ESR characters of intrinsic defects in epitaxial semi-insulating 4H-SiC illuminated by Xe light*

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Abstract: The intrinsic defects in epitaxial semi-insulating 4H-SiC prepared by low pressure chemical vapor deposition (LPCVD) are studied by electron spin resonance (ESR) with different illumination times. The results show that the intrinsic defects in as-grown 4H-SiC consist of carbon vacancy (V_C) and complex-compounds-related V_C. There are two other apexes presented in the ESR spectra after illumination by Xe light, which are likely to be V_{Si} and V_CC_{Si}. Illumination time changes the relative density of intrinsic defects in 4H-SiC; the relative density of intrinsic defects reaches a maximum when the illumination time is 2.5 min, and the ratio of V_C to complex compounds is minimized simultaneously. It can be deduced that some V_{Si} may be transformed to the complex-compounds-related V_C because of the illumination.

Key words: electron spin resonance; low pressure chemical vapor deposition; intrinsic defects; semi-insulating 4H-SiC

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1. Introduction

One of the key issues in SiC technology is to develop high-purity semi-insulating (HPSI) substrates for high-frequency high-power electronics. In addition, semi-insulating (SI) SiC is considered to be the best substrate for GaN-based microwave devices. So preparation of HPSI SiC is an all-important task. At the present time, HPSI SiC substrates with low concentrations of structural defects have been achieved, which are suitable for some device applications. So far, many intrinsic defects in SI 4H-SiC bulk substrates grown by physical vapor transport (PVT) and high-temperature chemical vapor deposition (HTCVD) have been revealed from magnetic resonance and Hall-effect studies. These point defects play an important role both in limiting performance and compensating shallow dopants in SI substrates[1]. Some intrinsic defects in SI SiC material have been identified using electron paramagnetic resonance (EPR) and photoluminescence (PL) spectroscopies[2−6]. It is well known that Xe light can excite part of the intrinsic defects in SI SiC[5, 7−9], but there are few results on whether Xe light can affect the characters of intrinsic defects in SI SiC. In order to find the relationship between Xe light and intrinsic defects of SI 4H-SiC, we use ESR to study the characters of native defects in epitaxial SI 4H-SiC substrates prepared by LPCVD under different illumination times. When the illumination time increases, the relative density of intrinsic defects in SI 4H-SiC exhibits a periodical transformation.

2. Experimental details

The samples used in this experiment were epitaxial HPSI 4H-SiC grown by LPCVD techniques. The 4H-SiC crystal substrates which were of two inch size, were supplied by the SiCrystal AG Company. The ESR measurements were obtained using a JES-FA200 spectrometer operating near 9.0 GHz equipped by a nitrogen gas flow system with temperature control. All the presented ESR data were taken with the external magnetic field B oriented along the crystal c-axis. Optimum data were obtained at 120 K. A 750 W xenon lamp and appropriate optical filters were used in these tests. To analyze the spectral characters, the line width was computed by magnetic distance between apex and valley in EPR spectra; the Y value is defined in Eq. (2), the g vector is expressed by Eq. (1) and the relative intensity of the intrinsic defects is obtained by Eq. (2).

3. Results and discussion

ESR results measured at 120 K in darkness and under illumination for SI 4H-SiC substrates grown by LPCVD are shown in Figs. 1 and 2 respectively. The result in darkness is identical to the findings of as-grown samples[10], but it does not fit with those of Son *et al.*[5] and Janzén[6]. We believe the key factor affecting the characters of the ESR spectra is test temperature[10]. Unlike Fig. 1, there are two other apexes presented in Fig. 2; in addition, the line width is wider and the

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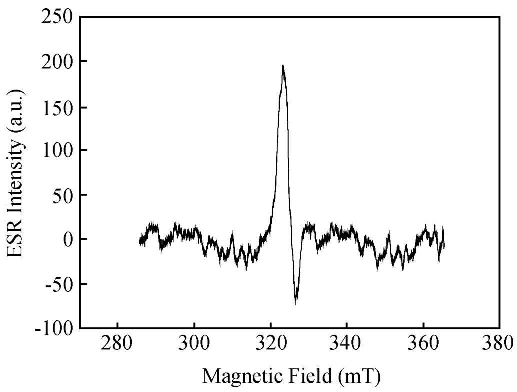

Fig. 1. ESR spectra measured at 120 K in darkness for SI 4H-SiC substrates grown by LPCVD.

