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Electrical Behavior of Mg in Mg-Implanted 4H-SiC Layer

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Because Al and B (elements of group III) in SiC are acceptors with deep energy levels and these acceptors cannot reduce the resistivity of p-type SiC very much, Mg (an element of group II) that may emit two holes into the valence band is investigated. Annealing at 1800 °C makes a Mg-implanted layer p-type. It is found that an Mg acceptor level in 4H-SiC is too deep to reliably determine the density and energy level of the Mg acceptor using the frequently used occupation probability, i.e., the Fermi–Dirac distribution function. Using the distribution function that accounts for the influence of the excited states of a deep-level acceptor, the density and energy level of Mg acceptors can be determined to be approximately 1×10^{19} cm^{-3} and 0.6 eV, respectively. These values are considered to be reliable because they agree well with the Mg implantation condition.

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1. Introduction

Silicon carbide (SiC) is attractive as semiconductor because of its wide band gap, high electron mobility, high electron saturation drift velocity, and high thermal conductivity. As a result, SiC has been identified as a promising candidate semiconductor for devices that operate at high power, high frequency, and high temperature.

The acceptor levels of Al and B in 4H-SiC were reported to be approximately 0.2 and 0.3 eV, respectively [1–9], and two N donor levels in 4H-SiC were reported to be approximately 0.05 and 0.1 eV [1, 10]. Because these accepter levels are much deeper than a B acceptor level in Si (0.045 eV) [11] as well as the N donor levels in 4H-SiC, it is difficult to lower the resistivity of p-type 4H-SiC, indicating that contact resistance between an electrode and p-type SiC is high. Since elements of group II can emit two holes into the valence band in SiC when these elements are replaced by Si or C, the associated acceptors might reduce the resistivity of p-type 4H-SiC. Two acceptor levels of Be in 6H-SiC were reported in p-type 6H-SiC prepared by the diffusion of Be [12]. However, because these acceptor levels determined by Hall-effect measurements were reported to be 0.4 and 0.6 eV [12], those were too deep.

To reliably determine the acceptor density and energy level of Mg (i.e., another element of group II) in 4H-SiC, in this study, we investigate the electrical properties in Mg-implanted 4H-SiC layers by Hall-effect measurements.

2. Experimental

Mg ions were implanted at 500 °C to 5 μm thick n-type 4H-SiC epilayers with N atoms of 5×10^{15} cm^{-3} on 0.36 mm thick n^+-type 4H-SiC substrate with the resistivity between 0.013 and 0.025 Ωcm. To obtain a box profile of the concentration of Mg atoms (C_{Mg}), tenfold Mg ion implantation was carried out by the implantation energies of 20, 40, 80, 120, 170, 230, 300, 400, 550, and 700 keV with the corresponding Mg doses of 1.3×10^{13}, 3.6×10^{13}, 5.0×10^{13}, 5.3×10^{13}, 7.2×10^{13}, 7.8×10^{13}, 9.5×10^{13}, 1.35×10^{14}, 1.40×10^{14}, and 1.95×10^{14} cm^{-2}, respectively. Judging from the depth profile of C_{Mg} simulated in the manner of Biersack [13] by the stopping and range of ion in matter (SRIM2006) using the Mg implantation condition mentioned above, this implantation formed an 800 nm thick Mg-implanted 4H-SiC layer with C_{Mg} of approximately 1×10^{19} cm^{-3}.

After the implantation, the sample covered with diamond-like carbon (DLC) was annealed at 1800 °C for 5 min. The DLC layers were removed and ohmic metal (Al/Ti) was deposited on four corners of one side of the sample. The sample was annealed at 900 °C for 1 min in an Ar atmosphere. The Hall-effect measurements were carried out between 300 and 800 K under a magnetic field of 0.45 T by a Toyo ResiTest8300.

