Enhancement of Ionization Efficiency of Acceptors by Their Excited States in Heavily Doped p-Type GaN and Wide Bandgap Semiconductors

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Our focus

Problem in heavily doped p-type wide bandgap semiconductors

The acceptor density, which is determined by the curve-fitting procedure using the temperature dependence of the hole concentration, is always **much higher** than **the doping density**.

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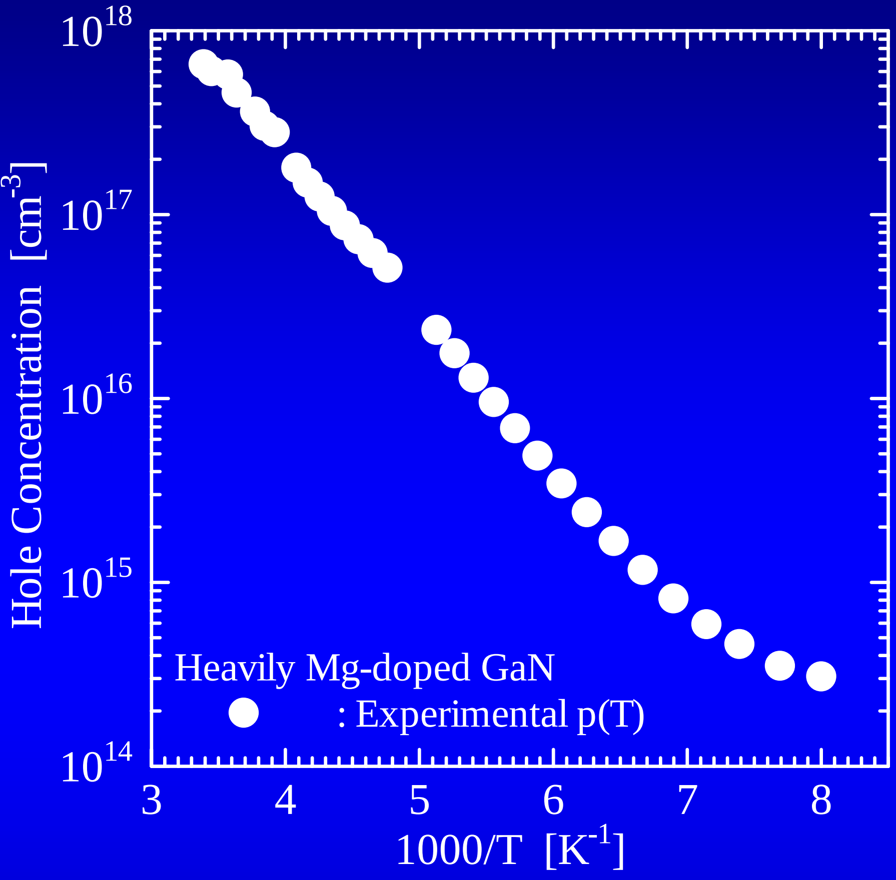
Why?

Acceptor density in heavily Mg-doped GaN



1. Hall-effect measurement

Fermi-Dirac (FD) distribution function

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

Results determined by **curve-fitting**

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

$$N_{\mathrm{A}} = 2.1 \times 10^{20} \quad \mathrm{cm}^{-3}$$

2. SIMS

Concentration of Mg in GaN: $2 \times 10^{19} \quad \mathrm{cm}^{-3}$

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

Contents

1. How to determine the densities and energy levels of impurities from p(T) or n(T) without any assumptions regarding the impurities.
2. How to investigate a distribution function suitable for acceptors in heavily doped p-type wide bandgap semiconductors
3. How do the excited states of deep acceptors influence p(T) in heavily doped case?

1. In order to determine the densities and energy levels of impurities from the temperature dependence of the majority-carrier concentration without any assumptions regarding the impurities.

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graphical peak analysis method

Free carrier concentration spectroscopy (FCCS)

Free Carrier Concentration Spectroscopy (FCCS)

