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

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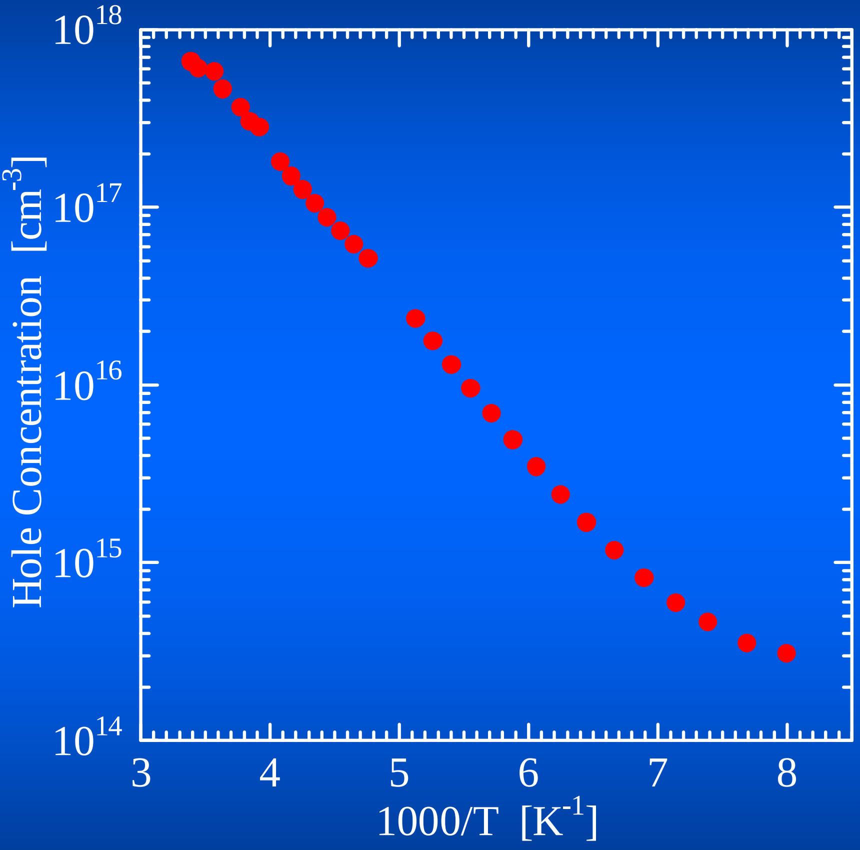
Acceptor density in Mg-doped GaN epilayer



1. Hall-Effect measurements

Fermi-Dirac (FD) distribution function

$$f_{\mathrm{FD}}(\Delta E_{\mathrm{A}}) = \frac{1}{1+4\exp\left(\frac{\Delta E_{\mathrm{A}}-\Delta E_{\mathrm{F}}}{kT}\right)}$$

Results determined by curve-fitting

$$N_{\mathrm{A}} = 2.1\times10^{20}\ \mathrm{cm}^{-3}$$

$$\Delta E_{\mathrm{A}} = 154\ \ \mathrm{meV}$$

2. SIMS

Concentration of Mg atoms in GaN is ~$2\mathrm{x}10^{19}$ cm^{-3}

Is the FD distribution function available for Mg acceptor in GaN?

Ground and excited states of Acceptor in GaN

Hydrogenic model

$$\Delta E_r = 13.6 \frac{m^*}{m_0 \varepsilon_s^2} \cdot \frac{1}{r^2} \ \ \text{eV}$$

Acceptor Level (ground state level)

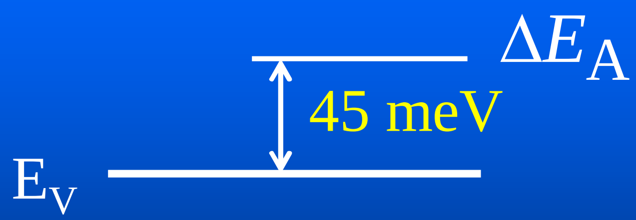
$$\Delta E_\text{A} = \Delta E_1 = 100 \ \ \text{meV}$$

First excited state level

$$\Delta E_2 = 25 \ \ \text{meV}$$

In the case of p-type GaN

In the case of B-doped Si



It is necessary to consider a distribution function including the influence of the excited states!!

Conventional distribution function including the influence of excited states

$$f_{\mathrm{conv}}(\Delta E_{\mathrm{A}}) = \frac{1}{1 + 4\left\{\exp\left(\frac{\Delta E_{\mathrm{A}} - \Delta E_{\mathrm{F}}}{kT}\right) + \sum_{r=2} g_r \exp\left(\frac{\Delta E_r - \Delta E_{\mathrm{F}}}{kT}\right)\right\}}$$

↓

Hardly any holes can be emitted into the valence band, because they are captured in the excited states.

