) V_{Si} generation with $E_e \geq 0.5$ MeV. Based on these observations it is reasonable to propose the following interpretation of the present data. At 0.2 MeV electron irradiation the energy transferred to the C and Si atoms is insufficient to cause atomic displacement on neither sublattice of *n*-type 6*H*-SiC. Increasing to 0.3 MeV the deep levels *ED*1, E_1/E_2, and E_i are generated and it is plausible to conclude that the defects associated with these levels are related in their origin to the displacement of a C atom in the SiC sublattice. Further increasing the irradiation energy causes defects by displacing the Si atom from the sublattice to occur. *ED*2 and the Z_1/Z_2 are seen as belonging to this category.

However, Steeds *et al.* [16,17] have irradiated the 6*H*-SiC materials with electrons having energies of 50–300 keV and studied the induced defects by performing the low temperature PL measurements. With $E_e \geq$ 200 keV, a 864.9 nm PL signal was observed. This signal was attributed to the *V*1 signal previously observed in Sörman *et al.* [18] and Wagner *et al.* [19] , in which the *V*1 (865 nm), *V*2 (887 nm), and the *V*3 (908 nm) signals were unambiguously related to the V_{Si} defects at different equivalent sites. The observation of Steeds *et al.* [16,17] contradicts with the findings of Rempel *et al.* [11] (i.e., V_{Si} was only created with $E_e \geq 500$ keV). Rempel *et al.* [20] have pointed out that the discrepancy is possibly due to the difference in the irradiation environments of the two studies, for which Rempel *et al.* and Steed *et al.* have used the accelerator and the electron microscope as the electron irradiation sources, respectively. In the accelerator based electron irradiation, sample temperature was usually well controlled and the electron flux was usually lower.

In order to resolve the uncertainty of any V_{Si} created in our 0.3 MeV electron irradiated sample, we have performed PL measurements at 10 K on our 300 keV and 1.7 MeV electron irradiated samples and the PL spectra were shown in Fig. 2. The samples used in the PL measurements are the same as those of the DLTS studies. The present electron irradiation was performed with the electron accelerator, which is similar to Rempel *et al.*'s work [11] . From Fig. 2, signals of ~865, ~887, and ~908 nm were clearly observed in the 1.7 MeV electron irradiated samples. These three PL signals are very similar to the *V*1, the *V*2, and the *V*3 peaks in Sörman *et al.* [18] in the sense that: (i) the peak positions coincide well with each other; (ii) the intensities of the three peaks follow the same order, in which *V*3 has the highest intensity and *V*2 has the lowest; and (iii) the peak intensities increase with increasing irradiation dosage (with dosage lower than 10^{17} cm^{-2} [18]) and this implies the three peaks are associated with the electron irradiation. This leads us to conclude the three peaks observed in the 1.7 MeV electron irradiated samples are *V*1, *V*2, and *V*3, and are thus related to the V_{Si} defects at different equivalent sites as reported in Sörman *et al.* [18]. In contrast with Steed *et al.*'s result that only the *V*1 signal was induced by the electron irradiation process [16,17], the signals corresponding to the three equivalent sites (i.e., *V*1, *V*2, and *V*3) were created by the electron irradiation in the present and the Sörman *et al.*'s studies [18]. From Fig. 2, it is clearly seen that neither the *V*1, the *V*2, nor the *V*3 signals were found in the 0.3 MeV electron irradiated sample. This result is consistent with that of Rempel *et al.* [11], but contradicts with that of Steed *et al.* [16,17]. The divergence may arise from different irradiation conditions and further investigation is required. Nevertheless, it is plausible to conclude the V_{Si} related PL signals *V*1, *V*2, and *V*3 was not induced in the present 0.3 MeV electron irradiated sample.