Using an experimental n(T), the FCCS signal is defined as

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

This FCCS has peaks corresponding to donor levels

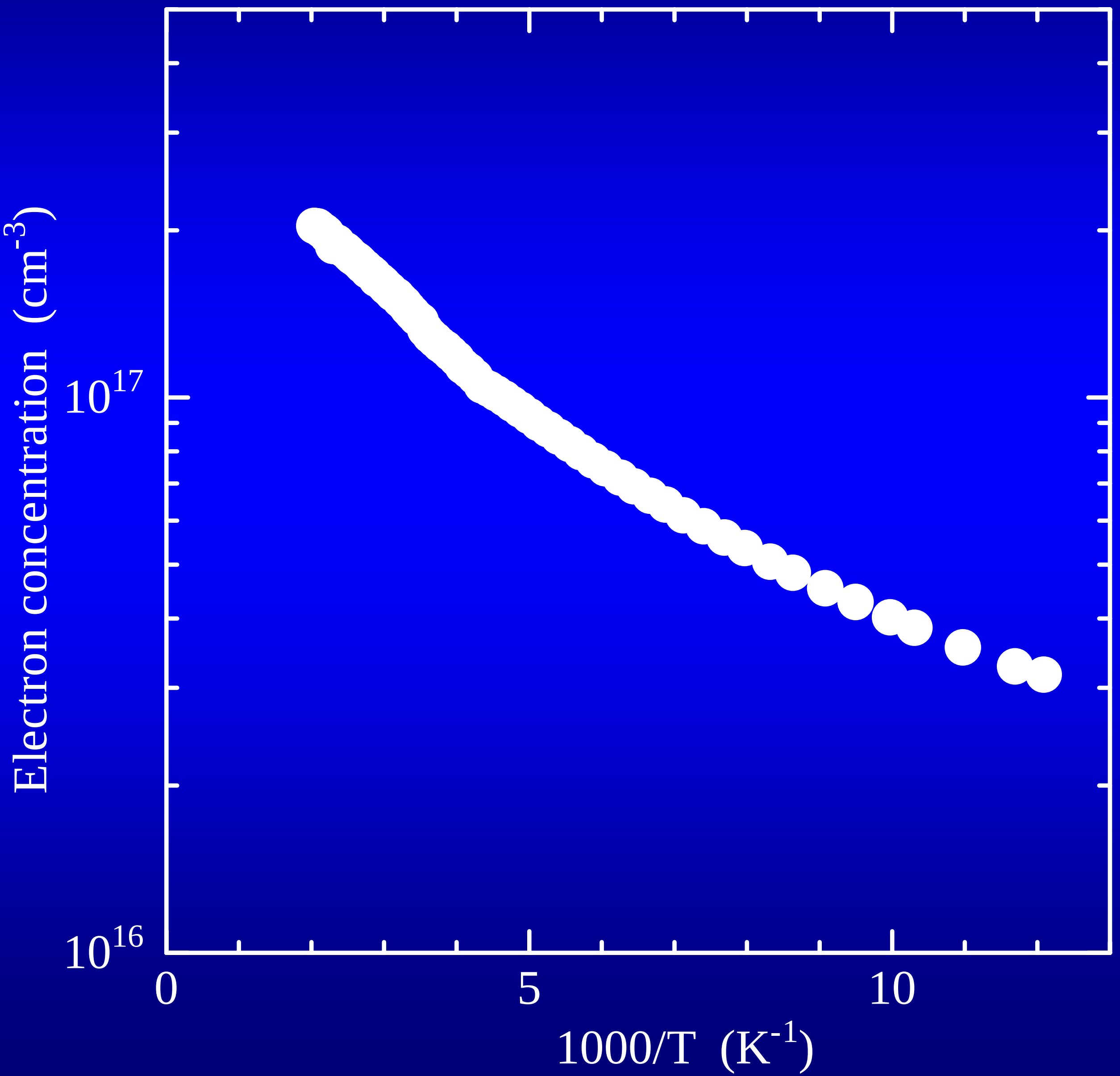
From each peak temperature and value,

$$\Delta E_{\mathrm{D},i} \cong kT_{\underline{\mathrm{peak},i}} + E_{\mathrm{ref}}$$

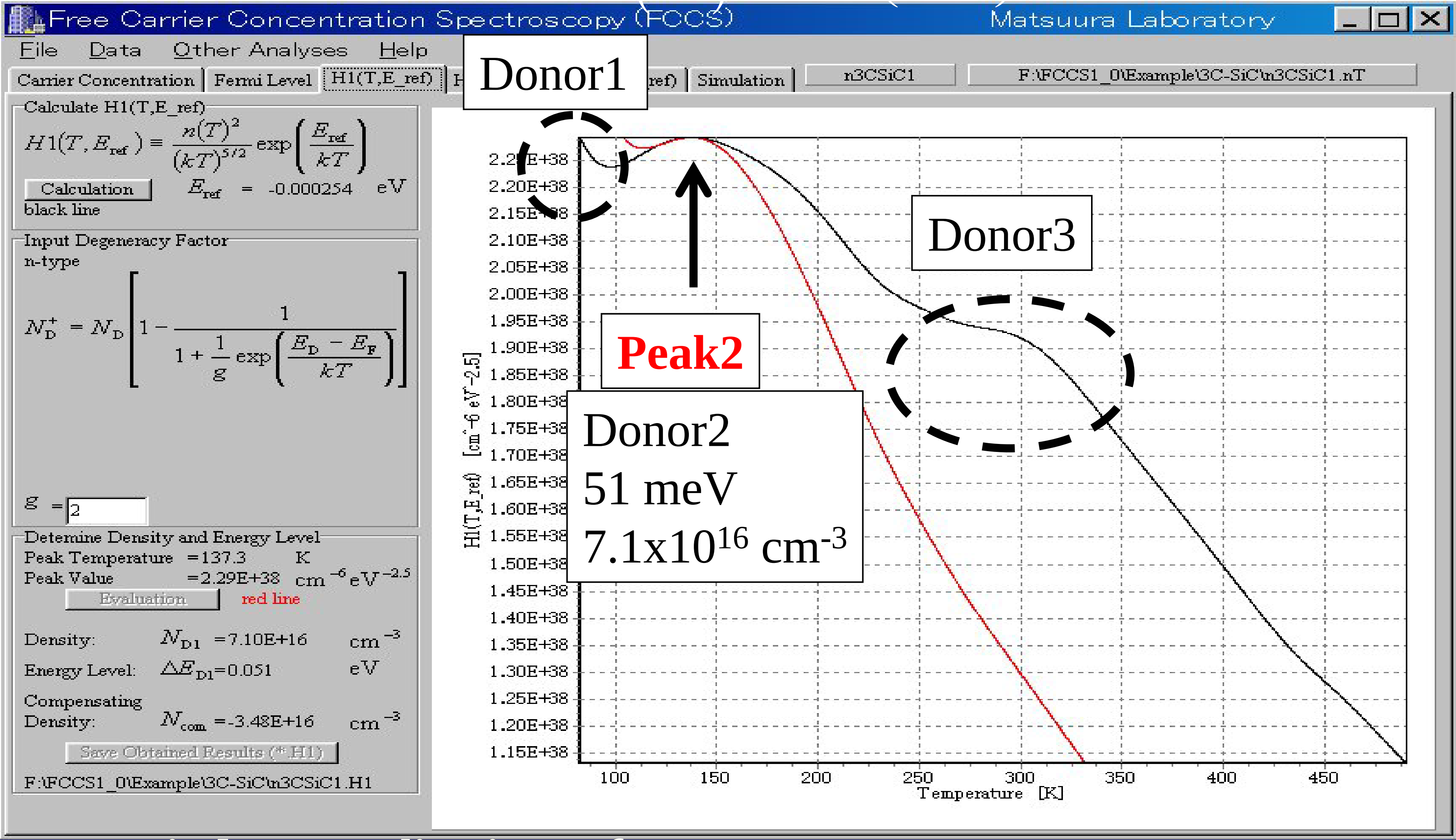
$$N_{\mathrm{D},i} \cong kT_{\underline{\mathrm{peak},i}} \underline{H\left(T_{\mathrm{peak},i}, E_{\mathrm{ref}}\right)} \exp(1)$$

