Materials Science Forum Vols. 433-436 (2003) pp. 447-450
Online at http://www.scientific.net

Real Relationship between Acceptor Density and Hole Concentration in Al-implanted 4H-SiC

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Keywords: acceptor density, acceptor level, Al implantation, excited states, Hall-effect measurement

Abstract. Al-implanted p-type 4H-SiC layers with different conditions of implantation and annealing temperatures are formed, and the temperature dependence of the hole concentration $p(T)$ in the p layer is obtained from Hall-effect measurements. In order to determine the reliable acceptor density (N_A) from $p(T)$, it is found that the Fermi-Dirac distribution function is not appropriate and that a distribution function including the influence of the excited states of Al acceptors is required. This is because the Al acceptor level in SiC is deep (~180 meV) and because its first excited state level, which is calculated by the hydrogenic model, is still deep (~35 meV), which is close to the acceptor level of B in Si. It is demonstrated that the proposed distribution function is suitable for obtaining the actual relationship between N_A and $p(T)$.

Introduction

The relationship between a dopant density and a temperature-dependent majority-carrier concentration in semiconductor is important for device simulations. Here, this relationship means a distribution function for dopants.

Excited states of a substitutional dopant in a semiconductor have been theoretically discussed using the hydrogenic model [1], and the existence of the excited states of B or P in Si has been experimentally confirmed from infrared absorption measurements at very low temperatures [1]. Since the Al acceptor level (ΔE_A) in SiC, measured from the valence band maximum (E_V), was reported to be ~180 meV from photoluminescence studies [2], the excited state levels should influence the temperature dependence of the hole concentration $p(T)$, indicating that a distribution function including the influence of the excited states of Al acceptors should be required.

Although an acceptor density (N_A) in Al-doped or Al-implanted p-type SiC was determined by a least-squares fit of the charge neutrality equation to $p(T)$ using the Fermi-Dirac (FD) distribution function $f_{FD}(\Delta E_A)$ that does not include the influence of the excited states, the value of N_A was much higher than the concentration of Al atoms (N_{Al}) in SiC [3-5]. This indicates that the obtained N_A is not reliable, because N_A, which means the density of Al atoms located at substitutional sites in SiC, is less than or equal to N_{Al}.

There are the following two reports to determine the actual acceptor density from Hall-effect measurements; (1) the experimental adjustment of Hall scattering factor for holes (γ) and (2) the theoretical introduction of a distribution function suitable for deep acceptors. Pensl has strongly insisted that γ should be temperature-dependent (0.5~1.2) [4]. On the other hand, we have proposed a distribution function including the influence of the excited states [5].

From a viewpoint of the latter, we discuss N_A, ΔE_A and the compensating density (N_{comp}) in Al-implanted p-type 4H-SiC with different implantation temperatures ($T_{implant}$) and annealing temperatures (T_{anneal}) using the FD and proposed distribution functions.

Distribution Functions

The proposed distribution function at ΔE_A in a forbidden band, which includes the influence of the excited states of acceptors, is described as [5]

$$f(\Delta E_A) = \frac{1}{1 + 4\exp\left(-\frac{\overline{E_{ex}}}{kT}\right)\cdot\left[\exp\left(\frac{\Delta E_A - \Delta E_F}{kT}\right) + \sum_{r=2} g_r \exp\left(\frac{\Delta E_r - \Delta E_F}{kT}\right)\right]}, \quad (1)$$

where ΔE_F is the Fermi level measured from E_V, k is the Boltzmann constant, T is the absolute temperature, ΔE_r is the $(r-1)$th excited state level measured from E_V, g_r is the $(r-1)$th excited state degeneracy factor ($g_r = r^2$), and $\overline{E_{ex}}$ is an ensemble average of the ground ($r = 1$) and excited state ($r \geq 2$) levels of the acceptor, which is given by [5,6]

$$\overline{E_{ex}} = \frac{\sum_{r=2}(\Delta E_A - \Delta E_r) g_r \exp\left(-\frac{\Delta E_A - \Delta E_r}{kT}\right)}{1 + \sum_{r=2} g_r \exp\left(-\frac{\Delta E_A - \Delta E_r}{kT}\right)}. \quad (2)$$

When the influence of the excited states is ignored (i.e., $r = 1$ and $\overline{E_{ex}} = 0$), Eq. 1 coincides with $f_{FD}(\Delta E_A)$. When $\overline{E_{ex}} = 0$ although the excited states are considered, on the other hand, Eq. 1 coincides with the conventional distribution function $f_{conv}(\Delta E_A)$ [5,7].