3. Results and discussion

The Mg-implanted 4H-SiC layer annealed at 1800 °C showed p-type conduction. Figure 1 shows the temperature dependence of the hole concentration ($p(T)$) in the Mg-implanted 4H-SiC layer annealed at 1800 °C, denoted by open circles, on the frequently used assumption that a Hall-scattering factor for holes ($\gamma_{\mathrm{H}}(T)$) is 1. It is clear from its temperature dependence that the Mg-implanted 4H-SiC layer is a non-degenerate semiconductor. The values of $p(T)$ increased as the temperature increased, and reached 3.0×10^{18} cm^{-3} at 800 K, which is close to C_{Mg}.

Figure 2 shows the temperature dependence of the hole mobility ($\mu_{\mathrm{h}}(T)$). Because at the same temperature $\mu_{\mathrm{h}}(T)$ in the Mg-implanted 4H-SiC layer was only a little bit lower than the value of $\mu_{\mathrm{h}}(T)$ in the Al-implanted

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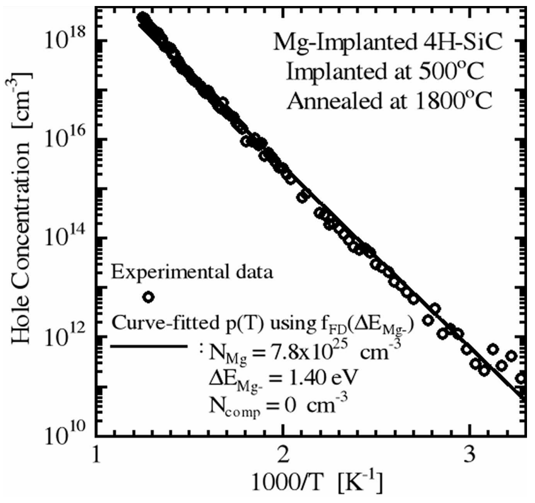

Fig. 1. Temperature dependence of hole concentration in Mg-implanted 4H-SiC, and $p(T)$ fitted by the method of least squares using the Fermi–Dirac distribution function without N_{comp}.

4H-SiC layer [3], the holes moved in the valence band, not by hopping. As a result, it is found that Mg atoms in 4H-SiC emit holes into the valence band and behave as an acceptor.

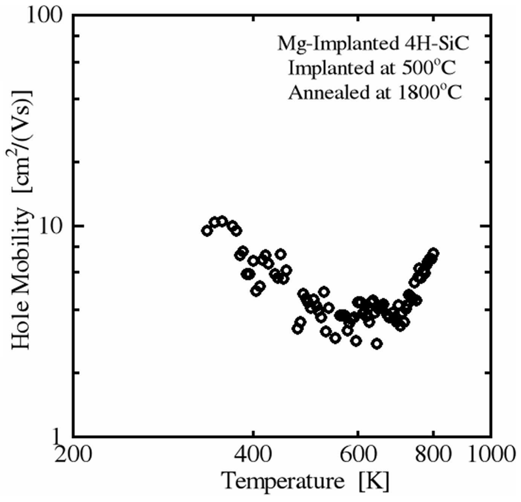

Fig. 2. Temperature dependence of hole mobility in Mg-implanted 4H-SiC.

Figure 3 shows the temperature dependence of the Fermi level ($\Delta E_{\mathrm{F}}(T)$) measured from the valence band maximum (E_{V}), given by [2, 4, 6]:

$$\Delta E_{\mathrm{F}}(T) = kT \ln\left(\frac{N_{\mathrm{V}}(T)}{p(T)}\right), \tag{1}$$

where $N_{\mathrm{V}}(T)$ is the effective density of states in the valence band, given by [2, 4, 6, 11]:

