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Enhancement of ionization efficiency of acceptors by their excited states in heavily doped wide bandgap semiconductors

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Abstract. The temperature dependence of the hole concentration $p(T)$ for heavily Al-doped 6H-SiC and Mg-doped GaN are obtained from Hall-effect measurements. The density and energy level (ΔE_{A}) of acceptors are determined by the graphical peak analysis method (free carrier concentration spectroscopy) using $p(T)$. Since their ΔE_{A} are deep, it is found that a distribution function including the influence of the excited states of acceptors is necessary to the analysis of $p(T)$ for the heavily doped samples. Moreover, it is proved that the excited states enhance the ionization efficiency of acceptors in the heavily doped case.

1. Introduction

GaN, SiC and diamond have been attractive wide bandgap semiconductors for devices operating at high powers, high frequencies, and high temperatures. In p-type cases, their acceptor energy levels (ΔE_{A}) are experimentally reported to be rather deep. According to the hydrogenic model, on the other hand, a ground state level corresponding to the theoretical ΔE_{A} of a substitutional acceptor in them is expected to be deep, because their dielectric constants are lower than that of Si and because their hole effective masses are heavier than their electron effective masses. For example, ΔE_{A} for SiC is calculated as 146 meV, and the first excited state level (ΔE_2) is estimated to be 36 meV that is close to ΔE_{A} of B in Si. Therefore, the excited states should affect the temperature dependence of the hole concentration $p(T)$ in p-type wide bandgap semiconductors.

In this article, a distribution function suitable for acceptors in heavily doped p-type SiC and GaN is investigated using $p(T)$ obtained by Hall-effect measurements. Since the Fermi levels in heavily doped samples are located between the valence band and the acceptor level, which indicates that the Fermi level is close to the excited state levels, there are a lot of holes at the excited states of acceptors. This suggests that a distribution function for acceptors should include the influence of the excited states of acceptors. Therefore, we here consider two distribution functions; (1) the Fermi-Dirac distribution function $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$ not including it and (2) our proposed distribution function $f(\Delta E_{\mathrm{A}})$ including it [1-4].

2. Distribution function

$f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$ is described as

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

(1)

where $\Delta E_{\mathrm{F}}(T)$ is the Fermi level measured from the valence band maximum (E_{V}), g_{A} is the acceptor degeneracy factor of 4, k is the Boltzmann constant, and T is the absolute temperature.

On the other hand, the distribution function considering the influence of the excited states of acceptors is given by [1-4]

$$f(\Delta E_{\mathrm{A}}) = \frac{1}{1 + g_{\mathrm{A}}(T) \exp\left(\dfrac{\Delta E_{\mathrm{A}} - \Delta E_{\mathrm{F}}(T)}{kT}\right)}, \tag{2}$$

where

$$g_{\mathrm{A}}(T) = g_{\mathrm{A}}\left[1 + \sum_{r=2} g_r \exp\left(\frac{\Delta E_r - \Delta E_{\mathrm{A}}}{kT}\right)\right] \exp\left(-\frac{\overline{E_{\mathrm{ex}}(T)}}{kT}\right), \tag{3}$$

g_r is the $(r-1)$ th excited state degeneracy factor of r^2, ΔE_r is the difference in energy between E_{V} and the excited state level [$\Delta E_r = 13.6 m_{\mathrm{h}}^* / (m_0 \varepsilon_{\mathrm{s}}^2 r^2)$ eV], $\overline{E_{\mathrm{ex}}(T)}$ is an ensemble average energy of the acceptor and excited state levels, given by [1-4]

$$\overline{E_{\mathrm{ex}}(T)} = \frac{\displaystyle\sum_{r=2} (\Delta E_{\mathrm{A}} - \Delta E_r) g_r \exp\left(-\frac{\Delta E_{\mathrm{A}} - \Delta E_r}{kT}\right)}{\displaystyle 1 + \sum_{r=2} g_r \exp\left(-\frac{\Delta E_{\mathrm{A}} - \Delta E_r}{kT}\right)}, \tag{4}$$

m_0 is the free space electron mass, m_{h}^* is the hole effective mass, and ε_{s} is the dielectric constant.

