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Electron Paramagnetic Resonance study on n-type electron-irradiated 3C-SiC.

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Abstract. Electron Paramagnetic Resonance (EPR) was used to study defects in n-type 3C-SiC films irradiated by 3-MeV electrons at room temperature with a dose of 2×10^{18} cm^{-2}. After electron irradiation, two new EPR spectra with an effective spin S = 1, labeled L5 and L6, were observed. The L5 center has C_{3v} symmetry with g = 2.004 and a fine-structure parameter D = 436.5×10^{-4} cm^{-1}. The L5 spectrum was only detected under light illumination and it could not be detected after annealing at ~550°C. The principal *z*-axis of the D tensor is parallel to the <111>-directions, indicating the location of spins along the Si-C bonds. Judging from the symmetry and the fact that the signal was detected under illumination in n-type material, the L5 center may be related to the divacancy in the neutral charge state. The L6 center has a C_{2v}-symmetry with an isotropic g-value of g=2.003 and the fine structure parameters D=547.7×10^{-4} cm^{-1} and E=56.2×10^{-4} cm^{-1}. The L6 center disappeared after annealing at a rather low temperature (~200°C), which is substantially lower than the known annealing temperatures for vacancy-related defects in 3C-SiC. This highly mobile defect may be related to carbon interstitials.

1. Introduction

Silicon carbide (SiC) is a promising material for high-power, high-frequency and high-temperature devices. The understanding of intrinsic defects in SiC – their origin, electronic structure, annealing behavior and influence on the electrical and optical properties of the material – is essential for defect control. Besides the potential application in electronics, the 3C polytype is also interesting for fundamental studies of defects due to its simple zincblende crystal structure.

In this study, Electron Paramagnetic Resonance (EPR) was used to study intrinsic defects introduced by electron irradiation in n-type 3C-SiC. The results on two new EPR centers and their annealing behavior are presented.

2. Experimental

The starting materials were single crystalline n-type 3C-SiC epilayers of thickness ~130 µm, grown by chemical vapor deposition (CVD). The freestanding films were irradiated by 3 MeV electrons at room temperature with a dose of 2×10^{18} cm^{-2}. EPR measurements were performed at 77 K on an X-band (~9.5 GHz) Bruker ELEXSYS E580 spectrometer. For optical excitation, a 150 W Xenon lamp with appropriate optical filters was used. For angular dependence measurements, the magnetic field was rotated in the $(0\bar{1}1)$ plane from the [100] to the [011] direction with steps of 5°. The annealing study was performed in Ar gas flow ambience in the temperature range from 150°C to 950°C with a step of 50°C. The annealing time was 10 minutes at each temperature.

3. Results and discussion

3.1. The L5 center

Figure 1(a) shows the EPR spectra measured at 77 K, under illumination with light of photon energies ~ 2.06-2.85 eV, for the magnetic field parallel to the three main directions [100], [111], and [011]. The strong line at ~338 mT belongs to the negatively charged silicon vacancy (V_{Si}^{-}) [1]. A new spectrum with an effective electron spin S=1 was detected and labeled as L5. In this n-type irradiated sample, the L5 center was detected only under illumination. The angular dependence of the center with the magnetic field rotating in the $(0\bar{1}1)$ plane is shown in figure 1(b).

