Deep level defects in unintentionally doped 4H-SiC homoepitaxial layer*

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Abstract: Unintentionally doped 4H-SiC homoepitaxial layers grown by hot-wall chemical vapor deposition (HWCVD) have been studied using photoluminescence (PL) technique in the temperature range of 10 to 240 K. A broadband green luminescence has been observed. Vacancies of carbon (V_C) are revealed by electron spin resonance (ESR) technique at 110 K. The results strongly suggest that the green band luminescence, as shallow donor-deep accepter emission, is attributed to the vacancies of C and the extended defects. The broadband green luminescence spectrum can be fitted by the two Gauss-type spectra using nonlinear optimization technique. It shows that the broadband green luminescence originates from the combination of two independent radiative transitions. The centers of two energy levels are located 2.378 and 2.130 eV below the conduction band, respectively, and the ends of two energy levels are expanded and superimposed each other.

Key words: 4H-SiC Homoepitaxial layers; broadband green luminescence; vacancies of carbon; deep level defects
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1. Introduction

Silicon carbide (SiC) exists as several different polytypes according to the stacking sequence of SiC atomic double layers in the crystal lattice. One of the most important polytypes is 4H-SiC, which has the largest energy gap (3.26 eV), highest electric critical breakdown field (3–5 MV/cm), and high thermal conductivity. With its electronic properties, 4H-SiC devices, such as MOSFET, Schottky diodes, BJT and PIN diodes, can be used at higher blocking voltage and higher temperatures than silicon devices. These lead to higher switching speed, higher operating frequency and lower switching loss in the applications of aerospace, hybrid electric vehicles and more efficient electric power control and transmission[1−4]. Due to the large bandgap of SiC, intrinsic defects often have their ground states and in many cases also excited states within the bandgap and can be electrically and/or optically active[5, 6]. Among these, many are deep levels, which may act as efficient recombination centers and play an important role in carrier compensation processes[7−10]. Lots of work has been done in theory and experiment to explain the formation of deep level energy defects, but there are also several attitudes in some different samples [5, 6, 8, 11, 12]. So it is very useful for the improvement of 4H-SiC epitaxial layers growth to understand the formation of deep level energy defects and to confirm the donor level and acceptor level of defects.

In this study, unintentionally doped 4H-SiC homoepitaxial layers on 8° off-axis substrates by hot-wall chemical vapor deposition (CVD) have been investigated. Photoluminescence (PL) and electron spin resonance (ESR) technique are used to study the deep level energy defects, and the broadband green luminescence spectrum is fitted and divided by using nonlinear optimization technique. A new explanation for the reason of the broadband green luminescence is presented and the deep level energy is discussed.

2. Experiments

4H-SiC homoepitaxial growth was carried out in reactor using the $SiH_4/C_3H_8/H_2$ system[13]. The reactor was a commercial low-pressure, hot-wall CVD (LP-HW-CVD) reactor (Epigress VP508 system). The unintentionally doped 4H-SiC epitaxial layers were deposited on the Si-face (0001) 4H-SiC substrates, purchased from the SiCrystal. AG, n-doping concentration of about 5×10^{18} cm^{-3}, with 8° off axis, inclined toward $[11\bar{2}0]$. SiH_4 and C_3H_8 in H_2 were used as source gases for Si and C, respectively. The donor concentration was about 1.1×10^{15} cm^{-3} due to N_2 in background.

The PL measurements were performed at temperature varied from 10 to 240 K. The emission was excited by the 325 nm line of a He–Cd laser. EPR spectra were obtained using a conventional 9.07 GHz spectrometer equipped at 110 K in the dark for B$\|$c.

3. Results and discussion

Figure 1 shows the 10–240 K PL measurement results of sample, and a broadband green luminescence is observed. The intensity of luminescence becomes weak and the luminescence band becomes broad as the temperature increases, which

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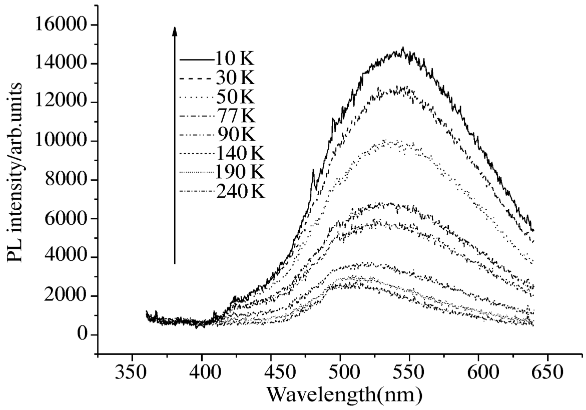

Fig. 1. PL measurements of sample at temperatures varied from 10 to 240 K.