Undoped 3C-SiC

The temperature dependence of the electron concentration



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



Calculate H1(T,E_ref)

$$H1(T,E_{\mathrm{ref}}) = \frac{n(T)^2}{(kT)^{5/2}}\exp\left(\frac{E_{\mathrm{ref}}}{kT}\right)$$

Calculation E_{ref} = -0.000254 eV

black line

Input Degeneracy Factor

n-type

$$N_{\mathrm{D}}^{+} = N_{\mathrm{D}}\left[1-\frac{1}{1+\frac{1}{g}\exp\left(\frac{E_{\mathrm{D}}-E_{\mathrm{F}}}{kT}\right)}\right]$$

g = 2

Determine Density and Energy Level

Peak Temperature =137.3 K

Peak Value =2.29E+38 $\mathrm{cm}^{-6}\,\mathrm{eV}^{-2.5}$

Evaluation red line

Density: N_{D1} =7.10E+16 cm^{-3}

Energy Level: ΔE_{D1}=0.051 eV

Compensating Density: N_{com} =-3.48E+16 cm^{-3}

Save Obtained Results (*.H1)

F:\FCCS1_0\Example\3C-SiC\n3CSiC1.H1

Donor1

Peak2

Donor2

51 meV

7.1×10^{16} cm^{-3}

Donor3

Free Windows Application software:

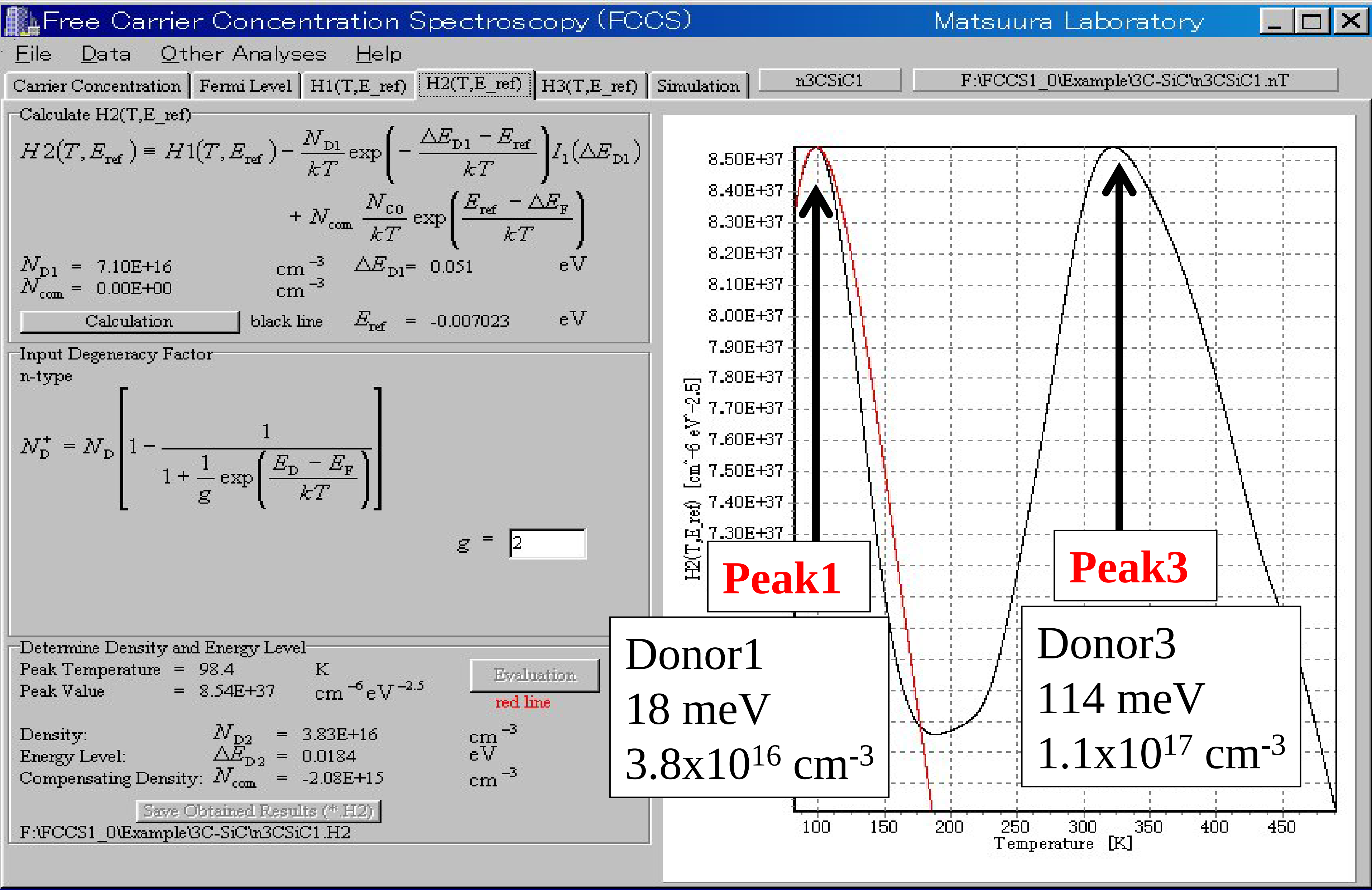
See at Web site http://www.osakac.ac.jp/labs/matsuura/

The FCCS signal is theoretically written as

$$H(T,E_{\mathrm{ref}}) = \sum_i \frac{N_{\mathrm{D}i}}{kT}\exp\left(-\frac{\Delta E_{\mathrm{D}i}-E_{\mathrm{ref}}}{kT}\right) I_{\mathrm{D}}\left(\Delta E_{\mathrm{D}i}\right) - \frac{N_{\mathrm{C0}}N_{\mathrm{A}}}{kT}\exp\left(\frac{E_{\mathrm{ref}}-\Delta E_{\mathrm{F}}}{kT}\right)$$

FCCS signal , in which the influence of the previously determined donor species is removed, is expressed as

$$H2\left(T,E_{\mathrm{ref}}\right) = \frac{n(T)^2}{(kT)^{5/2}}\exp\left(\frac{E_{\mathrm{ref}}}{kT}\right) - \frac{\underline{N_{\mathrm{D2}}}}{kT}\exp\left(-\frac{\underline{\Delta E_{\mathrm{D2}}}-E_{\mathrm{ref}}}{kT}\right) I_D\left(\underline{\Delta E_{\mathrm{D2}}}\right)$$