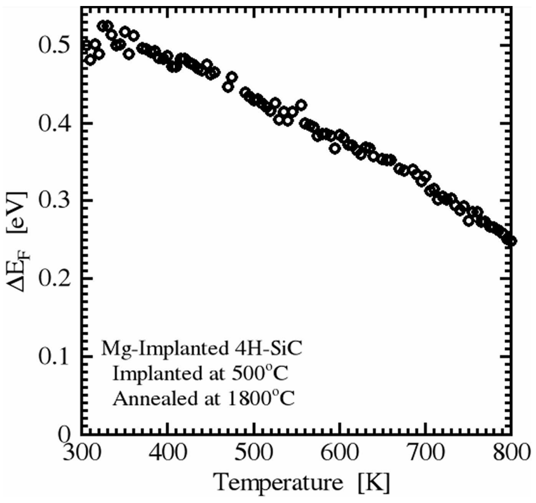

Fig. 3. Temperature dependence of the Fermi level in Mg-implanted 4H-SiC.

$$N_{\mathrm{V}}(T) = 2\left(\frac{2\pi m_{\mathrm{h}}^{*} kT}{h^2}\right)^{3/2}, \tag{2}$$

m_{h}^{*} is the hole-effective mass in 4H-SiC, k is the Boltzmann constant, and h is Planck's constant. From the figure, the Mg acceptor level (ΔE_{Mg}) measured from E_{V} seems to be deeper than 0.5 eV because $\Delta E_{\mathrm{F}}(T)$ at around 300 K were approximately 0.5 eV. This means that Mg in 4H-SiC behaves as a deep-level acceptor.

The density (N_{Mg}) of Mg acceptors and the energy level (ΔE_{Mg^-}) of negative singly-ionized Mg acceptors in the Mg-implanted 4H-SiC layer were investigated by testing the least-squares fit to the experimentally obtained $p(T)$ in Fig. 1. From the neutrality condition, $p(T)$ is given by [1–6, 11]:

$$p(T) = N_{\mathrm{Mg}} f_{\mathrm{FD}}(\Delta E_{\mathrm{Mg}^-}) - N_{\mathrm{comp}} \tag{3}$$

in the temperature range at which the electron concentration is much less than $p(T)$, where N_{comp} is a compensating density (e.g., donor density and density of hole traps deeper than ΔE_{Mg^-}). Here, the Fermi–Dirac distribution function ($f_{\mathrm{FD}}(\Delta E_{\mathrm{Mg}-})$) is expressed as [1–6, 11]:

$$f_{\mathrm{FD}}(\Delta E_{\mathrm{Mg}^-}) = \frac{1}{1 + g_{\mathrm{A}} \exp\left(\frac{\Delta E_{\mathrm{Mg}^-} - \Delta E_{\mathrm{F}}(T)}{kT}\right)}, \tag{4}$$

where g_{A} is the degeneracy factor for acceptors, and $g_{\mathrm{A}} = 4$ [1–6, 11].

Figure 1 also shows $p(T)$ fitted by the method of least squares using $f_{\mathrm{FD}}(\Delta E_{\mathrm{Mg}^-})$ without N_{comp}, denoted by a solid line. The obtained N_{Mg} and ΔE_{Mg^-} were 7.8×10^{25} cm^{-3} and 1.40 eV, respectively. In consideration of N_{comp}, on the other hand, N_{Mg}, ΔE_{Mg^-}, and N_{comp} were determined to be 4.4×10^{23} cm^{-3}, 0.68 eV, and 4.1×10^{20} cm^{-3}, respectively. As is clear from Fig. 1, the simulated $p(T)$ were in good agreement with the experimentally obtained $p(T)$. However, these values for N_{Mg} obtained from $f_{\mathrm{FD}}(\Delta E_{\mathrm{Mg}^-})$ exceeded not only $2C_{\mathrm{Mg}}$ but also the concentration (approximately

1×10^{23} cm^{-3}) of the matrix atoms (Si and C). Because this implanted layer behaves as a non-degenerate semiconductor, the density of defects induced by ion implantation should be much less than 1×10^{23} cm^{-3}. Moreover, the density of acceptors related to Mg should be less than $2C_{\mathrm{Mg}}$. Therefore, the obtained values of N_{Mg} were incorrect.