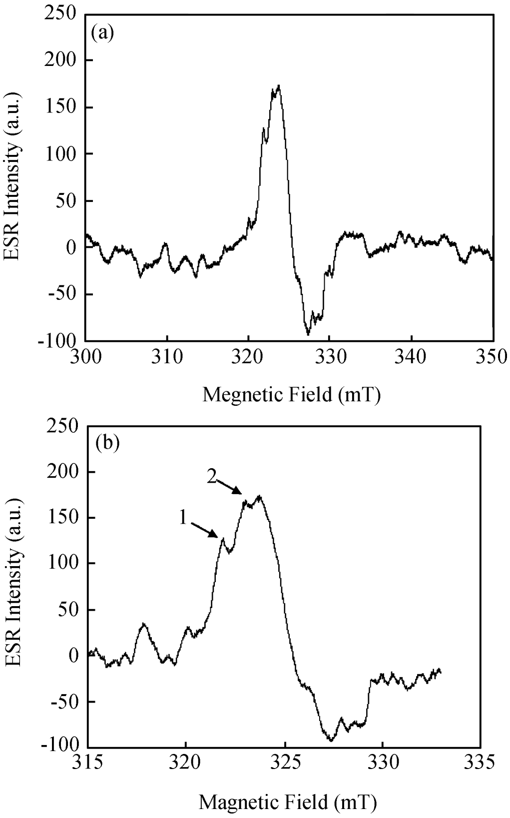

Fig. 2. ESR spectra measured at 120 K under illumination for SI 4H-SiC substrates grown by LPCVD: (a) ESR spectra in all magnetic field ranges; (b) Body of spectra in (a).