Calculate H2(T,E_ref)

$$H2(T,E_{ref}) = H1(T,E_{ref}) - \frac{N_{D1}}{kT}\exp\left(-\frac{\Delta E_{D1}-E_{ref}}{kT}\right)I_1(\Delta E_{D1}) + N_{com}\frac{N_{C0}}{kT}\exp\left(\frac{E_{ref}-\Delta E_F}{kT}\right)$$

N_{D1} = 7.10E+16 cm^{-3} ΔE_{D1}= 0.051 eV

N_{com} = 0.00E+00 cm^{-3}

Calculation black line E_{ref} = -0.007023 eV

Input Degeneracy Factor

n-type

$$N_D^+ = N_D\left[1 - \frac{1}{1+\frac{1}{g}\exp\left(\frac{E_D-E_F}{kT}\right)}\right]$$

g = 2

Determine Density and Energy Level

Peak Temperature = 98.4 K

Peak Value = 8.54E+37 cm^{-6}eV$^{-2.5}$

Evaluation

red line

Density: N_{D2} = 3.83E+16 cm^{-3}

Energy Level: ΔE_{D2} = 0.0184 eV

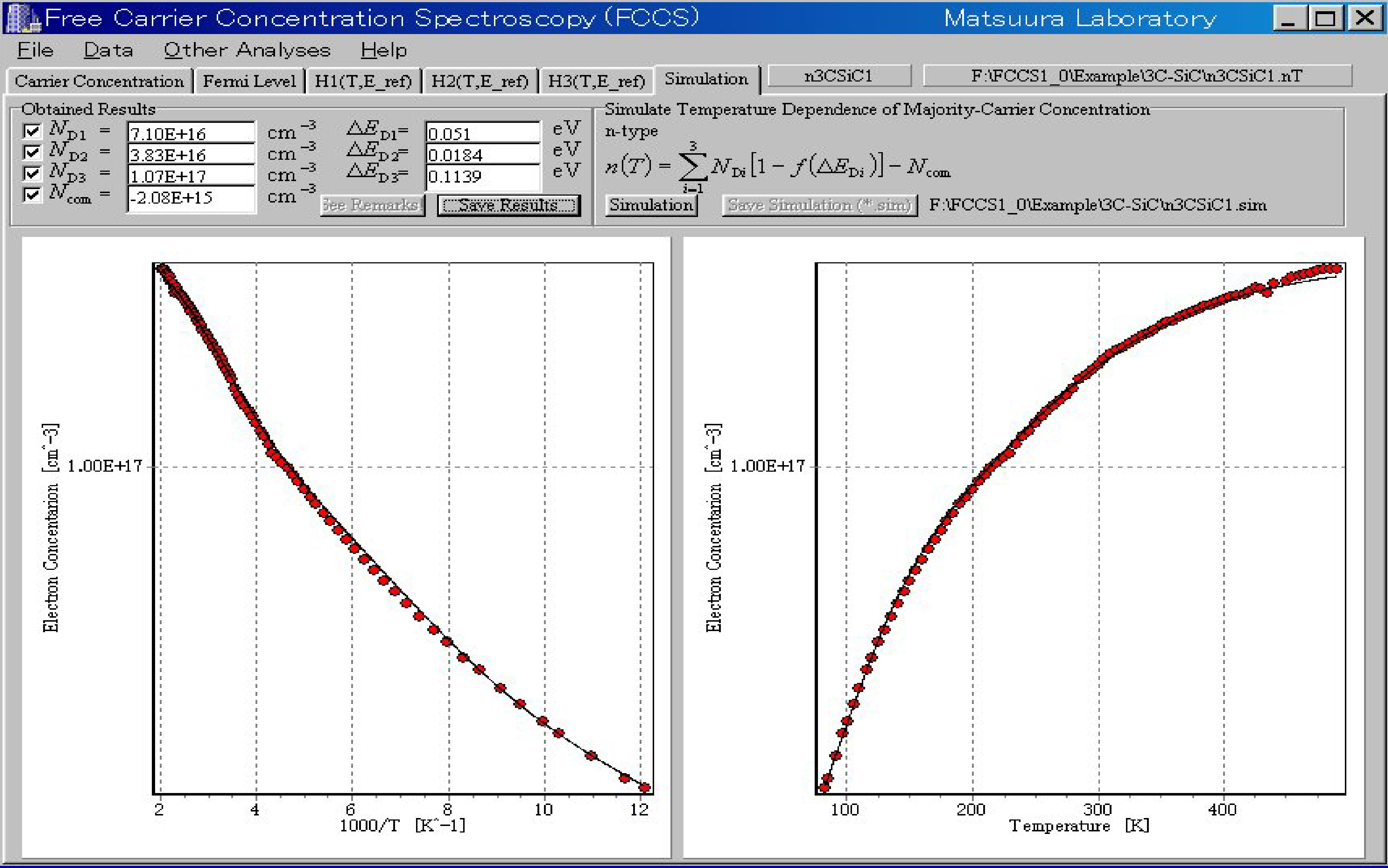
Compensating Density: N_{com} = -2.08E+15 cm^{-3}

Save Obtained Results (*.H2)

F:\FCCS1_0\Example\3C-SiC\n3CSiC1.H2

Donor1
18 meV
3.8x10^{16} cm^{-3}

Donor3
114 meV
1.1x10^{17} cm^{-3}



Obtained Results

☑ N_{D1} = 7.10E+16 cm $^{-3}$　ΔE_{D1}= 0.051 eV

☑ N_{D2} = 3.83E+16 cm $^{-3}$　ΔE_{D2}= 0.0184 eV

☑ N_{D3} = 1.07E+17 cm $^{-3}$　ΔE_{D3}= 0.1139 eV

☑ N_{com} = -2.08E+15 cm $^{-3}$

Simulate Temperature Dependence of Majority-Carrier Concentration

n-type

$$n(T) = \sum_{i=1}^{3} N_{Di}\left[1 - f(\Delta E_{Di})\right] - N_{com}$$

F:\FCCS1_0\Example\3C-SiC\n3CSiC1.sim

The n(T) simulation is in agreement with the experimental n(T).