The reason why N_{Mg} should be less than $2C_{\mathrm{Mg}}$ is mentioned below. Because the Mg acceptor might emit two holes into the valence band, Eq. (3) can approximate to

$$p(T) \cong 2N_{\mathrm{Mg}} f_{\mathrm{FD}}(\Delta E_{\mathrm{Mg}^-}) - N_{\mathrm{comp}}, \tag{5}$$

when the Mg acceptor would have negative-U properties. Therefore, the Mg acceptor density evaluated using Eq. (3) should be $2N_{\mathrm{Mg}}$. Because Mg acceptors are substitutive Mg atoms in SiC, therefore, the Mg acceptor density evaluated using Eq. (3) is less than $2C_{\mathrm{Mg}}$.

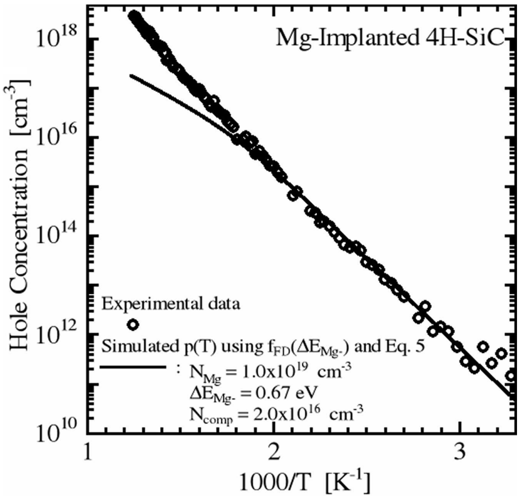

Fig. 4. Temperature dependence of hole concentration simulated by the Fermi–Dirac distribution function and Eq. (5) with N_{Mg} of 1×10^{19} cm^{-3}.

To reliably obtain N_{Mg}, ΔE_{Mg^-}, and N_{comp}, we investigate the influence of $\gamma_{\mathrm{H}}(T)$ on $p(T)$. The ratio of $p(T)$ simulated with N_{Mg} of 1.0×10^{19} cm^{-3} to the experimentally obtained $p(T)$ was calculated. In the literature [14, 15], this ratio corresponds to the empirical $\gamma_{\mathrm{H}}(T)$. Figure 4 shows $p(T)$ simulated by Eq. (5) with ΔE_{Mg^-} of 0.67 eV and N_{comp} of 2.0×10^{16} cm^{-3} denoted by a solid line. These values of $p(T)$ were used to calculate $\gamma_{\mathrm{H}}(T)$. The obtained $\gamma_{\mathrm{H}}(T)$ decreased from 1.56 to 0.057 as T increased from 300 to 800 K. Typical theoretical values of $\gamma_{\mathrm{H}}(T)$ are 1.18 for phonon scattering and 1.93 for ionized-impurity scattering [11]. Because the calculated values of $\gamma_{\mathrm{H}}(T)$ at higher temperatures are too small, these values are unreliable.

Finally, to reliably obtain N_{Mg}, ΔE_{Mg^-}, and N_{comp}, we investigate the influence of the excited states of the acceptor on $p(T)$. The distribution function that accounts for the influence of the excited states of the Mg acceptor ($f_{\mathrm{MC}}(\Delta E_{\mathrm{Mg}^-})$) is given by [1–6]:

$$f_{\mathrm{MC}}(\Delta E_{\mathrm{Mg}^-}) = \frac{1}{1 + g_{\mathrm{A,MC}}(T) \exp\left(\frac{\Delta E_{\mathrm{Mg}^-} - \Delta E_{\mathrm{F}}(T)}{kT}\right)}, \tag{6}$$

where $g_{\mathrm{A,MC}}(T)$ is called the effective degeneracy factor for Mg acceptors given by

$$g_{\mathrm{A,MC}}(T) = 4\left[1 + \sum_{r=2}^{l} g_r \times \exp\left(-\frac{\Delta E_{\mathrm{Mg}^-} - \Delta E_{r,\mathrm{Mg}^-}}{kT}\right)\right] \times \exp\left(-\frac{\overline{E_{\mathrm{ex,Mg}^-}(T)}}{kT}\right). \tag{7}$$