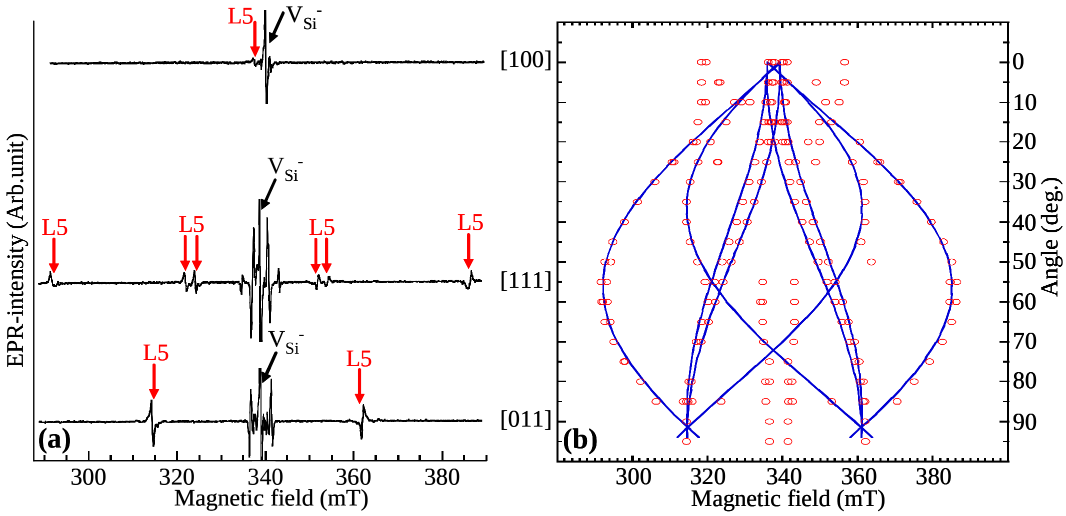

Figure 1. (a) EPR spectra measured under illumination at 77 K with the applied magnetic field parallel to three main directions: [100], [111], and [011]. For clarity, the main peak is cropped. (b) The measured (open circle) and simulated (solid curves) angular dependence. The magnetic field was rotated in the $(0\bar{1}1)$ plane. The angles 0° and 90° correspond to the [100] and [011] directions, respectively.

The L5 center has a trigonal symmetry (C_{3v}). The angular dependence can be described by the spin-Hamiltonian

$$H=\mu_B \mathbf{BgS}+\mathbf{SDS}, \quad (1)$$

where μ_B is the Bohr magneton and the D-tensor represents the spin-spin interaction. The D-tensor can be diagonalized with the principal terms: $D_{xx}=-(1/3)D+E$, $D_{yy}=-(1/3)D-E$ and $D_{zz}=(2/3)D$. D and E are the fine-structure parameters, representing the crystal field splitting due to the trigonal and orthorhombic fields, respectively. From the fit to the experimental data, using spin-Hamiltonian Eq.(1), the parameters of the L5 centers were obtained as: g=2.004 and $D=436.5\times10^{-4}cm^{-1}$. The principal z-axis of the D-tensor is parallel to the <111> directions, indicating the location of the spins along the Si–C bonds. The results are summarized in table 1.

Due to relatively weak signals in thin films, no clear hyperfine structure could be detected. The center was not detected after annealing at 550°C. Judging from the symmetry of the defect, possible candidates could be a paired defect with both the constituencies aligned along the Si-C bonds. The fine structure parameters of the L5 center ($D=436.5\times10^{-4}$ cm^{-1}) is almost coincident to that of the P6'b center in 4H-SiC ($D=436\times10^{-4}$ cm^{-1}), which was recently identified as a C_{3v} configuration of the neutral divacancy [2]. This similarity suggests that the divacancy in the neutral charge state ($V_CV_{Si}^0$) is a possible defect model for the L5 center.

3.2. The L6 center

Figure 2(a) shows the EPR spectra measured in darkness at three main crystal directions. The L6 center can also be detected under illumination with photon energies in the range 2.06–2.85 eV. The angular dependence of the center is shown in figure 2(b).