Free Carrier Concentration Spectroscopy

Free carrier concentration spectroscopy (FCCS) can accurately determine the densities and energy levels of impurities and traps from Hall-effect measurements [8]. Using an experimental $p(T)$, the FCCS signal is defined as [8]

$$H(T, E_{ref}) \equiv \frac{p(T)^2}{(kT)^{5/2}} \exp\left(\frac{E_{ref}}{kT}\right). \quad (3)$$

The FCCS signal has a peak at the temperature corresponding to each acceptor level or hole trap level, where E_{ref} is the parameter that can shift the peak temperature of $H(T, E_{ref})$ within the temperature range of the measurement. From each peak value and peak temperature, the density and energy level of the corresponding acceptor or hole trap can be accurately determined. FCCS can adopt any distribution function to the determination of the densities and energy levels from $p(T)$. When $f_{FD}(\Delta E_A)$ is adopted, the values obtained by FCCS coincides with those determined by the curve-fitting procedure of $p(T)$.

Experimental

In order to form p-type 4H-SiC layers, Al ions were implanted at room temperature or 1000 °C to 5-μm-thick n-type 4H-SiC epilayers with N atoms of 2.5×10^{15} cm^{-3} on n-type 4H-SiC {0001} substrate with 8° off to $<11\bar{2}0>$ direction. In order to obtain a box profile of N_{Al}, seven-fold Al ion implantation was carried out with different energies onto the SiC epilayer surface tilted to 7° to normal. Each dose of Al ions was 3.0×10^{14} cm^{-2}, and the implantation energies were 1.0, 1.6, 2.4, 3.3, 4.4, 5.6 and 7.0 MeV. After the implantation, the sample was annealed at 1443 °C or 1575 °C for 1 hr in an Ar atmosphere. The Rutherford backscattering spectroscopy (RBS) spectra were measured using 2 MeV He ions.

The 1.3-μm-thick layer from the surface was removed by reactive ion etching, and then the sample was cut into a 4×4 mm^2 size. Ohmic metal (Al/Ti) was deposited on four corners of the etched surface, and the sample was annealed. $p(T)$ was measured by the van der Pauw method at temperatures between 100 K and 420 K and in a magnetic field of 1.4 T.

Table 1 Sample preparation conditions and obtained results.

Sample number	$T_{implant}$ [°C]	T_{anneal} [°C]	N_A [cm^{-3}]	ΔE_A [eV]	N_{comp} [cm^{-3}]
pSiC(HH)	1000	1575	1.21×10^{19}	0.177	2.29×10^{17}
pSiC(HL)	1000	1443	9.49×10^{18}	0.187	1.62×10^{17}
pSiC(LH)	Room temp.	1575	7.14×10^{18}	0.178	6.44×10^{16}
pSiC(LL)	Room temp.	1443	5.44×10^{18}	0.183	1.23×10^{17}

Results and Discussion

The profile of N_{Al} was calculated by the Monte Carlo simulation (SRIM-2000). The box profile of Al atoms was confirmed and the average N_{Al} in the p layer was ~1×10^{19} cm^{-3}. The RBS spectrum in the sample implanted at 1000 °C was substantially below that in the sample implanted at room temperature. The RBS spectra of the annealed samples were close to the virgin level.

Four p-type 4H-SiC layers with different $T_{implant}$ and T_{anneal} were investigated, as shown in Table 1. Two $p(T)$ in pSiC(HH) and pSiC(LH) are higher than those in pSiC(HL) and pSiC(LL). While $p(T)$ in pSiC(LH) is the highest at < 290 K, $p(T)$ in pSiC(HH) is the highest at > 290 K.

The open circles in Fig. 1 represent the experimental $H(T,E_{ref})$ with $E_{ref} = 0.231$ eV for pSiC(HH). In the FCCS analyses, $H(T,E_{ref})$ was calculated by interpolating $p(T)$ with a cubic smoothing natural spline function at intervals of 0.1 K. The peak temperature and peak value are 381.8 K and 5.86×10^{42} cm^{-6}eV$^{-2.5}$, respectively. From this peak, the values of N_A determined by FCCS using $f(\Delta E_A)$, $f_{FD}(\Delta E_A)$ and $f_{conv}(\Delta E_A)$ are 1.21×10^{19}, 4.85×10^{19} and 4.69×10^{20} cm^{-3}, respectively, where in $f(\Delta E_A)$ or $f_{conv}(\Delta E_A)$ the highest excited state considered in the FCCS analyses was the fourth excited state. The value of N_A determined using $f(\Delta E_A)$ is close to N_{Al}, while the others are much higher than N_{Al}, suggesting that $f(\Delta E_A)$ is appropriate.

In Fig. 1, the solid, broken and dotted curves represent $H(T,E_{ref})$ simulated using N_A, ΔE_A and N_{comp} corresponding to $f(\Delta E_A)$, $f_{FD}(\Delta E_A)$ and $f_{conv}(\Delta E_A)$, respectively. Although all the peaks of three simulated $H(T,E_{ref})$ coincide with the peak of the experimental $H(T,E_{ref})$, the solid curve is in better agreement with the experimental $H(T,E_{ref})$ than the others. This indicates that the values determined using $f(\Delta E_A)$ are more reliable than the others.