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The values determined by FCCS are reliable.

2. In order to investigate a distribution function suitable for deep acceptors in heavily doped semiconductors

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A distribution function including the influence of excited states of acceptors

Acceptor level and excited state levels

$$\Delta E_r = 13.6 \frac{1}{\underline{\varepsilon_s}^{2}} \cdot \frac{\underline{m_h}^{*}}{m_0} \cdot \frac{1}{r^{2}} \quad \mathrm{eV}$$

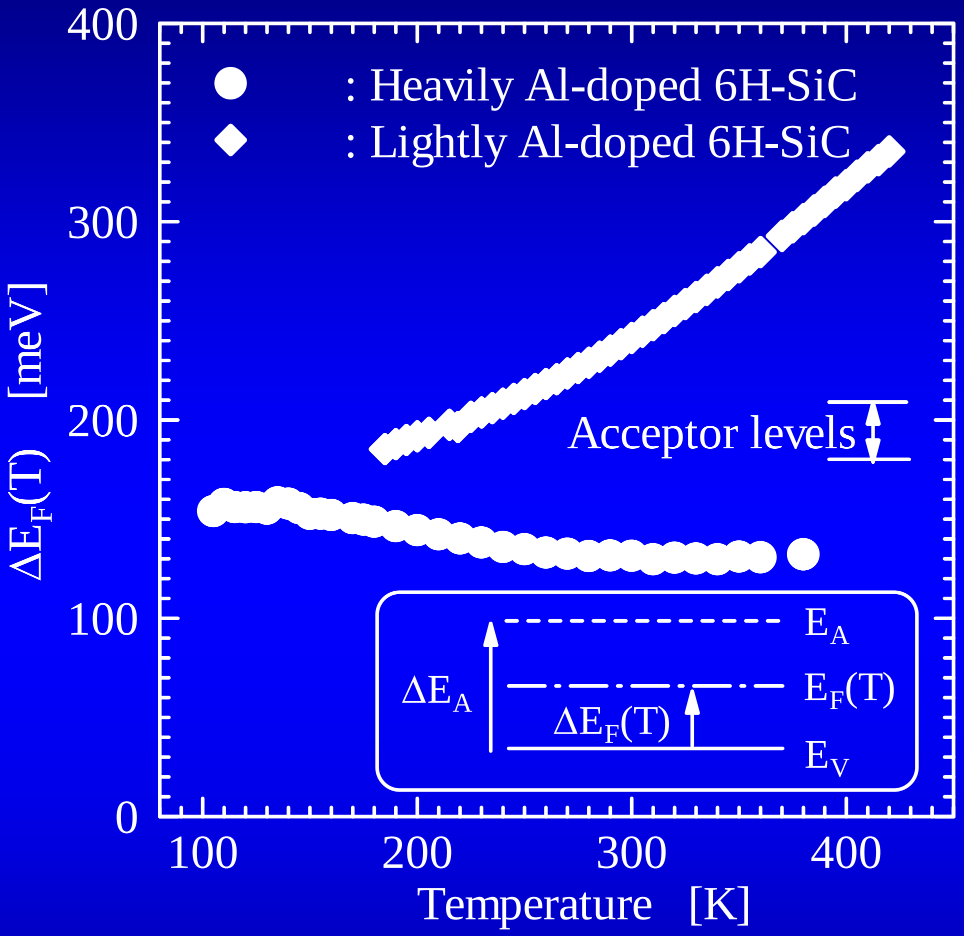
p-type wide bandgap semiconductors (GaN, SiC, diamond)

1. Their **dielectric constants** are lower than that of Si
2. Their **hole effective masses** are heavier than their electron effective masses

Semiconductor	Acceptor level (r=1)	1st excited state level (r=2)
SiC	146 meV	37 meV
GaN	101 meV	25 meV

The acceptor levels become deep, and also the excited state levels are still close to acceptor levels in Si.

Position of Fermi level in heavily doped p-type case



Heavily doped case

- - - Acceptor level

— · — Fermi level

········ 1^{st} excited state

········ 2^{nd} excited state

—— Valence band

Since the Fermi level is close to the excited state levels, a lot of holes exist at the excited states.

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The excited states should affect p(T)!

A distribution function suitable for deep acceptors

1. Fermi-Dirac distribution function not including the influence of excited states of acceptors

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

2. The distribution function including the influence of excites states of acceptors

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

The difference between two functions is only the acceptor degeneracy factor, g_{A} and $g_{\mathrm{A}}(T)$.

