Effects of growth pressure on point defects in unintentionally doped 4H-SiC epitaxial layers

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Unintentionally doped 4H-SiC (0001) epilayers were performed on 4°off-axis substrates under varied pressures condition by CVD. It has been founded that the main point defects in 4H-SiC epitaxial layers performed under varied pressures are carbon vacancy and related complexes. A magnetic method is employed to precisely calculate the concentration of point defects in specimen. The concentration of carbon vacancy has been reduced from 2.17×10^{17} g^{-1} to 8.69×10^{16} g^{-1} with reduced growth pressure. Reduction of carbon vacancy in epilayers by decreasing the growth pressure is demonstrated. The reduction mechanism of the carbon vacancies is discussed.

1. Introduction

Silicon carbide (SiC) is a very desirable semiconductor material for applications of high power electronic devices owing to its superior physical properties such as wide bandgap, high thermal conductivity and high breakdown electric field strength [1]. However, high quality SiC layers still contain intrinsic defects acting as carrier traps or recombination centers under the current growth techniques, which degrade the minority carrier lifetime and lead to the reduction in conductivity. The $Z_{1/2}$ center has been recognized as one of the most important deep levels in 4H-SiC, known as a major lifetime killer [2,3]. Kawahara *et al.* reported that the $Z_{1/2}$ center originates from carbon vacancy (V_C), which is one of the intrinsic defects in 4H-SiC epitaxial layer [4]. Consequently, the minimization of the concentration of $Z_{1/2}$ center is to reduce the density of V_C essentially. Current strategies to reduce the density of V_C are mainly by post-growth processing such as thermal oxidation [5,6] or carbon implantation followed by thermal annealing [7,8]. Moreover, it has been founded that higher C/Si ratio [9-12] and reduction of growth temperature [10,11] during chemical vapor deposition (CVD) growth are effective ways to reduce density of point defects. However, new deep levels [5] which can affect lifetimes are generated after thermal oxidation or carbon implantation and growth parameters in CVD process should be carefully optimized to reduce extended defects and to maintain a good morphology. In our previous work, the effects of growth pressure on morphological and structural defects of 4H-SiC epilayers were investigated and it was founded that morphological defects reduce with the decreasing of growth pressure [13]. However, as a significant growth parameter in CVD growth process, there are few reports

about impacts of growth pressure on point defects in 4H-SiC epilayers.

In this study, the authors have investigated the effects of growth pressure on point defects in unintentionally doped 4H-SiC epilayers. The concentration of point defects with charged state which is related to the density of paramagnetic centers is determined by fitting the paramagnetic component of the specimen with the Brillouin function. It was found that the concentration of point defects can be reduced by the reduction of growth pressure. The correlation between point defects and growth pressure is discussed based on the results.

2. Experimental details

The authors prepared unintentionally doped epitaxial layers on 4° off-axis 4H-SiC (0001) n+ substrate by a commercial hot wall CVD Epigress VP508 with a standard chemistry of SiH_4-C_3H_8-H_2 [13]. The susceptor used in this study is TaC coated. To minimize the influence of substrate defects, all samples were performed on substrates cut from the same substrate. The growth temperature and C/Si ratio were 1580 ℃ and 1.0 for all samples, respectively. The growth pressures were varied from 40 to 100mbar. The growth rate and thickness of samples prepared at different growth pressures are approximately 10μm/h and 20 μm, respectively [13]. The net doping concentrations (N_d -N_a) of the epitaxial layers for each growth at different pressure were determined to be approximately 1×10^{15} cm^{-3} by C–V measurement. Low temperature photoluminescence (LTPL) with a 325 nm

He-Cd excitation laser was used to investigate the presence and change of intrinsic defects in epilayers performed at varied growth pressure. Electron spin resonance (ESR) measurements were performed on a X-band (~9.2 GHz) JES-FA200 ESR spectrometer at 130K. The magnetic measurements were carried out with a superconducting quantum interference device magnetometer (SQUID, MPMS-3, Quantum Design, Inc).