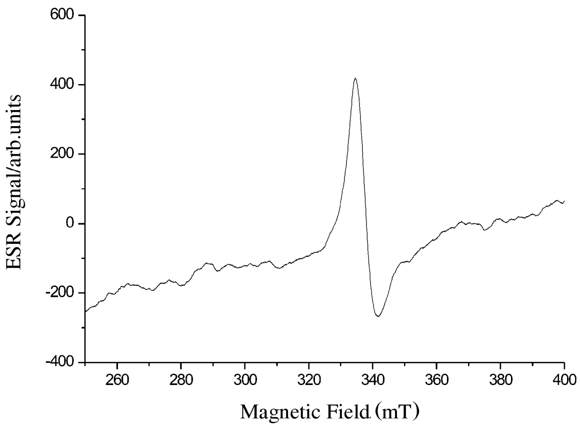

Fig. 2. ESR measurement of sample at 110 K in the dark for B||c.

are attributed to the lattice vibration and lattice scattering. Due to the luminescence caused by the recombination of donor and acceptor, the following equation can be obtained,

$$h\nu = E_g - (E_A + E_D) + e^2/\varepsilon_r. \tag{1}$$

Here the wave of luminescence is about 390.85 nm calculated according to Eq. (1) with $E_g = 3.23$ eV, $E_A = 0$ eV, $E_D = E_N = 0.06$ eV. The results obtained are different between the calculation and experiments. An energy level E_x may be located in the bandgap of SiC, and the green luminescence is caused by the recombination of shallow donor and deep acceptor level E_x.

There are different attitudes on the green luminescence[14–16], and several explanations are given. To confirm the origin of deep acceptor level E_x, electron spin resonance (ESR) measurement is used at 110 K in the dark for B||c, as shown in Fig. 2. Lots of carbon vacancies exist in the sample according to the intensity and location of ESR signal[8, 11, 12], which lead to many point defects. The broadband green luminescence depends on both the vacancies of carbon and its extended point defects. For this reason, the broadband green luminescence exists consistently, and the intensity and wavelength of luminescence change with the temperature variation.

The PL spectrum at 10 K is asymmetrical because of the asymmetrical distribution of the vacancies of carbon and its extended defects, as shown in Fig. 3. It indicates that the broadband green luminescence originates from the

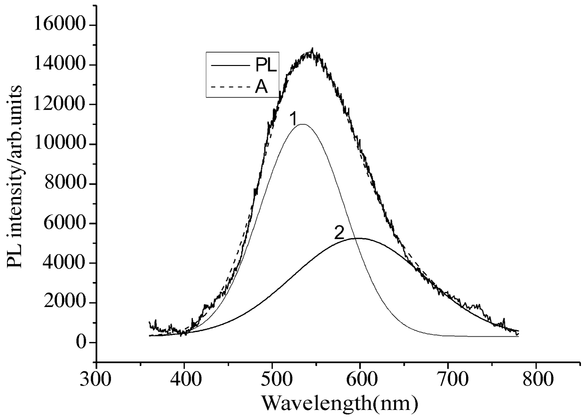

Fig. 3. PL spectrum at 10 K and fitting result with two Gauss-type spectra.

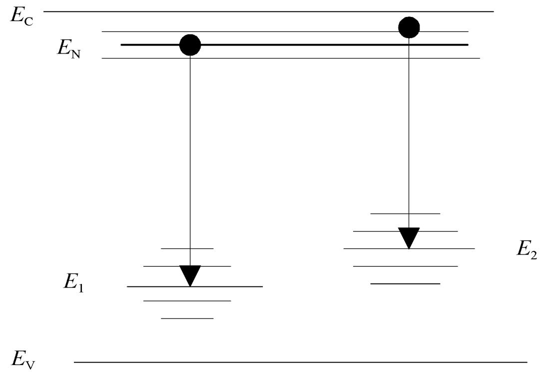

Fig. 4. Radiative model of the broadband green luminescence.

combination of several independent radiative transitions. Several pieces of Gauss-type spectra are attempted to fit the PL spectrum using nonlinear optimization technique, and it can be fitted by the two pieces of Gauss-type spectra, shown in Fig. 3. The combination of spectra 1 and 2 leads to the spectrum A, which is represented by the dotted line, as shown in Fig. 3. The spectrum A almost overlaps with the broadband green luminescence, which indicates that the broadband green luminescence is the combination of two independent radiative transitions. The centers of two energy levels are located 2.378 and 2.130 eV below the conduction band, respectively.

The radiative model of the broadband green luminescence can be given based on the spectra 1 and 2, as shown in Fig. 4. E_C, E_V and E_N stand for the conduction band, valence band and N shallow donor level, respectively. E_N is located 0.06 eV below the conduction band, and in fact it connects with the conduction band when extended. It is the reason that the luminous efficiency of green band is high and can compete with the transition of bandgap. The spectra 1 and 2 are Gauss distribution caused by deep level energy defects, so the level E_1 and E_2 are extended and superimposed each other, which lead to the emission spectrum superimposed each other and the broadband green luminescence is observed.

Based on the above analysis, to weaken or avoid the generation of green luminescence, vacancies of carbon should be suppressed. So in the process of 4H-SiC homoepitaxial growth, C/Si ratio should be increased under the condition that others of crystal, such as the quality of crystal, concentration of doping and roughness of surface, are not influenced.

4. Summary

Unintentionally doped 4H-SiC homoepitaxial layer have been investigated using photoluminescence and electron spin resonance (ESR) technique. It is shown that the broadband green luminescence is shallow donor-deep acceptor luminescence caused by vacancies of carbon and its extended point defects. Using nonlinear optimization technique, the broadband green luminescence spectrum can be fitted by the two Gauss-type spectra, which indicate that it originates from the combination of two independent radiative transitions. The centers of two energy levels are located 2.378 and 2.130 eV below the conduction band, respectively, and the ends of two energy levels are expanded and superimposed each other.

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