A graphical peak analysis method for characterizing impurities in SiC, GaN and diamond from temperature-dependent majority-carrier concentration

Hideharu Matsuura
matsuura@isc.osakac.ac.jp
Osaka Electro-Communication University

ABSTRACT

A method for uniquely determining the densities and energy levels of impurities from the temperature dependence of the majority-carrier concentration in wide band gap semiconductors is discussed. It is demonstrated that the proposed graphical analysis method can evaluate the number of impurity species and can determine those densities and energy levels uniquely. In the case that the Fermi levels in p-type SiC, GaN and diamond are located between E_A and E_V, the excited states of acceptors strongly affect the hole concentration, indicating that the distribution function including the influence of the excited states should be applied to determining the density and energy level of acceptor from the temperature – dependent hole concentration.

Determination of densities and energy levels of impurities from n(T) or p(T) obtained from Hall-effect measurements

ln n(T)-1/T or ln p(T)-1/T

The analysis of ln n(T)-1/T or ln p(T)-1/T curve cannot be applied to semiconductors with more than one types of impurities or compensated semiconductors.

Curve-fitting

It is difficult to obtain reliable densities and energy levels of impurities by fitting an n(T) or p(T) simulation to the experimental data, because it is necessary to assume the number of impurity species before the curve-fitting procedure.

A graphical peak analysis method can determine the densities and energy levels of impurities without any assumptions regarding impurities species.

Free Carrier Concentration Spectroscopy (FCCS)

FCCS

Definition

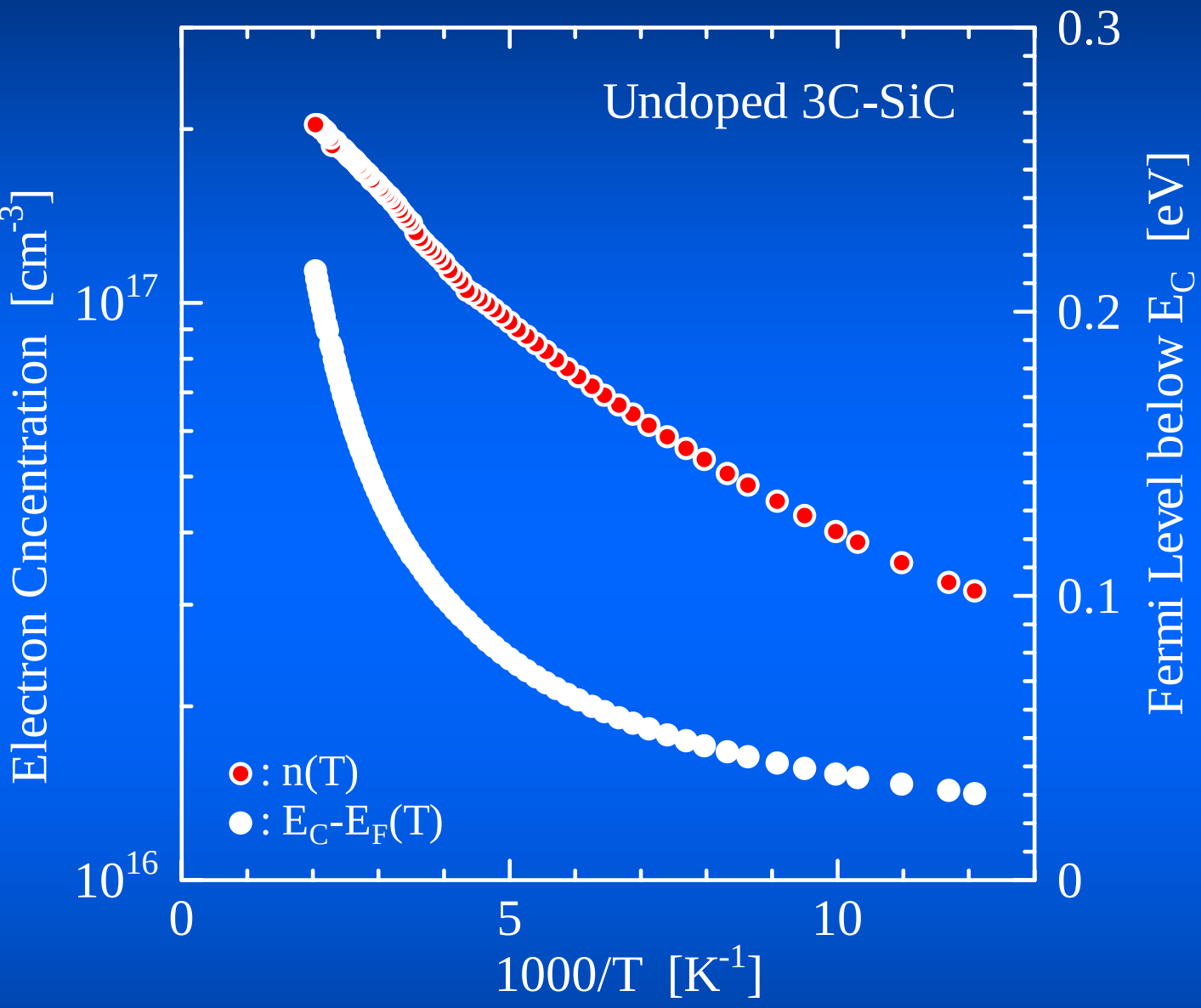
$$H\left(T, E_{\mathrm{ref}}\right) \equiv \frac{n(T)^2}{k^{5/2} T^{5/2}} \exp\left(\frac{E_{\mathrm{ref}}}{kT}\right)$$