↓

N_A higher than N_A obtained by the FD distribution function is required in order to meet p(T).

R. A. Smith, Semiconductors, 2^{nd} ed. (Cambridge University Press, 1978) p. 92.

Proposed distribution function including the influence

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

This term makes acceptors release holes at high temperatures more easily than $f_{\mathrm{conv}}(\Delta E_{\mathrm{A}})$.

Ensemble average of ground and excited state levels

$$\overline{E_{\mathrm{ex}}} = \frac{\sum_{r=2} (\Delta E_{\mathrm{A}} - \Delta E_r)\, g_r \exp\left(-\frac{\Delta E_{\mathrm{A}} - \Delta E_r}{kT}\right)}{g_1 + \sum_{r=2} g_r \exp\left(-\frac{\Delta E_{\mathrm{A}} - \Delta E_r}{kT}\right)}$$

Average acceptor level: $\overline{\Delta E_{\mathrm{A}}} = \Delta E_{\mathrm{A}} - \overline{E_{\mathrm{ex}}}$

H. Matsuura, New Journal of Physics, 4 (2002) 12.1 (http://www.njp.org/)

Experimental

Conditions of Mg-doped GaN epilayer

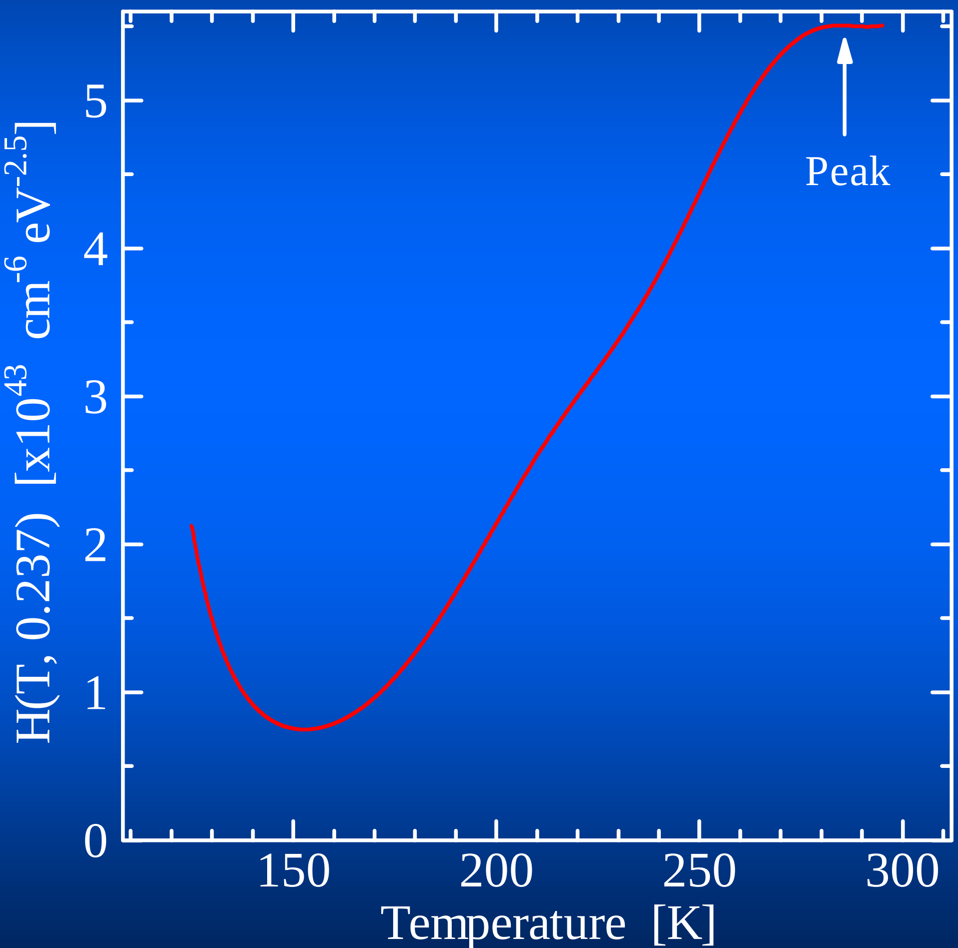
	T_s [^oC]	TMGa [μmol/min]	CP_2Mg [μmol/min]	V/III	Thickness [μm]
Mg-doped GaN	1025	360.3	5	1700	2
Undoped GaN	1025	360.3	0	1700	1
GaN buffer	515	131.3	0	4600	0.03
Sapphire (0001)					