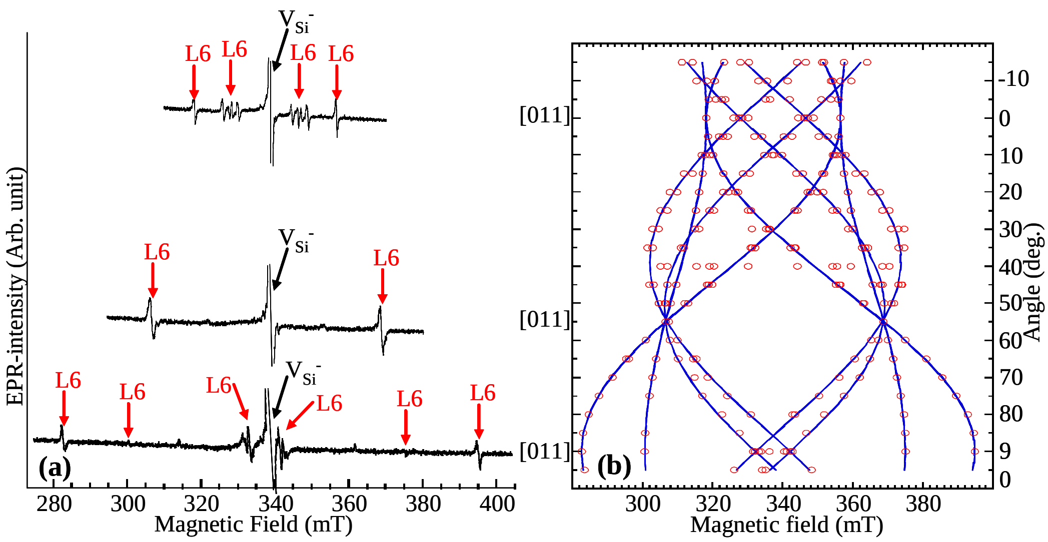

Figure 2. (a) EPR spectra measured in darkness at 77 K with the magnetic field parallel to three main directions: [100], [111], and [011]. For clarity, the main peak is cropped. (b) The measured (open circles) and simulated (solid curves) angular dependence. The magnetic field was rotated in the $(0\bar{1}1)$ plane.

The L6 center is also a spin S=1 center with orthorhombic-I symmetry (C_{2v}). Its angular dependence can be described by the spin-Hamiltonian equation (1) with an isotropic g=2.003 and the fine-structure parameters: $D=547.7\times10^{-4}$ cm^{-1} and $E=56.2\times10^{-4}$ cm^{-1}. The obtained parameters are also summarized in Table 1.

The L6 center disappeared after annealing at ~200°C, which is substantially lower than the known annealing temperatures for vacancy related defects in 3C-SiC. The low symmetry and low annealing temperature of the center indicate that it may be a carbon-interstitial (C_i) related defect.

Table 1. The parameters and properties of the L5 and L6 centers in n-type irradiated 3C-SiC.

	L5	L6
Hamiltonian	$H=\mu_B\mathbf{BgS}+\mathbf{SDS}$	$H=\mu_B\mathbf{BgS}+\mathbf{SDS}$
Defect symmetry	C_{3v}	C_{2v}
Effective spin	S=1	S=1
g-value	2.004	2.003
Fine structure parameter	$D=436.5\times10^{-4}$cm^{-1} E=0	$D=547.7\times10^{-4}$cm^{-1} $E=56.2\times10^{-4}$cm^{-1}
Measuring conditions	77 K, illumination (photon energies: 2.06–2.85 eV)	77 K, in darkness
Annealing temperature	~550°	~200°
Tentative model	$V_CV_{Si}^0$	C_i related defect

4. Summary

Two new EPR-centers with an effective electron spin S=1, L5 and L6, were observed in n-type 3C-SiC irradiated by 3-MeV electrons at room temperature with a dose of 2×10^{18} cm^{-2}. L5 had C_{3v}-symmetry with an isotropic g value g=2.004 and the fine-structure parameter $D=436.5\times10^{-4}$ cm^{-1}. The center disappears after annealing at ~550°C. Based on the similarity in the fine structure parameter of L5 and the P6'b center in 4H-SiC, the center is suggested to be the neutral divacancy. L6 had C_{2v} symmetry, with g=2.003 and the fine-structure parameters $D=547.7\times10^{-4}$ cm^{-1} and $E=56.2\times10^{-4}$ cm^{-1}. The center has low symmetry and low annealing temperature (~200°C). Therefore, a tentative model of a carbon-interstitial related defect is suggested for the L6 center. A conclusive identification of these two defects requires further investigations.

References

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