g_r is the $(r-1)$-th excited state degeneracy factor described as

$$g_r = r^2, \tag{8}$$

$\Delta E_{r,\mathrm{Mg}^-}$ is the energy level of the $(r-1)$-th excited state of the Mg acceptor measured from E_{V} given by

$$\Delta E_{r,\mathrm{Mg}^-} = 13.6 \frac{m_{\mathrm{h}}^*}{m_0} \frac{1}{\varepsilon_{\mathrm{s}}^2} \frac{1}{r^2}, \tag{9}$$

m_0 is the free-space electron mass, ε_{s} is a dielectric constant of 4H-SiC, and $\overline{E_{\mathrm{ex,Mg}^-}(T)}$ is the ensemble average of the ground and excited state levels of the Mg acceptor measured from the acceptor level, and is given by

$$\overline{E_{\mathrm{ex,Mg}^-}(T)} = \frac{\sum_{r=2}^{l} \left(\Delta E_{\mathrm{Mg}^-} - \Delta E_{r,\mathrm{Mg}^-}\right) g_r \exp\left(-\frac{\Delta E_{\mathrm{Mg}^-} - \Delta E_{r,\mathrm{Mg}^-}}{kT}\right)}{1 + \sum_{r=2}^{l} g_r \exp\left(-\frac{\Delta E_{\mathrm{Mg}^-} - \Delta E_{r,\mathrm{Mg}^-}}{kT}\right)}. \tag{10}$$

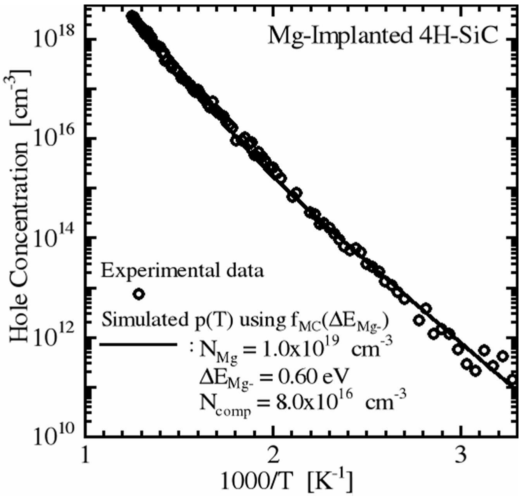

Fig. 5. Temperature dependence of hole concentration simulated by the distribution function that accounts for the influence of the excited states of an Mg acceptor.

Figure 5 shows $p(T)$ simulated from $f_{\mathrm{MC}}(\Delta E_{\mathrm{Mg}^-})$ with N_{Mg} of 1.0×10^{19} cm^{-3}, ΔE_{Mg^-} of 0.60 eV, N_{comp} of 8.0×10^{16} cm^{-3}, and l of 35. It is clear from the figure that the simulated $p(T)$ is in good agreement with the experimentally obtained $p(T)$. Moreover, the determined N_{Mg} is close to C_{Mg}. In the case of Mg acceptors in SiC, therefore, the distribution function that accounts for the excited states of a deep-level acceptor should be used to determine its density and energy level.

4. Summary

Mg ions were implanted at 500 °C to n-type 4H-SiC epilayers. Annealing at 1800 °C made a Mg-implanted 4H-SiC layer p-type. The temperature dependence of the hole concentration in the Mg-implanted 4H-SiC layer annealed at 1800 °C suggested that the Mg acceptor was a deep-level acceptor. We tried to reliably determine the density and energy level of Mg acceptors from the experimentally obtained $p(T)$. When we adopted the distribution function that accounts for the influence of the excited states of a deep-level acceptor instead of the Fermi–Dirac distribution function, we could reliably determine the density and energy level of the Mg acceptor from the experimentally obtained $p(T)$.

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