3. Results and discussion

Photoluminescence measurements were performed at 18 K to identify the defect type in unintentionally doped epilayers as shown in Fig. 1. The band edge part of LTPL spectra for the grown epilayers are assigned to zero-phonon lines of neutral donor bound exciton and phonon replicas of free and bound exciton. A broad PL peak, peaking in the vicinity of 2.2 eV, covering yellow–green spectral range is observed in low energy part of the LTPL spectra for all samples. The yellow–green luminescence of unintentionally doped 4H-SiC epilayers could be attributed to shallow donor-deep acceptor pair (DAP) emission [14] and our previous work reported that deep acceptor related to V_C and related complex defects [15]. The LTPL results demonstrate the existence of intrinsic defects in unintentionally doped 4H-SiC epilayers, principally carbon vacancies and related complex defects. In addition, it is clearly noted that the V_C and its complex defects related PL intensity is decreased as growth pressure decreases from 100 mbar to 40 mbar, indicating the reduction of intrinsic defects at lower growth pressure. It is clearly note that the PL spectra is relatively high in low energy part of the LTPL spectra for all samples, which may attribute to the following reason: SiC has relatively low absorption coefficients in the visible region, and gives large penetration depth for PL probe lasers. However, the depth rapidly decreases when UV lasers are used and the penetration depth for 325 nm (He-Cd excitation laser used in this study) is approximate 30 μm, which is thicker than the epilayers of 20 μm. It means part of photoluminescence intensity is contributed by the n$^+$ substrate. The high DAP emission in heavily doped 4H-SiC is reported by Ivanov *et al.* [14]. Besides, the PL results indicates that the concentration of carbon vacancy and related complex defects are relatively high in epilayers performed under high growth pressure conditions. Meanwhile, the higher measurement temperature may be a cause for the lower PL spectra of P and Q photon replica when comparing to PL spectra of DAP.
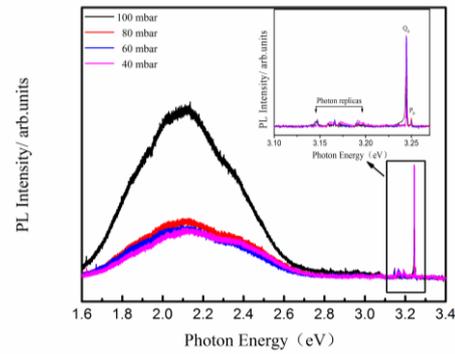

Fig. 1. Photoluminescence spectra of unintentionally doped 4H–SiC epilayers measured at T=18 K. The band edge part of the low temperature photoluminescence is shown in the inset

The ESR spectra of unintentionally doped 4H-SiC epilayers are shown in Fig. 2 with the magnetic field B parallel to the c-axis at 130K. The values of g factor of epilayers grown at varied pressures are in the range of 1.9943-2.0012 (shown in Table 1), which is the characteristic of carbon vacancies [16]. The ESR characterization further indicates that intrinsic defects in unintentionally doped 4H-SiC are mainly carbon vacancies and related complexes. The peak-to-peak width, ΔBpp, of epilayers grown from 40-100 mbar are 4.20127 mT, 4.88519 mT, 4.88520 mT and 5.37371 mT, respectively, indicating the variation of defect concentrations with varied growth pressures. Meanwhile, the ESR spectra of samples exhibit a line shape of nearly Lorentzian form, which can be attributed to the existence of isolated magnetic moments [17]. Therefore, carbon vacancies are responsible for the existence of magnetic moments, which agrees with previous investigation reported by Jenny et al. [18].
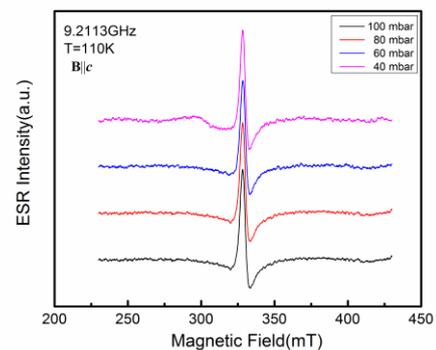

Fig. 2. ESR spectra of the unintentionally doped 4H-SiC epilayers grown at varied pressures

Table 1. The density of paramagnetic centers N and the value of g and J

Samples	g_J	J	$N(g^{-1})$
40 mbar	1.9943	1	8.69×10^{16}
60 mbar	1.9964	1	9.53×10^{16}
80 mbar	1.9959	1	1.83×10^{17}
100 mbar	2.0012	1	2.17×10^{17}