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

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

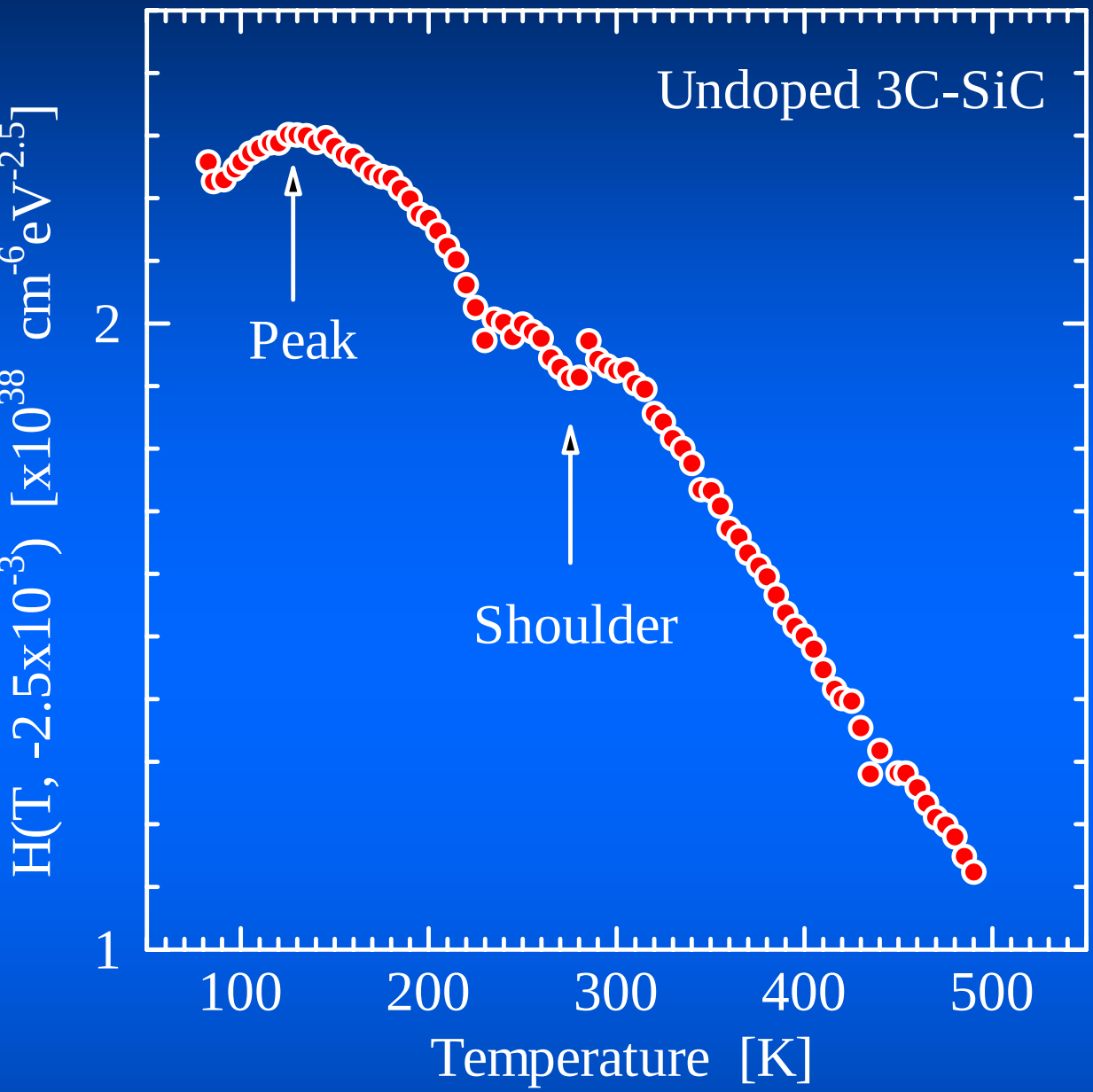
From each peak, the density and energy level of the corresponding impurity can be accurately determined.