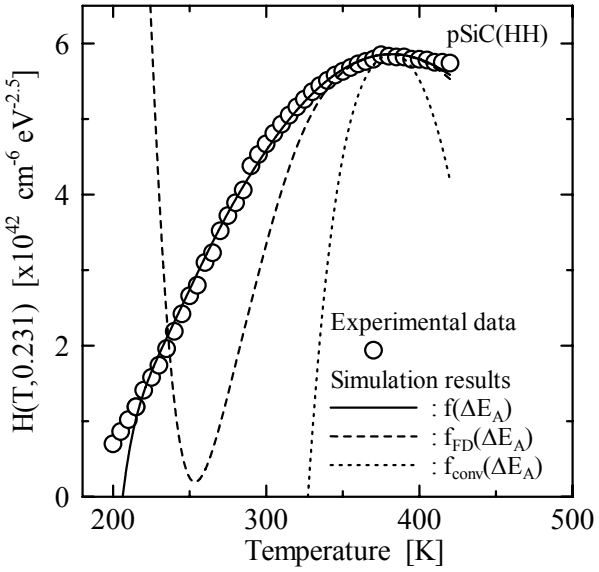

Fig. 1 Experimental and simulated $H(T,E_{ref})$.

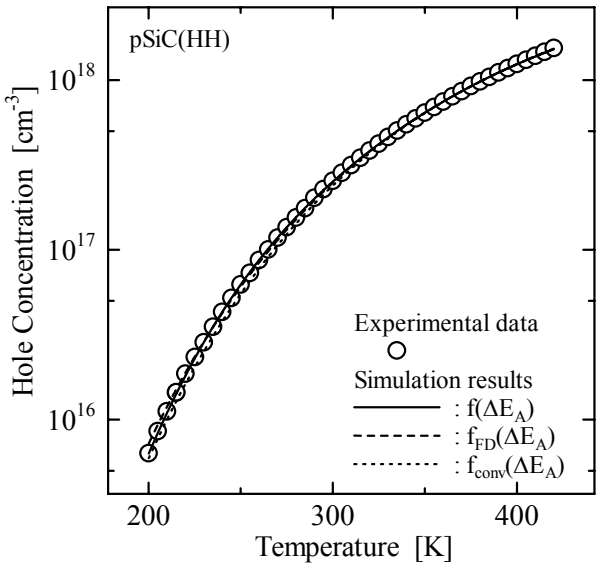

Fig. 2 Experimental and simulated $p(T)$.

In Fig. 2, the open circles represent the experimental $p(T)$, and the solid, broken and dotted curves show $p(T)$ simulated using N_A, ΔE_A and N_{comp} corresponding to $f(\Delta E_A)$, $f_{FD}(\Delta E_A)$ and $f_{conv}(\Delta E_A)$, respectively. Since all the simulated $p(T)$ are in good agreement with the experimental $p(T)$, it is difficult to investigate the influence of the excited states of Al acceptors on $p(T)$ by the curve-fitting procedure of $p(T)$.

Table 1 also shows N_A, ΔE_A and N_{comp} determined using $f(\Delta E_A)$ for all the samples. All the obtained values are considered to be reliable, because all the N_A are less than or close to N_{Al} and because all the ΔE_A are close to ΔE_A obtained from PL. Here, all the N_A determined using $f_{FD}(\Delta E_A)$ and $f_{conv}(\Delta E_A)$ were much higher than N_{Al}. Almost all implanted Al atoms in pSiC(HH) act as an acceptor, while only an half of them in pSiC(LL) behave like an acceptor. By making a comparison between two N_A in pSiC(HH) and pSiC(LH), $T_{implant}$ is effective in forming acceptors in SiC.

Summary

Although there have been two reports to determine the actual N_A from Hall-effect measurements, a theoretical introduction of a distribution function suitable for deep acceptors was adopted here. Al-implanted p-type 4H-SiC layers with different $T_{implant}$ and T_{anneal} were fabricated, and $p(T)$ in those layers were obtained from Hall-effect measurements. Then, N_A, ΔE_A and N_{comp} were determined using three kinds of distribution functions for Al acceptors. It was found that the proposed distribution function considering the influence of the excited states of acceptors was the most suitable. Moreover, it was demonstrated that the proposed FCCS could study the influence of the excited states of acceptors in detail, while the curve-fitting procedure of $p(T)$ could not. When $T_{implant} = 1000$ °C and $T_{anneal} = 1575$ °C, almost all implanted Al atoms were found to behave like an acceptor in 4H-SiC.

Acknowledgments

The authors would like to thank Dr. H. Sugimoto in Mitsubishi Electric Corp. and Dr. K. Sekine in Ion Engineering Research Institute Corp. for the sample preparation and RBS measurements. This work was partially supported by the Academic Frontier Promotion Projects of the Ministry of Education, Culture, Sports, Science and Technology, and it was also partially supported by the R&D Association of Future Electron Devices (FED) and the New Energy and Industrial Technology Development Organization (NEDO).

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