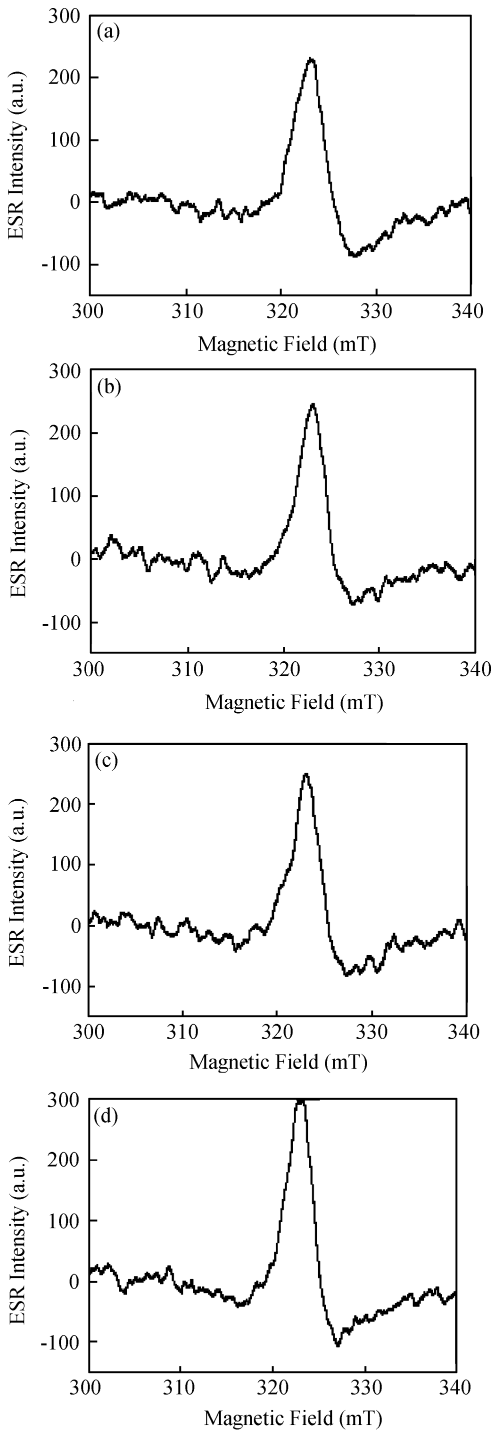

Fig. 3. ESR spectra measured under different illumination times at 120 K: (a) 2.5 min; (b) 5 min; (c) 8 min; (d) 10 min.

peak value is a little larger than that in darkness. Figure 3 illustrates the ESR results with different illumination times, from which we can conclude that the results seem to be in accordance with that of Fig. 1. That is to say, the intrinsic defects in SI 4H-SiC exposed in Xe light for certain times are the same as those in darkness, while momentary Xe light can excite some kinds of native defects, as identified in Refs. [3, 5, 6, 8, 9].

Based on the ESR theory, the g vector that exists in ESR spectra can be obtained by[11]

$$g = \frac{h\nu}{\beta H} = 0.714484\frac{\nu(\mathrm{MHz})}{H(\mathrm{G})}, \qquad (1)$$

where h is the Planck constant, ν is the microwave frequency, β is the Bohr magnetic and H is called the center magnetic field of the ESR signal. According to Eq. (1), the g vectors of the two side apexes in Fig. 2 are 2.013875 and 2.006690 respectively. It can be deduced that apex 1 is likely to be V_{Si} and apex 2 is likely to be $V_C C_{Si}$, referred to in Refs. [7, 8, 12, 13]; meanwhile the intrinsic defects of epitaxial SI 4H-SiC comprise the V_C and the complex-compounds-related V_C.

With longer illumination time, the ESR results are changed compared with Fig. 1. The two other apexes become faint. The correlative parameters under different test conditions, including the peak value Y, line width, g vector and relative density of intrinsic defects, are listed in Table 1.

Table 1. Correlative parameters of epitaxial SI 4H-SiC under different test conditions.

Parameter	As-grown	After illumination	Illumination 2.5 min	Illumination 5 min	Illumination 8 min	Illumination 10 min
Y (a.u)	264.25	267.88	319.75	318.86	335.38	406.75
Line width (mT)	3.20351	3.65279	4.80405	4.04102	4.37676	3.87011
g vector	1.995340	1.991100	1.989283	1.991240	1.991015	1.991000
Intensity ϑ	2711.859	3574.289	7379.477	5204.934	6424.549	6092.200

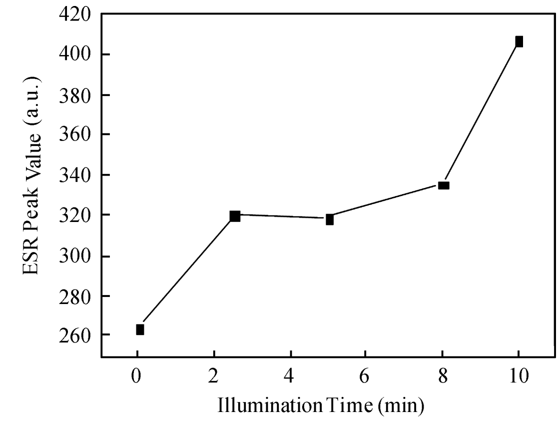

Fig. 4. Relationship between ESR peak illumination time in as-grown 4H-SiC.