32 μm-thick undoped 3C-SiC



$$E_C - E_F(T) = kT \ln\left[\frac{N_C(T)}{n(T)}\right]$$

FCCS signal



From peak

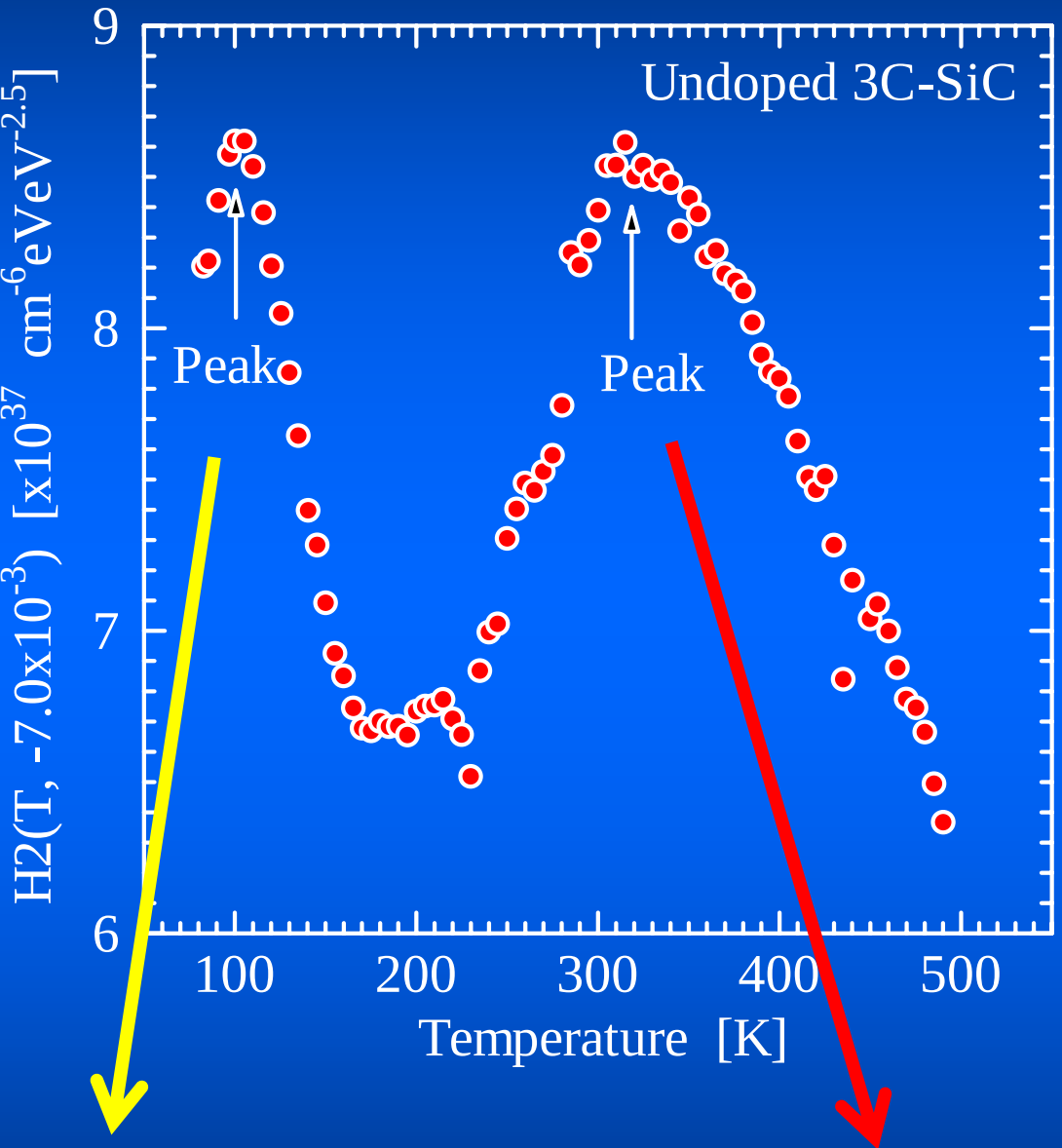
$T_{peak} = 137\ K$

$H(T_{peak}, E_{ref}) = 2.3\times10^{38}\ \mathrm{cm^{-6}eV^{-2.5}}$

$\rightarrow$ $E_{D2} = E_C - 0.051\ \mathrm{eV}$

