Influence of Excited States of Mg Acceptor on Hole Concentration in GaN

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Experimental acceptor levels (ΔE_{A}) in GaN, measured from the valence band maximum (E_{V}), are reported to be deeper than 150 meV [1]. Theoretically, the ground and first excited state levels of acceptors in GaN, calculated by hydrogenic dopant model [$\Delta E_r = 13.6(m^* / \varepsilon_s^2 r^2)$ eV], are 101 meV and 25 meV, respectively. The experimental ΔE_{A} corresponds to ΔE_1, while it is deeper than ΔE_1 due to central cell corrections. Since the Fermi level (ΔE_{F}) is between E_{V} and ΔE_{A}, the excited states $(r \geq 2)$ should affect the hole concentration $p(T)$. Here, all the energy levels are measured from E_{V}. Using both of the Fermi-Dirac distribution function $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$ and the proposed distribution function $f(\Delta E_{\mathrm{A}})$ including the influence of the excited states, we experimentally investigate the influence of the excited states on $p(T)$.

The proposed distribution function for electrons is expressed as [2]

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

where g_r is the $(r-1)$th excited state degeneracy factor and $\overline{E_{\mathrm{ex}}}$ is the ensemble average of the ground and excited state levels, which increases from 0 with T. Here, the average acceptor level $\overline{\Delta E_{\mathrm{A}}}$ is expressed as $\overline{\Delta E_{\mathrm{A}}} = \Delta E_{\mathrm{A}} - \overline{E_{\mathrm{ex}}}$. When the influence of the excited states is ignored (i.e., $r = 1$ and $\overline{E_{\mathrm{ex}}} = 0$), Eq. (1) corresponds to $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$.

2 µm-thick Mg-doped p-type GaN epilayers were grown at 1025 °C by metalorganic chemical vapor deposition on undoped GaN/sapphire, and they were annealed at 800 °C for 20 min. The Mg concentration (C_{Mg}) in the epilayers, determined by secondary ion mass spectroscopy, was 2×10^{19} cm^{-3}. $p(T)$ was obtained by Hall-effect measurements. Using Free Carrier Concentration Spectroscopy (FCCS) [2,3], ΔE_{A}, the acceptor density (N_{A}) and the compensating density (N_{comp}) were determined, and are shown in Table 1. Figure 1 shows the experimental and simulated $p(T)$.

Since Mg atoms at Ga sites act as acceptors, N_{A} should be lower than or equal to C_{Mg}. In $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$, although the simulated $p(T)$, shown by the broken line, is in agreement with the experimental $p(T)$, N_{A} is much higher than C_{Mg}, indicating that this N_{A} is not reliable. In $f(\Delta E_{\mathrm{A}})$, on the other hand, the simulated $p(T)$, shown by the solid line, is in agreement with the experimental $p(T)$, and also N_{A} is lower than C_{Mg}. Therefore, N_{A} and ΔE_{A} obtained using $f(\Delta E_{\mathrm{A}})$ are considered to be reasonable.

[1] D. J. Kim, D. Y. Ryu, N. A. Bojarczuk, J. Karasinski, S. Guha, S. H. Lee and J. H. Lee: J. Appl. Phys. **88** (2000) 2564.
[2] H. Matsuura: New J. Phys. **4** (2002) 12.1. (http://www.njp.org/).
[3] H. Matsuura, Y. Masuda, Y. Chen and S. Nishino: Jpn. J. Appl. Phys. **39** (2000) 5069.

Table 1 Results determined by FCCS.

	N_{A} [cm^{-3}]	ΔE_{A} [meV]	N_{com} [cm^{-3}]
$f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$	2.1x10^{20}	154	2.2x10^{18}
$f(\Delta E_{\mathrm{A}})$	8.9x10^{18}	149	1.5x10^{17}

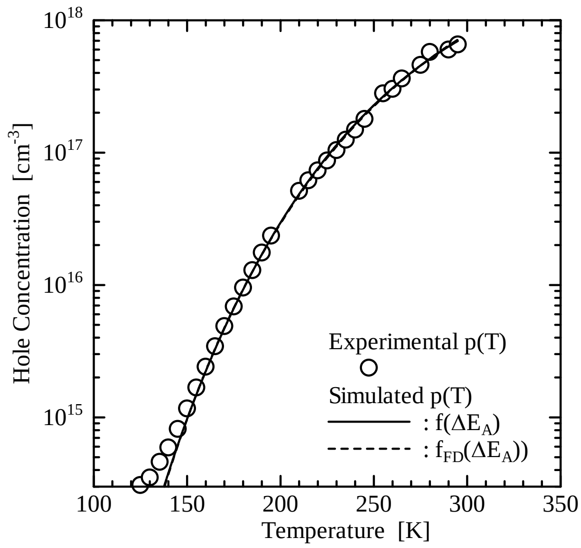

Fig. 1 Experimental and simulated $p(T)$.