Acceptor degeneracy factor

$\ln f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$

$$g_{\mathrm{A}} = 4$$

Degeneracy factors of excited states

Excited state levels

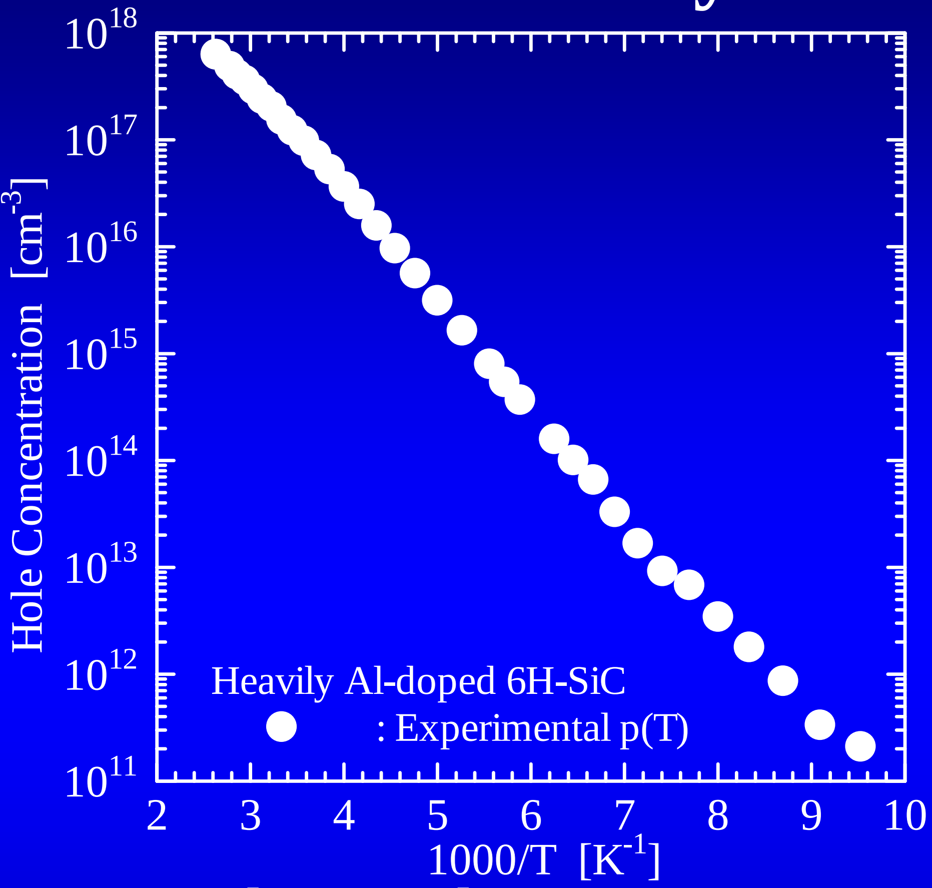
$\ln f(\Delta E_{\mathrm{A}})$

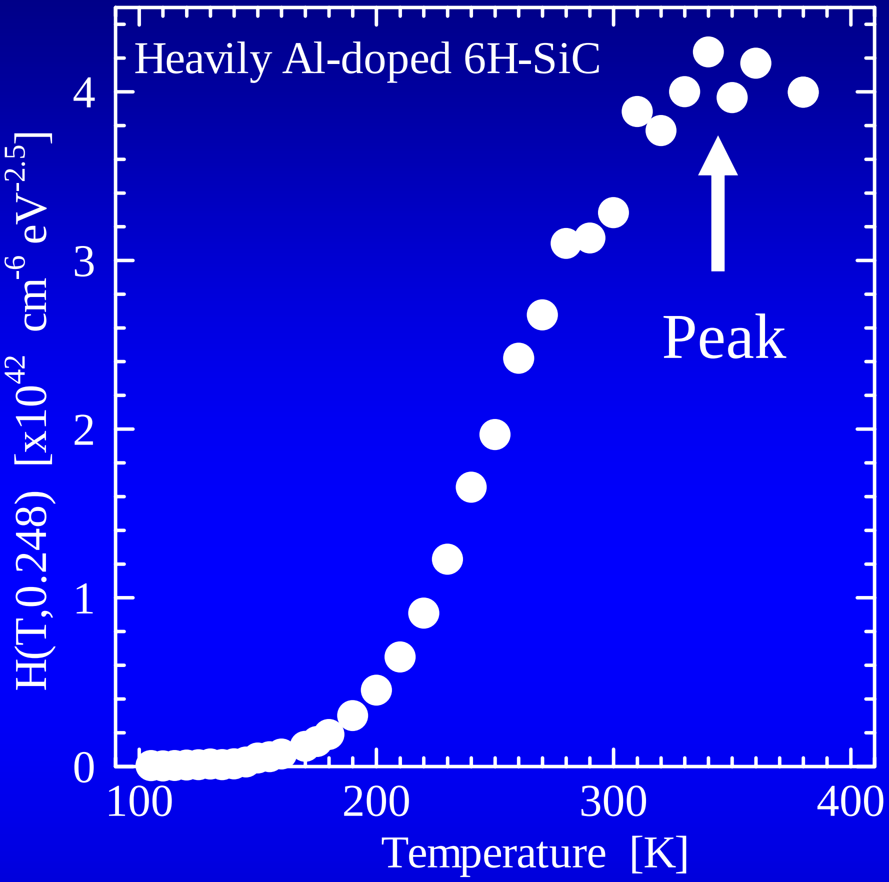
$$g_{\mathrm{A}}(T) = g_{\mathrm{A}}\left[1 + \sum_{r=2} g_r \exp\left(\frac{\Delta E_r - \Delta E_{\mathrm{A}}}{kT}\right)\right]\exp\left(-\frac{\overline{E_{\mathrm{ex}}(T)}}{kT}\right)$$

Average energy of acceptor level and excited state levels

$$\overline{E_{\mathrm{ex}}(T)} = \frac{\sum\limits_{r=2} (\Delta E_{\mathrm{A}} - \Delta E_r) g_r \exp\left(-\frac{\Delta E_{\mathrm{A}} - \Delta E_r}{kT}\right)}{1 + \sum\limits_{r=2} g_r \exp\left(-\frac{\Delta E_{\mathrm{A}} - \Delta E_r}{kT}\right)}$$

Heavily Al-doped 6H-SiC





From this peak,

$N_A = 2.5 \times 10^{19}$ cm^{-3} and $\Delta E_A = 180$ meV for $f_{FD}(\Delta E_A)$

$N_A = 3.2 \times 10^{18}$ cm^{-3} and $\Delta E_A = 180$ meV for $f\ (\Delta E_A)$

Since the Al-doping density is 4×10^{18} cm^{-3},

the influence of excited states on p(T) should be considered.

Comparison between Heavily and lightly Al-doped 6H-SiC

	Heavily doped		Lightly doped	
	$f(\Delta E_A)$	$f_{FD}(\Delta E_A)$	$f(\Delta E_A)$	$f_{FD}(\Delta E_A)$
N_A [cm^{-3}]	$3.2x10^{18}$	$2.5x10^{19}$	$4.1x10^{15}$	$4.9x10^{15}$
ΔE_A [meV]	180	180	212	199
Doping density [cm^{-3}]	$4.2x10^{18}$		$\sim 6x10^{15}$	

In lightly doped case, holes at the excited states are few because the Fermi level is far from E_V.