$N_{D2} = 7.1\times10^{16}\ \mathrm{cm^{-3}}$

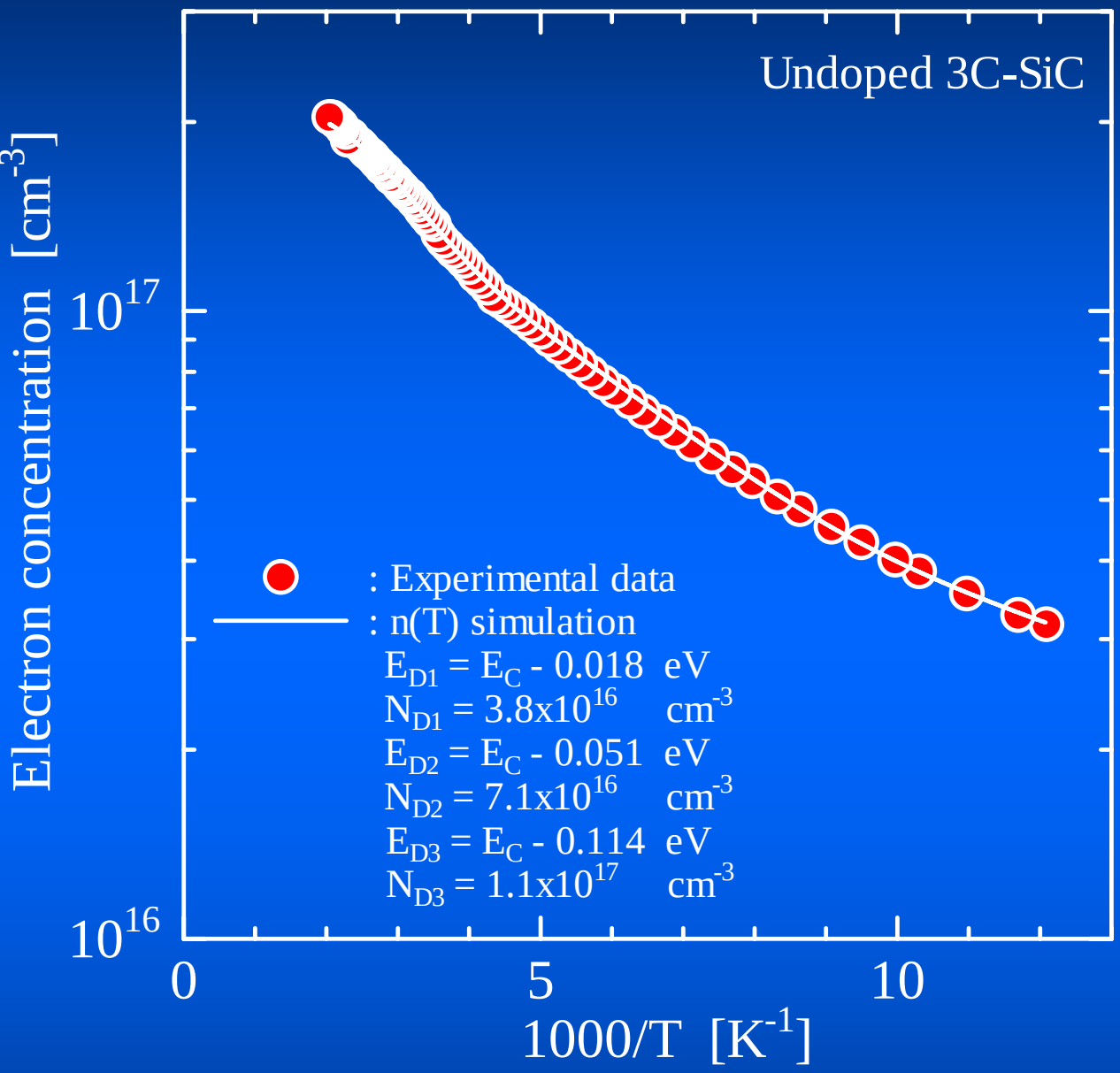
FCCS signal in which the influence of donor with E_{D2} is removed



$E_{D1} = E_C - 0.018$ eV $\quad E_{D3} = E_C - 0.114$ eV

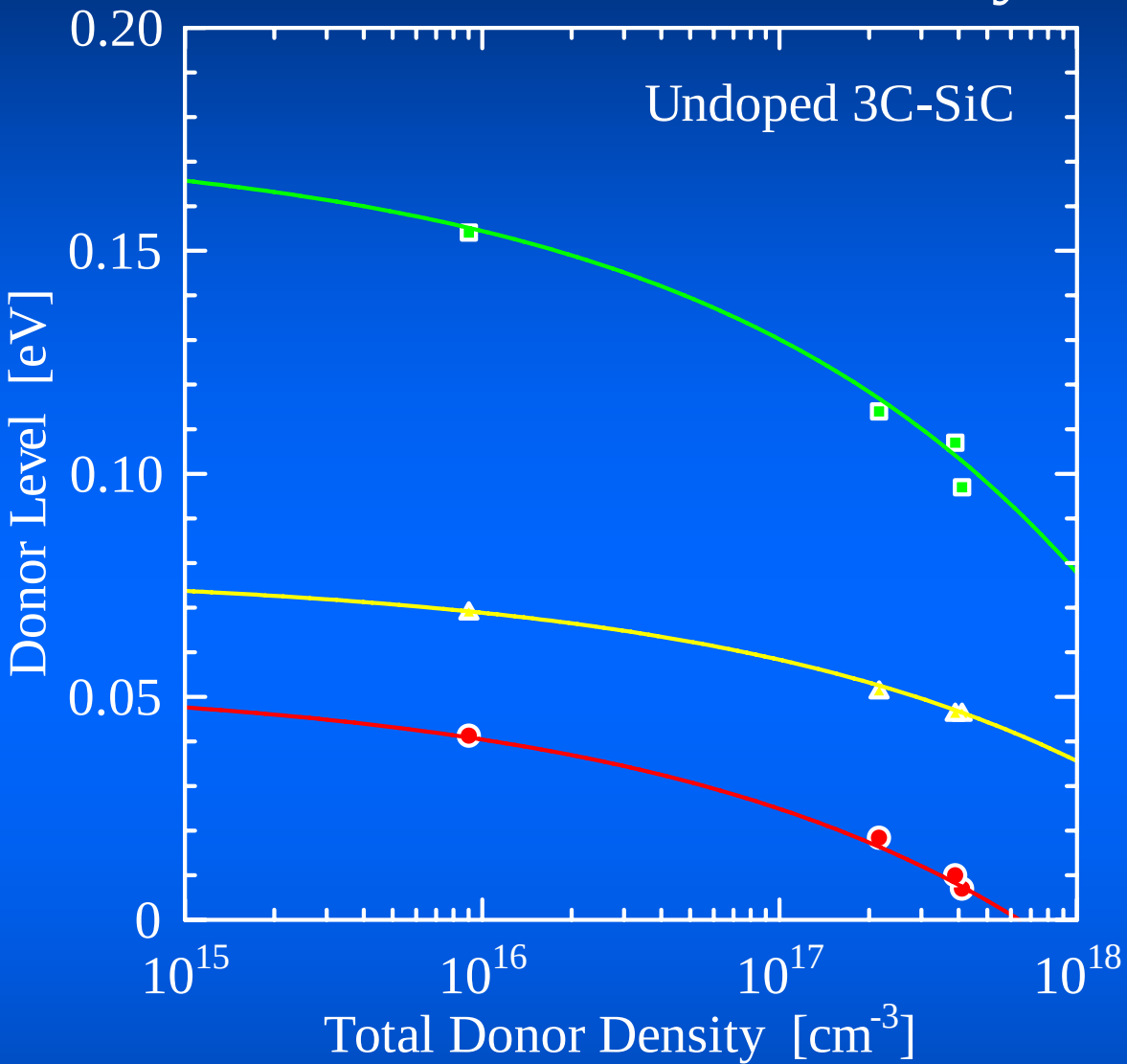
$N_{D1} = 3.8 \times 10^{16}$ cm^{-3} $\quad N_{D3} = 1.1 \times 10^{17}$ cm^{-3}