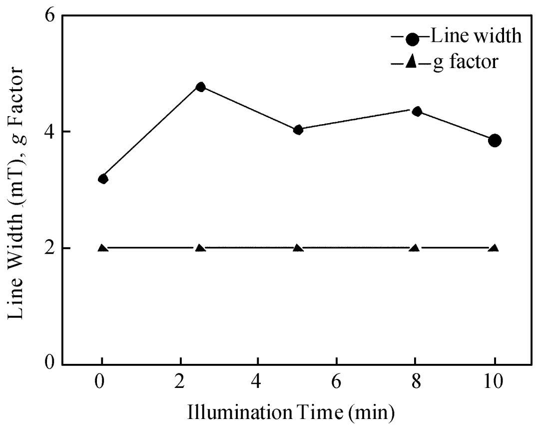

Fig. 5. Relationships between line width, g value and vector and illumination time in as-grown 4H-SiC.

According to Table 1, Figure 4 shows the changing trend of the ESR peak value as illumination time increases, and the variety of line widths and g vectors with different illumination times in epitaxial SI 4H-SiC are shown in Fig. 5. In Fig. 4, the ESR peak value increases rapidly in the first 2.5 min and between 8 and 10 min, descends appreciably from 2.5 to 5 min and ascends slowly between 5 and 8 min. In Fig. 5, the line width alters periodically and the range becomes smaller, while the g vectors remain almost constant during different illumination times. The g vectors only have a relative change within 0.111% and 0.193%, as shown in Table 1 and Fig. 5. This makes us believe that the intrinsic defects of epitaxial SI 4H-SiC comprise V_C and the complex-compounds-related V_C under different illumination times.

The results in Figs. 4 and 5 demonstrate that the duration of Xe light can change the intrinsic defects in SI 4H-SiC. The

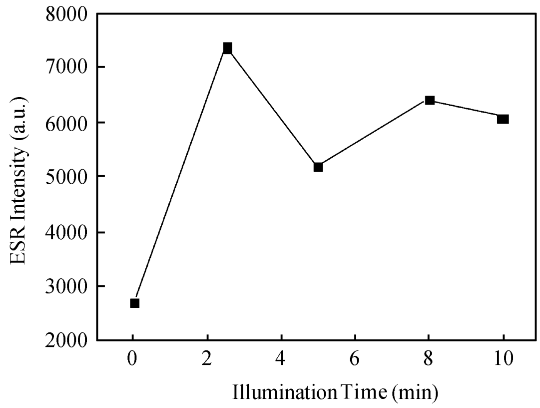

Fig. 6. Relationship between relative density of intrinsic defects and illumination time in SI 4H-SiC.

interrelation of the relative density of intrinsic defects and the illumination time in epitaxial SI 4H-SiC is shown in Fig. 6. The ESR intensity can be deduced[11] by Eq. (2).

$$\vartheta \propto Y\left(\Delta H_{pp}\right)^2, \tag{2}$$

where ϑ represents the ESR spectral intensity, Y is the sum of peak value and valley value, and ΔH_{pp} expresses the magnetic distance between apex and valley.

In Fig. 6, when the illumination time increases, the g vector changes a little, which should be caused by mutual transform between V_{Si} and the complex-compounds-related V_C[9]. At the illumination time of 2.5 min, the relative density of intrinsic defects reaches the maximum, while the g vector is minimized. It can be concluded that most intrinsic defects may be complex-compounds-related V_C at an illumination time of 2.5 min. Meanwhile, the longer the illumination time is, the lower the value of the observed curve inflexion is.

4. Summary

The intrinsic defect characters of epitaxial SI 4H-SiC substrates prepared by LPCVD are studied by the ESR technique. The results show that Xe light has an important effect on intrinsic defects of SI 4H-SiC. Firstly, the intrinsic defects in epitaxial SI 4H-SiC are V_C and the complex-compounds-related V_C in darkness. After illumination, there are two other apexes in the ESR spectra that are likely to be V_{Si} and V_CC_{Si}. Secondly, when the illumination time increases, the relative density of intrinsic defects in epitaxial SI 4H-SiC exhibits a periodical transformation. Finally, when the relative density of intrinsic defects is maximized at the illumination time of

2.5 min, the ratio of V_C to the complex-compounds-related V_C may be minimized. That is to say, some V_{Si} have been transformed to the complex-compounds-related V_C at the illumination time of 2.5 min.

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