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

H. Matsuura, K. Sugiyama, K. Nishikawa, T. Nagata and N. Fukunaga

Department of Electronic Engineering and Computer Science, Osaka Electro-Communication University, 18-8 Hatsu-cho, Neyagawa, Osaka 572-8530, Japan

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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 \( N_\Lambda \) 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 \( N_\Lambda \) 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 \( \Delta E_\Lambda \) 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 \( N_\Lambda \) 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 \( f_{\text{FD}}(\Delta E_\Lambda) \) that does not include the influence of the excited states, the value of \( N_\Lambda \) was much higher than the concentration of Al atoms \( N_{\text{Al}} \) in SiC [3-5]. This indicates that the obtained \( N_\Lambda \) is not reliable, because \( N_\Lambda \), which means the density of Al atoms located at substitutional sites in SiC, is less than or equal to \( N_{\text{Al}} \).

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 \( \gamma \) and (2) the theoretical introduction of a distribution function suitable for deep acceptors. Pensl has strongly insisted that \( \gamma \) 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 \( N_\Lambda, \Delta E_\Lambda \) and the compensating density \( N_{\text{comp}} \) in Al-implanted p-type 4H-SiC with different implantation temperatures \( T_{\text{implant}} \) and annealing temperatures \( T_{\text{anneal}} \) using the FD and proposed distribution functions.
Distribution Functions

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

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

where $\Delta E_f$ is the Fermi level measured from $E_v$, $k$ is the Boltzmann constant, $T$ is the absolute temperature, $\Delta E_r$ 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 $E_{ex}$ 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]

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

When the influence of the excited states is ignored (i.e., $r=1$ and $E_{ex} = 0$), Eq. 1 coincides with $f_{FD}(\Delta E_A)$. When $E_{ex} = 0$ 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]

$$H(T, E_{ref}) = \frac{p(T)^2}{(kT)^2} \exp\left(\frac{E_{ref}}{kT}\right).$$

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 $2.5 \times 10^{15}$ cm$^{-3}$ on n-type 4H-SiC {0001} substrate with 8° off to <1120> 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 $3.0 \times 10^{14}$ 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.
Results and Discussion

The profile of 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 $\sim 1 \times 10^{19}$ 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 $5.86 \times 10^{42}$ 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 $1.21 \times 10^{19}$, $4.85 \times 10^{19}$ and $4.69 \times 10^{20}$ 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 $N_A$, $\Delta E_A$ 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.

<table>
<thead>
<tr>
<th>Sample number</th>
<th>$T_{implant}$ [°C]</th>
<th>$T_{anneal}$ [°C]</th>
<th>$N_A$ [cm$^{-3}$]</th>
<th>$\Delta E_A$ [eV]</th>
<th>$N_{comp}$ [cm$^{-3}$]</th>
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<tbody>
<tr>
<td>pSiC(HH)</td>
<td>1000</td>
<td>1575</td>
<td>$1.21 \times 10^{19}$</td>
<td>0.177</td>
<td>$2.29 \times 10^{17}$</td>
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<tr>
<td>pSiC(HL)</td>
<td>1000</td>
<td>1443</td>
<td>$9.49 \times 10^{18}$</td>
<td>0.187</td>
<td>$1.62 \times 10^{17}$</td>
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<tr>
<td>pSiC(LH)</td>
<td>Room temp.</td>
<td>1575</td>
<td>$7.14 \times 10^{18}$</td>
<td>0.178</td>
<td>$6.44 \times 10^{16}$</td>
</tr>
<tr>
<td>pSiC(LL)</td>
<td>Room temp.</td>
<td>1443</td>
<td>$5.44 \times 10^{18}$</td>
<td>0.183</td>
<td>$1.23 \times 10^{17}$</td>
</tr>
</tbody>
</table>

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 $N_A$, $\Delta E_A$ and $N_{\text{comp}}$ corresponding to $f(\Delta E_A)$, $f_{\text{FD}}(\Delta E_A)$ and $f_{\text{conv}}(\Delta E_A)$, 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 $N_A$, $\Delta E_A$ and $N_{\text{comp}}$ 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 $\Delta E_A$ are close to $\Delta E_A$ obtained from PL. Here, all the $N_A$ determined using $f_{\text{FD}}(\Delta E_A)$ and $f_{\text{conv}}(\Delta E_A)$ 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(LL), $T_{\text{implant}}$ 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. AI-implanted p-type 4H-SiC layers with different $T_{\text{implant}}$ and $T_{\text{anneal}}$ were fabricated, and $p(T)$ in those layers were obtained from Hall-effect measurements. Then, $N_A$, $\Delta E_A$ and $N_{\text{comp}}$ 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 $T_{\text{implant}}=1000$ °C and $T_{\text{anneal}}=1575$ °C, almost all implanted Al atoms were found to behave like an acceptor in 4H-SiC.

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References