3. Free carrier concentration spectroscopy

Free carrier concentration spectroscopy (FCCS) is a graphical peak analysis method for determining the acceptor density (N_{A}) and ΔE_{A} from $p(T)$ using any distribution function. Using an experimental $p(T)$, the FCCS signal is defined as [1-4]

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

where E_{ref} is the parameter that can shift the peak temperature within the temperature range of the measurement. On the other hand, the FCCS signal is theoretically described as [1-4]

$$H(T, E_{\mathrm{ref}}) = \frac{N_{\mathrm{A}}}{kT} \exp\left(-\frac{\Delta E_{\mathrm{A}} - E_{\mathrm{ref}}}{kT}\right) I(\Delta E_{\mathrm{A}}) - \frac{N_{\mathrm{D}} N_{\mathrm{V0}}}{kT} \exp\left(\frac{E_{\mathrm{ref}} - \Delta E_{\mathrm{F}}(T)}{kT}\right), \tag{6}$$

where

$$I(\Delta E_{\mathrm{A}}) = N_{\mathrm{V0}} \exp\left(\frac{\Delta E_{\mathrm{A}} - \Delta E_{\mathrm{F}}(T)}{kT}\right) F(\Delta E_{\mathrm{A}}), \tag{7}$$

$F(\Delta E_{\mathrm{A}})$ represents $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$ or $f(\Delta E_{\mathrm{A}})$, N_{D} is the total donor density, $N_{\mathrm{V0}} = 2(2\pi m_{\mathrm{h}}^* / h^2)^{3/2}$, and h is Planck's constant.

Since the FCCS signal has a peak at the temperature corresponding to ΔE_{A}, the values of N_{A} and ΔE_{A} can be determined from the peak.

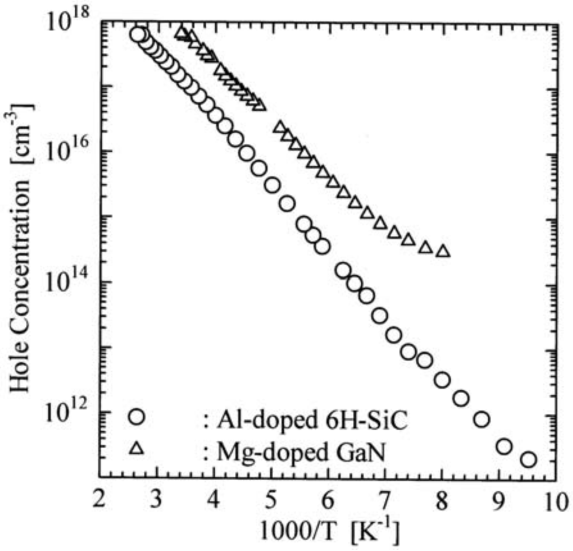

Figure 1. Experimental $p(T)$.

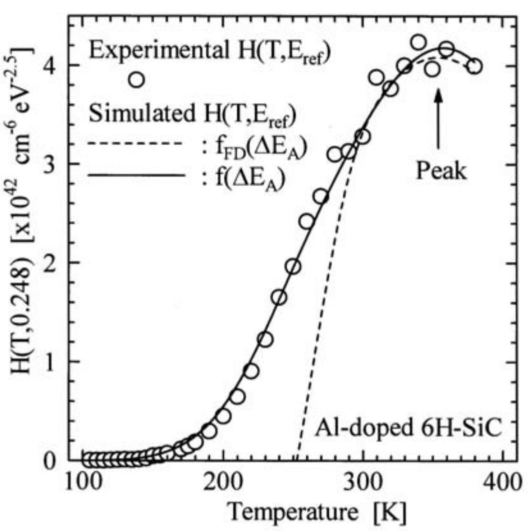

Figure 2. FCCS signal.

4. Experiment

A 400-μm-thick heavily Al-doped 6H-SiC wafer with a resistivity of 1.4 Ωcm and a 2-μm-thick heavily Mg-doped GaN epilayer on undoped GaN/sapphire were used. The $p(T)$ was obtained by Hall-effect measurements in a magnetic field of 1.4 T.

5. Results and discussion

Figure 1 shows two $p(T)$ for Al-doped 6H-SiC (circles) and Mg-doped GaN (triangles). Using these $p(T)$, the FCCS signals are calculated from Eq. (5).

Figure 2 depicts $H(T, E_{\mathrm{ref}})$ with $E_{\mathrm{ref}} = 0.248$ eV for Al-doped 6H-SiC. From the peak of the FCCS signal, the values of N_{A}, ΔE_{A} and N_{D} are determined as 2.5×10^{19} cm^{-3}, 180 meV and 7.3×10^{17} cm^{-3} for $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$, respectively, and 3.2×10^{18} cm^{-3}, 180 meV and 9.0×10^{16} cm^{-3} for $f(\Delta E_{\mathrm{A}})$, respectively. The broken and solid lines in Fig. 2 represent the $H(T, E_{\mathrm{ref}})$ simulations for $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$ and $f(\Delta E_{\mathrm{A}})$ using Eq. (6). The solid line is in better agreement with the circles than the other, indicating that the excited states affect $p(T)$ obviously. Moreover, since $N_{\mathrm{A}} - N_{\mathrm{D}}$ determined by capacitance-voltage characteristics was 4.2×10^{18} cm^{-3}, the values