Annealing conditions: 800 ^oC, 20 min

Hall-effect measurement: 125 K~295 K
1.4 T

How to determine ΔE_A and N_A using $p(T)$

Free Carrier Concentration Spectroscopy (FCCS)



Definition of FCCS signal:

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

The FCCS signal has a peak at the temperature corresponding to each acceptor.

$$T_{\mathrm{peak}} \cong \frac{\Delta E_A - E_{\mathrm{ref}}}{k}$$

$$H(T_{\mathrm{peak}}, E_{\mathrm{ref}}) \cong \frac{N_A}{kT_{\mathrm{peak}}} \exp(-1)$$

FCCS: H. Matsuura et. al., Jpn. J. Appl. Phys. 41 (2002) 496.

Results obtained by FCCS in GaN

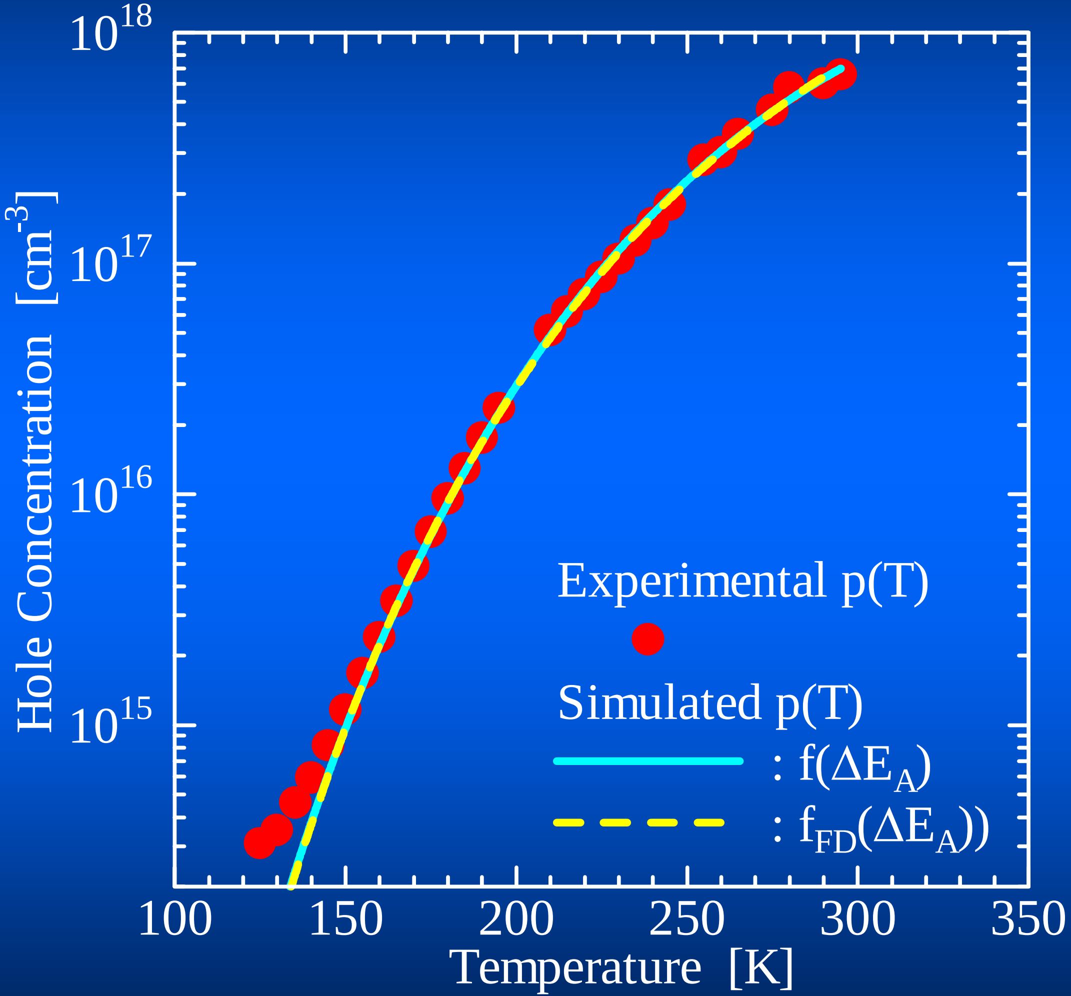
	N_A [cm^{-3}]	ΔE_A [meV]	N_{comp} [cm^{-3}]
$f(\Delta E_A)$	8.9×10^{18}	149	1.5×10^{17}
$f_{FD}(\Delta E_A)$	**2.1×10^{20}**	154	2.2×10^{18}

The concentration of Mg is **~2×10^{19}** cm^{-3} determined by SIMS

↓

In the case of $f(\Delta E_A)$, N_A is reasonable.
(44.5 % of Mg atoms are located at the substitutional sites in GaN)
In the case of $f_{FD}(\Delta E_A)$, N_A is rather high.

p(T) simulated using the obtained values



All the simulated p(T) are in good agreement with the experimental p(T).