Verification of the values obtained by FCCS



The n(T) simulation is in good agreement with the experimental n(T), indicating that the values determined by FCCS are reliable.

Relationship between each donor level and the total donor density

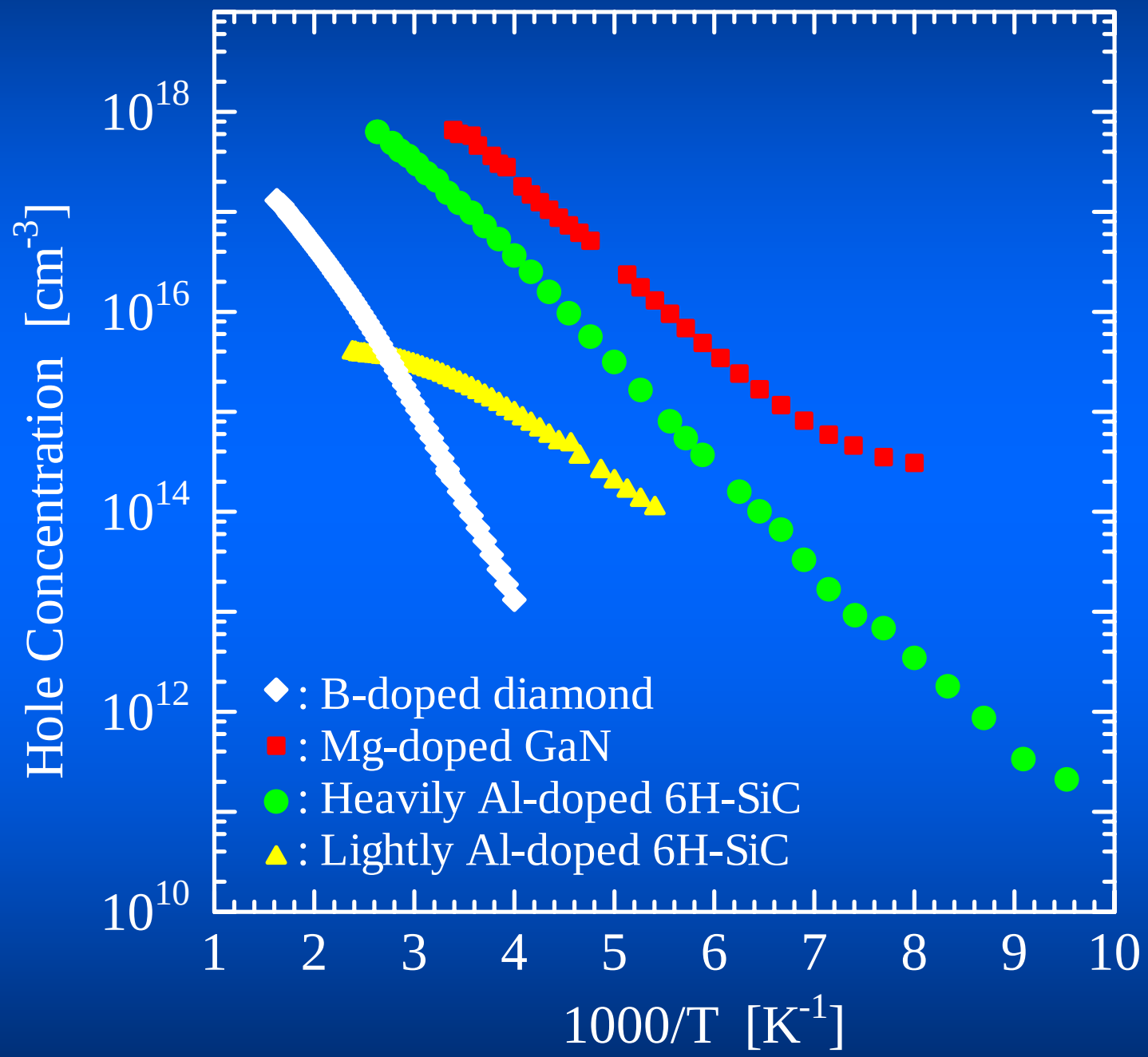


$$E_C - E_{D1} = 0.054 - 6.3\times10^{-8}\sqrt[3]{N_{D,total}}$$

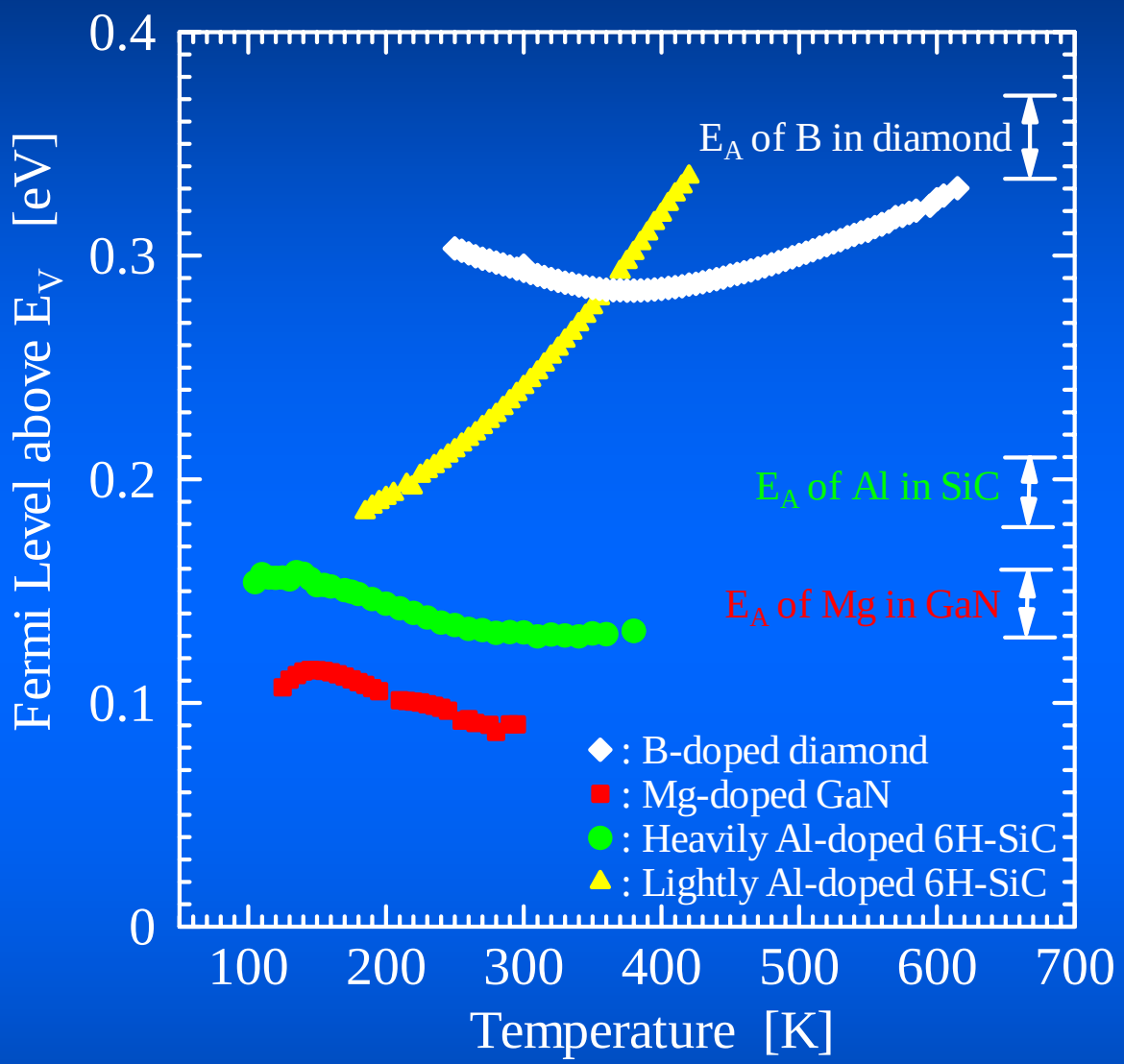
$$E_C - E_{D2} = 0.078 - 4.2\times10^{-8}\sqrt[3]{N_{D,total}}$$

$$E_C - E_{D3} = 0.176 - 9.8\times10^{-8}\sqrt[3]{N_{D,total}}$$

Heavily doped p-type wide band gap semiconductor



Comparison of Fermi level with acceptor level



Except for lightly Al-doped 6H-SiC, the Fermi levels are located between E_A and E_V.

↓

The excited states of acceptors should affect p(T).