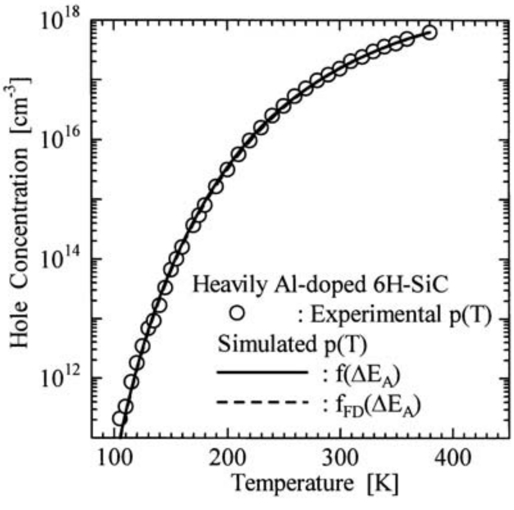

Figure 3. $p(T)$ simulations using values determined by FCCS. Since the $p(T)$ simulation using $f(\Delta E_{\mathrm{A}})$ is very close to the $p(T)$ simulation using $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$, the solid line overlaps with the broken line.

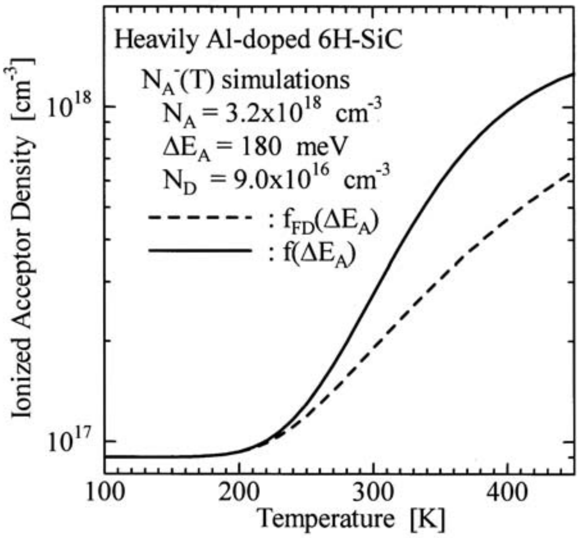

Figure 4. Ionized acceptor density for $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$ and $f(\Delta E_{\mathrm{A}})$ with the same values.

determined using $f(\Delta E_{\mathrm{A}})$ are more reliable than those using $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$.

From the peak of the FCCS signal for Mg-doped GaN, the values of N_{A}, ΔE_{A} and N_{D} are determined as 2.1×10^{20} cm^{-3}, 154 meV and 2.2×10^{18} cm^{-3} for $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$, respectively, and 8.9×10^{18} cm^{-3}, 149 meV and 1.5×10^{17} cm^{-3} for $f(\Delta E_{\mathrm{A}})$, respectively. Since the Mg concentration determined by secondary ion mass spectroscopy was 2×10^{19} cm^{-3}, the values obtained using $f(\Delta E_{\mathrm{A}})$ are more reasonable than the other.

Figure 3 shows the $p(T)$ simulations for Al-doped 6H-SiC with the determined values for $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$ (broken line) and $f(\Delta E_{\mathrm{A}})$ (solid line). From the figure, both the $p(T)$ simulations using $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$ and $f(\Delta E_{\mathrm{A}})$ coincide with the experimental $p(T)$. Therefore, it is difficult to determine which distribution function is suitable for acceptors.

Figure 4 depicts the ionized acceptor density $N_{\mathrm{A}}^-(T)$ simulated with the same values of N_{A}, ΔE_{A} and N_{D} for $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$ (broken line) and $f(\Delta E_{\mathrm{A}})$ (solid line) for the heavily Al-doped 6H-SiC. Both the $N_{\mathrm{A}}^-(T)$ are constant and equal to 9.0×10^{16} cm^{-3} at <170 K, because some of acceptors are negatively charged for the ionization of all the donors. On the other hand, $N_{\mathrm{A}}^-(T)$ for $f(\Delta E_{\mathrm{A}})$ is higher than $N_{\mathrm{A}}^-(T)$ for $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$ at high temperatures. Therefore, it is found that the excited states enhance the ionization efficiency of Al acceptors. The situation in heavily Mg-doped GaN is the same.

6. Conclusion

The $p(T)$ for heavily Al-doped 6H-SiC and heavily Mg-doped GaN were investigated. Since the acceptor levels in them are rather deep, the distribution function including the influence of the excited states of acceptors was required to analyze $p(T)$. From the discussion, it is proved that the excited states of acceptors enhance the ionization efficiency of acceptors.

References

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