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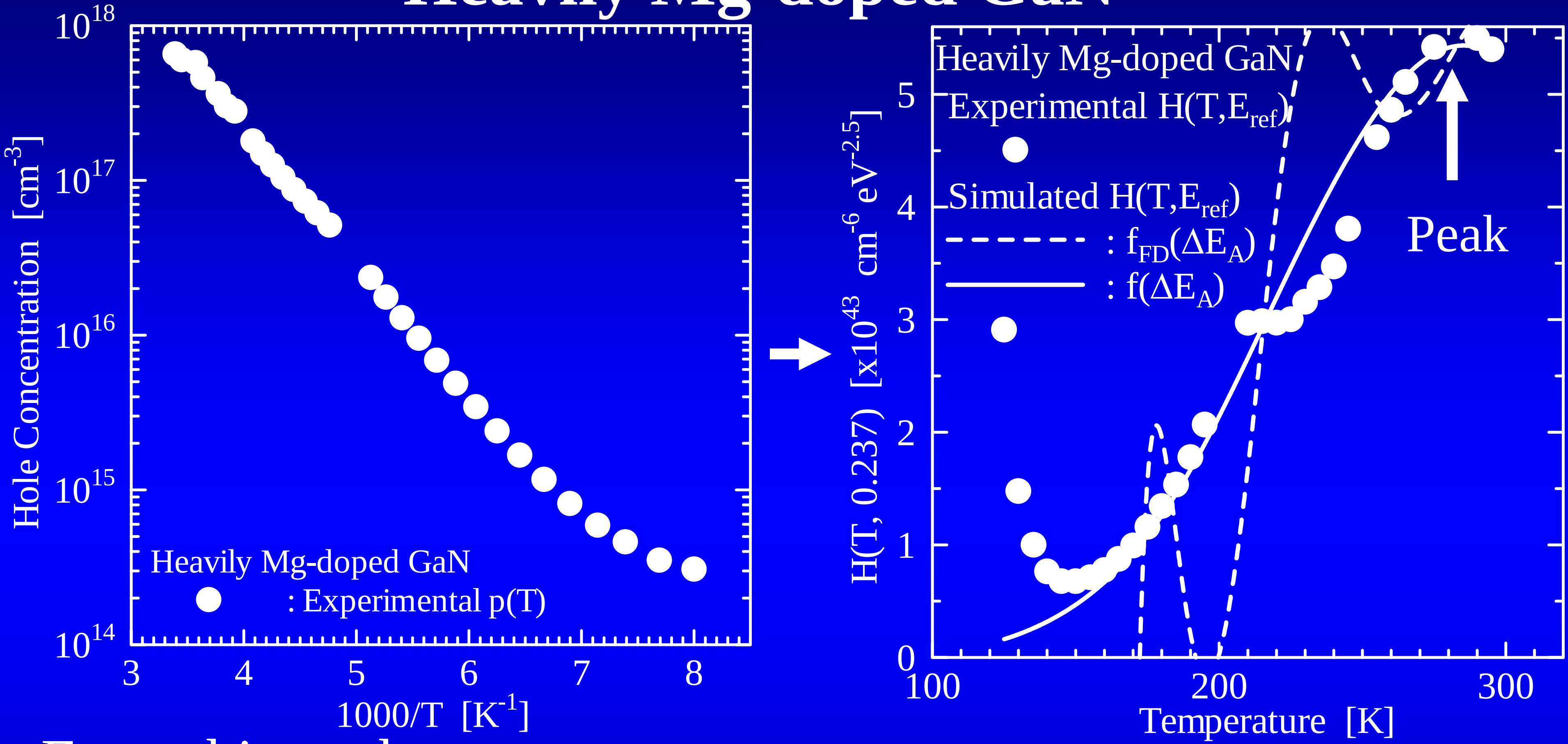
Using each distribution function, the reasonable acceptor density is obtained.

Only in heavily doped samples,
$f_{FD}(\Delta E_A)$ cannot be used to analyze p(T).

Heavily Mg-doped GaN



From this peak,

$N_A=2.1\times10^{20}$ cm^{-3} and ΔE_A=154 meV for $f_{FD}(\Delta E_A)$

$N_A=8.9\times10^{18}$ cm^{-3} and ΔE_A=149 meV for $f(\Delta E_A)$

Since the Mg-doping density is **2×10^{19} cm^{-3}**, $f(\Delta E_A)$ is suitable for heavily doped GaN.