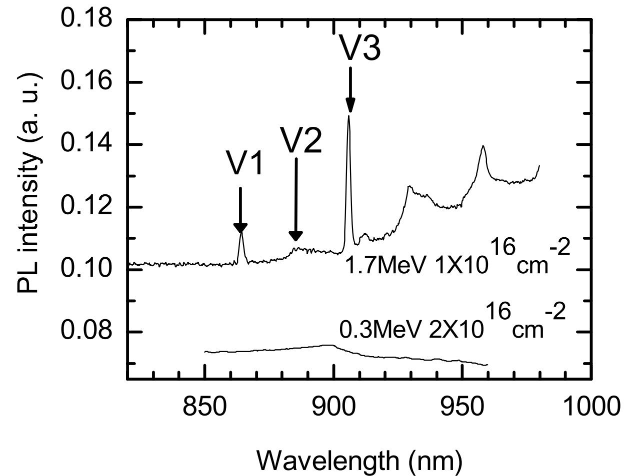

FIG. 2. PL spectra of the 0.3 and the 1.7 MeV electron irradiated 6*H*-SiC (dosage of 10^{16} cm^{-2}). The *V*1, the *V*2, and the *V*3 signals, which are related to the V_{Si} defect, are only seen in the 1.7 MeV electron irradiated sample but not in the 0.3 MeV sample.

The defect microstructure of the E_1/E_2 doublet is still controversial. Suggestions have ranged from the $V_C V_{Si}$ divacancy [5], the negatively charged V_C [6], the V_{Si} complex [8], the $V_C C_{Si}$ defect [9], or the N_i-C_i [10]. As discussed, the observed 0.3 MeV threshold for the E_1/E_2 gives strong evidence that these defects originate from the displacement of the C atom in the SiC sublattice. With electron irradiation energy just enough to displace the C atom like the 0.3 MeV in the present study, the displaced atom is not likely to have sufficient energy to induce further defects. This implies the E_1/E_2 have microstructure containing a carbon vacancy or a carbon interstitial. Moreover, this energy being below that required to displace a Si atom implies no involvement of the V_{Si} as, for example, in a V_{Si} complex. Further to this the involvement of $V_C V_{Si}$ can be largely ruled out based on the observation of E_1/E_2 being the dominant peaks in the

0.3 MeV spectrum and the production rate of $V_C V_{Si}$ being expected lower than that of monovacancy such as V_C. Further evidence for excluding E_1/E_2 being the $V_C V_{Si}$ comes from a recent positron lifetime measurement, in which the $V_C V_{Si}$ lifetime component in the Lely grown n-type 6H-SiC sample persists until 1400 °C, but in the DLTS study of neutron irradiated n-type 6H-SiC epi sample, the E_1/E_2 DLTS signals nearly completely disappear after the 1400 °C annealing [9,21].

In neutron irradiated n-type 6H-SiC the E_1/E_2 levels are found to form with a low relative intensity that increases as the samples are 600 °C annealed [9]. As noted in Ref. [9] such annealing behavior is identical to that of the $P6/P7$ EPR signal [22] making it likely that both E_1/E_2 and $P6/P7$ originate from the same defect structure. Theoretical modeling of EPR signal suggested that the most likely candidate for the $P6/P7$ signal was the $V_C C_{Si}$ center and it was further suggested that this could form via the V_{Si} through the reaction $V_{Si} + C_C \rightarrow V_C C_{Si}$ during thermal annealing process [22,23]. Here we point out that this proposed structure of E_1/E_2 center is also consistent with the present findings that the E_1/E_2 center is related to primary C-atom displacement. Under electron irradiation it is possible for the primary induced V_C to combine with a carbon antisite to form the $V_C C_{Si}$ (i.e., $V_C + C_{Si} \rightarrow V_C C_{Si}$). In support of this formation process we point out that C_{Si} is known to be an electrical and optical inactive defect having a low formation energy and is thus likely to be the abundant native defect in as-grown SiC [24]. Theoretical calculation shows that at all positions of the Fermi level, the formation energy of the $V_C C_{Si}$ pair is lower than the sum of formation energies of the isolated carbon antisite and the isolated V_C [22]. On the other hand, Eberlein *et al.* [10] using first principle calculations have studied the dicarbon interstitial complex next to a nitrogen atom termed N_i-C_i in 4H-SiC. Z_1/Z_2 in 4H-SiC (or E_1/E_2 in 6H-SiC) was proposed to have a structure of N_i-C_i because from calculation, N_i-C_i has similar properties to the high thermal stability and negative-U behavior to those of Z_1/Z_2 in 4H-SiC. Moreover, the calculated levels are close to those of the defects. The present experimental result is also consistent with this model.

In conclusion, deep level defects induced by electron irradiation have been studied with a range of irradiation energies and with isochronal thermal annealing. Deep levels $ED1$, E_1/E_2, and E_i are created with $E_e \geq 0.3$ MeV and have been associated with primary atom displacement on the C atom of SiC sublattice and have microstructure containing the carbon vacancy or the carbon interstitial.

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