Distribution function for acceptors

Fermi-Dirac distribution function

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

Distribution function including the influence of the excited states of the acceptor

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

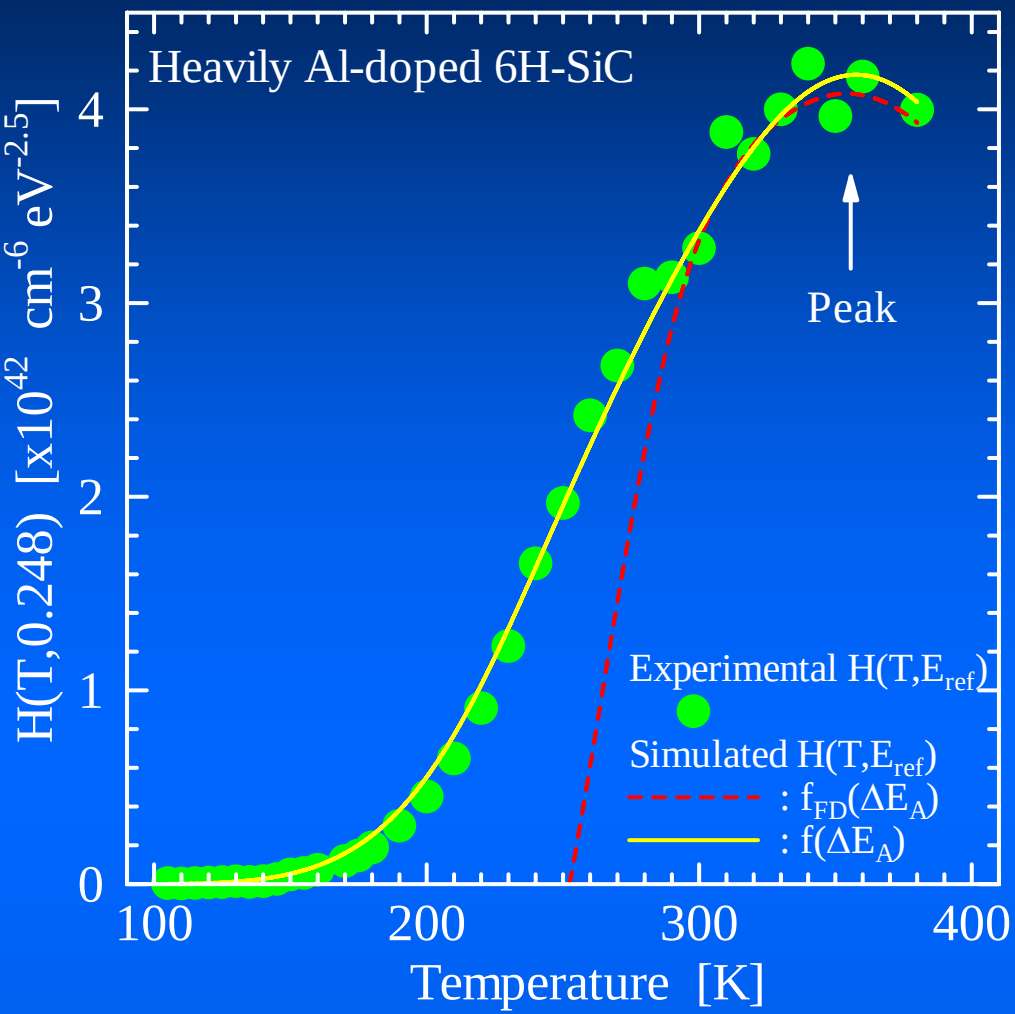
Effective acceptor degeneracy factor

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

Ensemble average energy of holes at the ground and excited state levels

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

FCCS of heavily Al-doped 6H-SiC

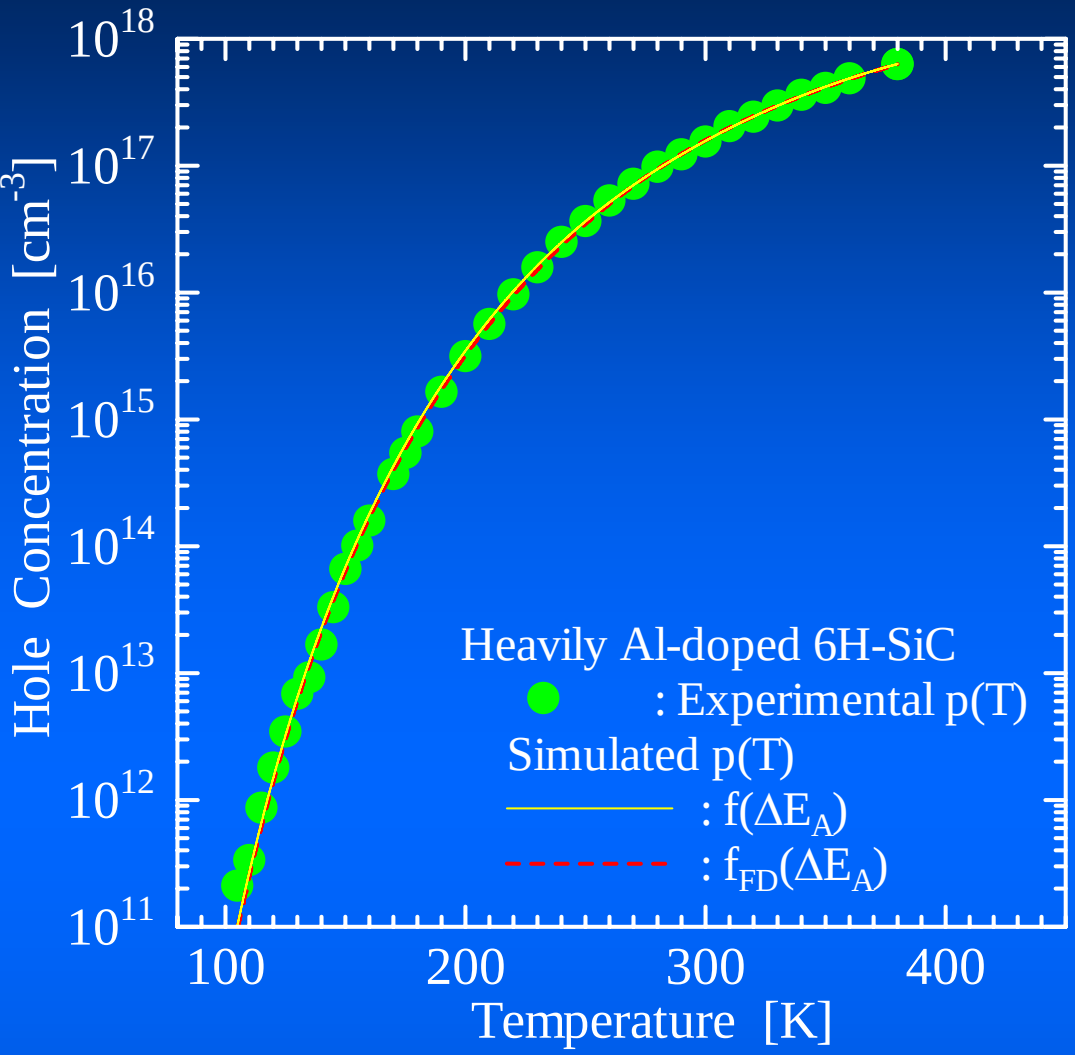


From peak

$f_{FD}(E_A)$	$f(E_A)$
$E_A = E_V + 0.18$ eV	$E_A = E_V + 0.18$ eV
$N_A = 2.5\times10^{19}$ cm^{-3}	$N_A = 3.2\times10^{18}$ cm^{-3}
$N_D = 7.3\times10^{17}$ cm^{-3}	$N_D = 9.0\times10^{16}$ cm^{-3}

The yellow line is in agreement with the experimental FCCS better than the red line.

Curve-fitting procedure



1. **The red line overlaps with the yellow line.**
2. **Both the lines are in good agreement with the experimental p(T).**
3. **N_A for $f_{FD}(E_A)$ is much higher than N_A for $f(E_A)$.**

↓

It is difficult to determine N_A, E_A and N_D by the curve-fitting procedure.

Comparison of N_A with doping density

	$f_{FD}(E_A)$	$f(E_A)$	Doping density [cm^{-3}]
	N_A [cm^{-3}]	N_A [cm^{-3}]	
Heavily doped 6H-SiC	2.5×10^{19}	3.2×10^{18}	4×10^{18}
Lightly doped 6H-SiC	4.9×10^{15}	4.1×10^{15}	6×10^{15}
Mg-doped GaN	8.5×10^{19}	6.0×10^{18}	2×10^{19}
B-doped diamond	9.7×10^{17}	2.8×10^{17}	2×10^{17}

N_A should be less than or equal to the doping density, because N_A is the density of dopant atoms at substitutional sites