3. How do the excited states of acceptors influence $p(T)$?

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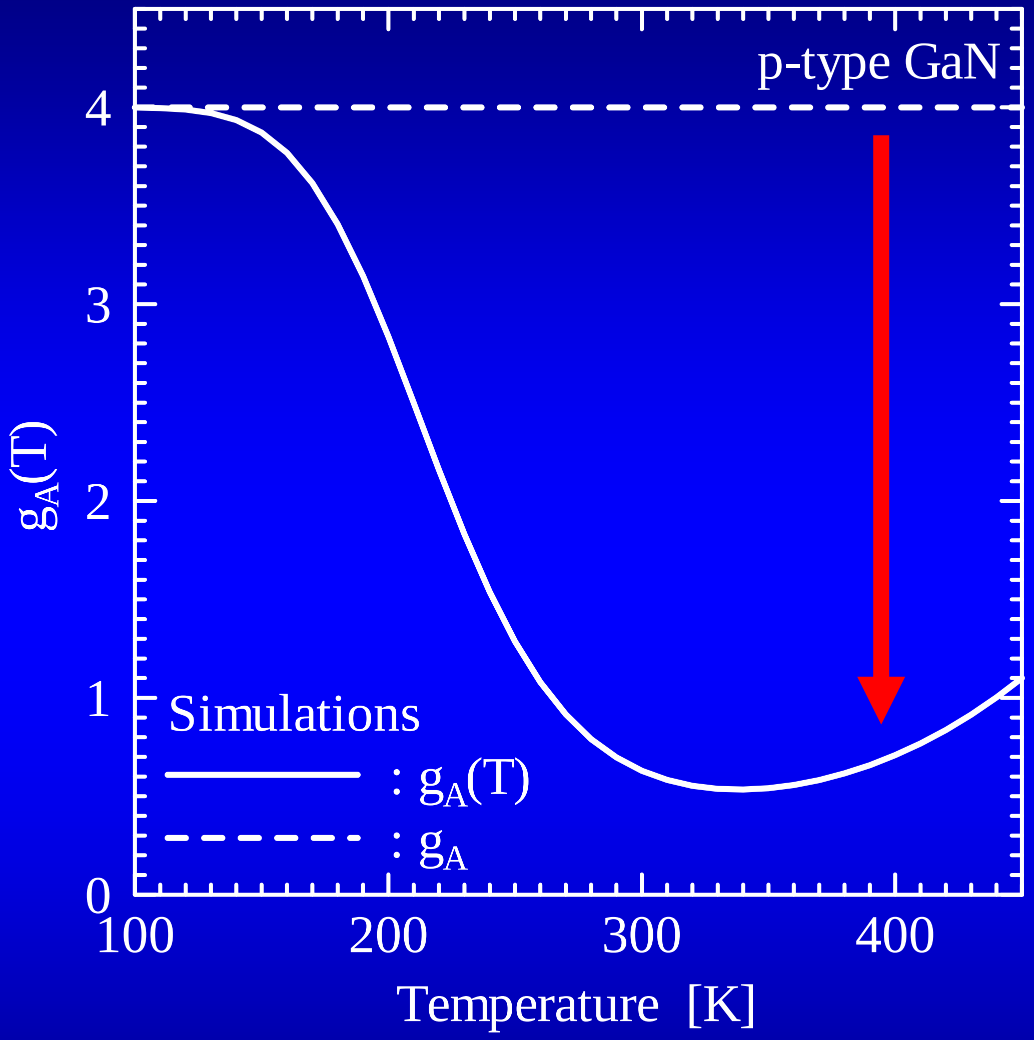
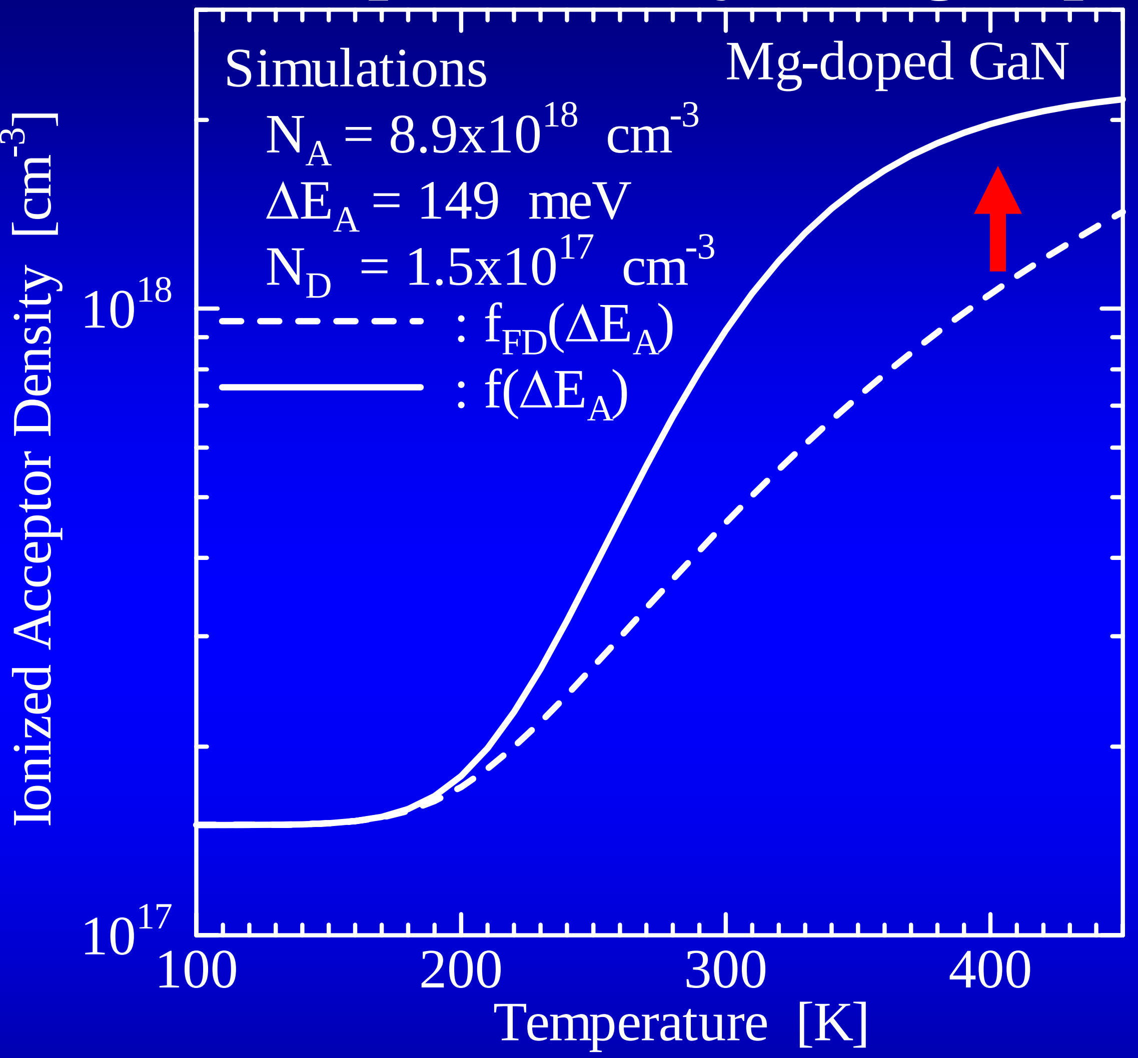
Do the excited states enhance the ionization efficiency of acceptors, or not?

Temperature dependence of acceptor degeneracy factor



$g_A(T)$ is less than g_A of 4 at high temperatures, which enhances the ionization efficiency at high temperatures.

Ionized acceptor density in Mg-doped GaN



Since $g_A(T)$ is less than g_A at high temperatures, the ionized acceptor density for $f(\Delta E_A)$ is higher than that for $f_{FD}(\Delta E_A)$.

Summary

- The distribution function suitable for deep acceptors has been proposed and tested.
- This distribution function is necessary for determining N_A in heavily doped p-type wide bandgap semiconductors.
- The excited states of acceptors enhance the ionization efficiency of acceptors at high temperatures.