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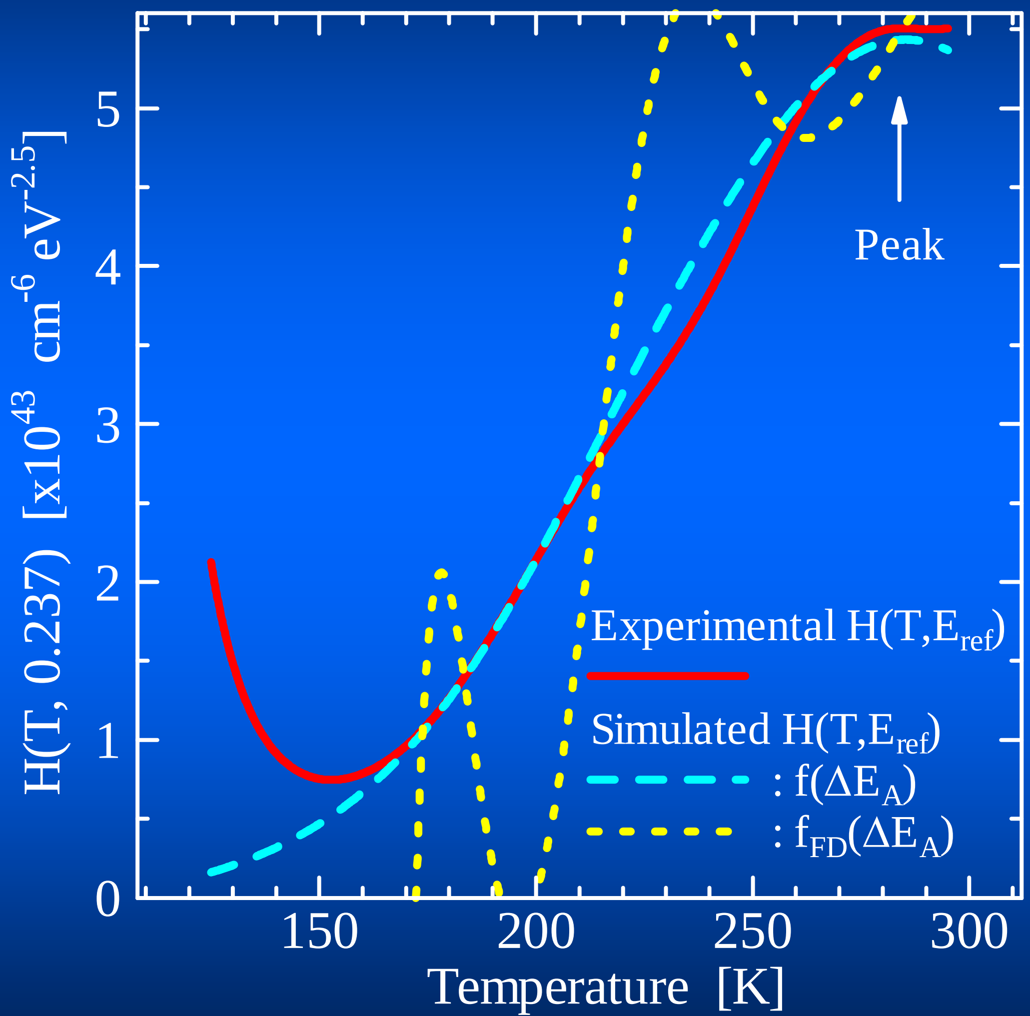
The curve-fitting procedure of p(T) is not suitable for investigating the influence of the excited states on p(T).

Simulated FCCS signals



The broken line is in better agreement with the experimental FCCS signal than the dotted line.

↓

FCCS is appropriate for investigating the influence of the excited states on p(T).

Summary

In order to obtain the reliable acceptor density from p(T), a distribution function including the influence of the excited states of acceptors is found to be required.

In order to investigate the influence of the excited states, FCCS is considered to be more appropriate than the curve fitting procedure of p(T).

In the conditions of this Mg-doped epilayer, 44.5 % of the doped Mg atoms are found to behave like an acceptor in GaN.