$f(E_A)$ is more appropriate for the distribution function for acceptors in heavily doped p-type SiC, GaN and diamond

Summary

1. It was demonstrated that FCCS (a graphical peak analysis method without any assumptions regarding impurity species) is a powerful method for determining densities and energy levels of impurities.
2. In undoped 3C-SiC, FCCS could detect three types of donor species, and could determine those densities and energy levels.
3. In p-type SiC, GaN and diamond whose $E_F(T)$ were located between E_A and E_V, p(T) was strongly affected by the influence of the excited states of acceptors.
4. In order to determine the density and energy level of acceptors from p(T), the proposed distribution function including the influence of the excited states of acceptors was required.

References

1. H. Matsuura, et al., Jpn. J. Appl. Phys. 35 (1996) L555.
2. H. Matsuura, et al., Jpn. J. Appl. Phys. 39 (2000) 5069.
3. H. Matsuura, et al., Phys. Status Solidi C 0 (2003) 2214.
4. H. Matsuura, J. Appl. Phys. 95 (2004) 4213.
5. H. Matsuura, et al., J. Appl. Phys. 96 (2004) 2708.
6. S. Kagamihara, H. Matsuura, et al., J. Appl. Phys. 96 (2004) 5601.
7. H. Matsuura, et al., J. Appl. Phys. 96 (2004) 7346.
8. H. Matsuura, et al., Jpn. J. Appl. Phys. 45 (2006) 6376.
9. H. Matsuura, Phys. Rev. B 74 (2006) 245216.
10. H. Matsuura, et al., Physica B 376-377 (2006) 34.

WINDOWS application software

FCCS (Free Carrier Concentration Spectroscopy)
DCTS (Discharge Current Transient Spectroscopy)

Downloaded freely at our web site
(http://www.osakac.ac.jp/labs/matsuura/)