The magnetization-field curves of typical epitaxial specimen at 5K and 300K are shown in Fig. 3(a). For a precise calculation, the magnetization of substrates had been subtracted. The minus slopes for all curves indicate a typical diamagnetic behavior. However, clear deviations can be observed between the curves at 5K and 300K, which demonstrates the existence of paramagnetism in 4H-SiC epilayers [19]. As a first order of approximation, the paramagnetic component can be extracted by subtracting the diamagnetism measured at 300 K, since the diamagnetism is essentially temperature independent, as shown in Fig. 3(b). The paramagnetic component can be fitted by the Brillouin function:

$$M(x) = N J \mu_B g_J \left[\frac{2J+1}{2J} coth \left(\frac{2J+1}{2J} x \right) - \frac{1}{2J} coth \left(\frac{1}{2J} x \right) \right] \quad (1)$$

$$x = g_J \mu_B J \mu_0 H / k_B T \quad (2)$$

Where M(x) is the magnetization, μB is the Bohr magneton, J=1 is the total angular momentum of the paramagnetic center, the Landé factor gJ is obtained from ESR measurement and N is the density of paramagnetic centers. As revealed in ESR characterization, V_C is the main intrinsic paramagnetic defects in specimen. Therefore, the concentration of point defects is represented by the density of paramagnetic centers. The calculated densities of paramagnetic centers in specimen are shown in Table 1. It is found that the value of N decreases with the reduction of growth pressure, which agrees well with the results obtained from photoluminescence and ESR measurements.
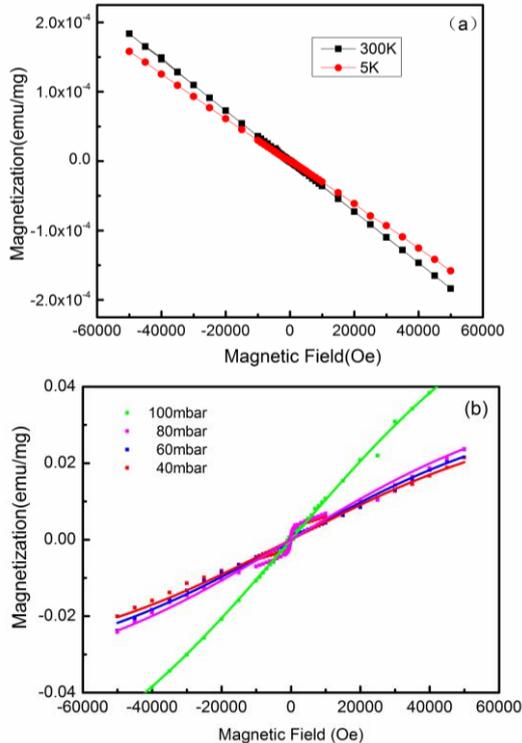

Fig. 3. (a) M-H curves of a typical epitaxial specimen at 5 K and 300 K. (b) paramagnetic component of specimens performed at varied growth pressures and the Brillouin fitting curves

The reduction of point defects with decreased growth pressure may attribute to the following reasons: Firstly, the researches of modeling simulation [20] and experiments [21, 22] have demonstrated that the relative mole fraction of C-containing gaseous species increases with reduced growth pressure in a CVD reactor with a standard chemistry of SiH_4-C_3H_8-H_2, which means the effective C/Si ratio on the growth surface increases at lower pressure even though the inlet C/Si ratio is kept constant. It had been reported [9-12] that reduction of point defects was observed in atmosphere with higher C/Si ratio. On the other hand, owing to the decreased supersaturation at lower growth pressure, step-flow growth mode is enhanced by lowering growth pressure [13]. It is reasonable to believe that the enhancement of step-flow growth increases surface migration of absorbed adatoms and the possibility of incorporation of carbon atoms. As a consequence, the formation of intrinsic defects is suppressed at lower growth pressure.

4. Conclusions

4H-SiC epilayers are performed under varied pressures. Photoluminescence and electron spin resonance spectra reveal that carbon vacancy and related complexes, the main point defects in 4H-SiC epitaxial layers, are suppressed with reduction of the growth pressure. Point defects concentrations are precisely characterized by Brillouin fitting of paramagnetic component of the epilayers. The concentration of carbon vacancy has been reduced from 2.17×10^{17} g^{-1} to 8.69×10^{16} g^{-1}, which verifies the tendency obtained from Photoluminescence and electron spin resonance spectra. The authors propose that phenomenon observed above may attributed to the increase of effective C/Si ratio on the growth surface and enhancement of step-flow growth at lower pressure, which increases the possibility of incorporation of carbon atoms and suppresses the formation of point defects. It is experimentally demonstrated that growth pressure plays a significant role in the formation of point defects and the authors suggest that lower pressure growth is a strategy for the reduction of carbon vacancy.

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