Background

In order to use SiC wafers or epilayers for electronic devices, an accurate evaluation of densities and energy levels of electrically active impurities and defects is essential.

Electrical method for characterizations

For deep impurities or defects

a. deep level transient spectroscopy (DLTS)

b. isothermal capacitance transient spectroscopy (ICTS)

For shallow impurities or defects ??

The temperature dependence of the majority-carrier concentration $n(T)$ includes a lot of important information on shallow impurities or defects.

Curve-fitting method $\longrightarrow$ unique solution is not obtained

Aim

1. To know the number of types of shallow impurities or defects in SiC.
2. To determine the densities and energy levels of these impurities or defects.

DLTS or ICTS can uniquely determine the densities and energy levels of deep impurities or defects.

This is because each peak in the signal corresponds to a one-to-one impurity or defect.

In ICTS, the signal is defined as

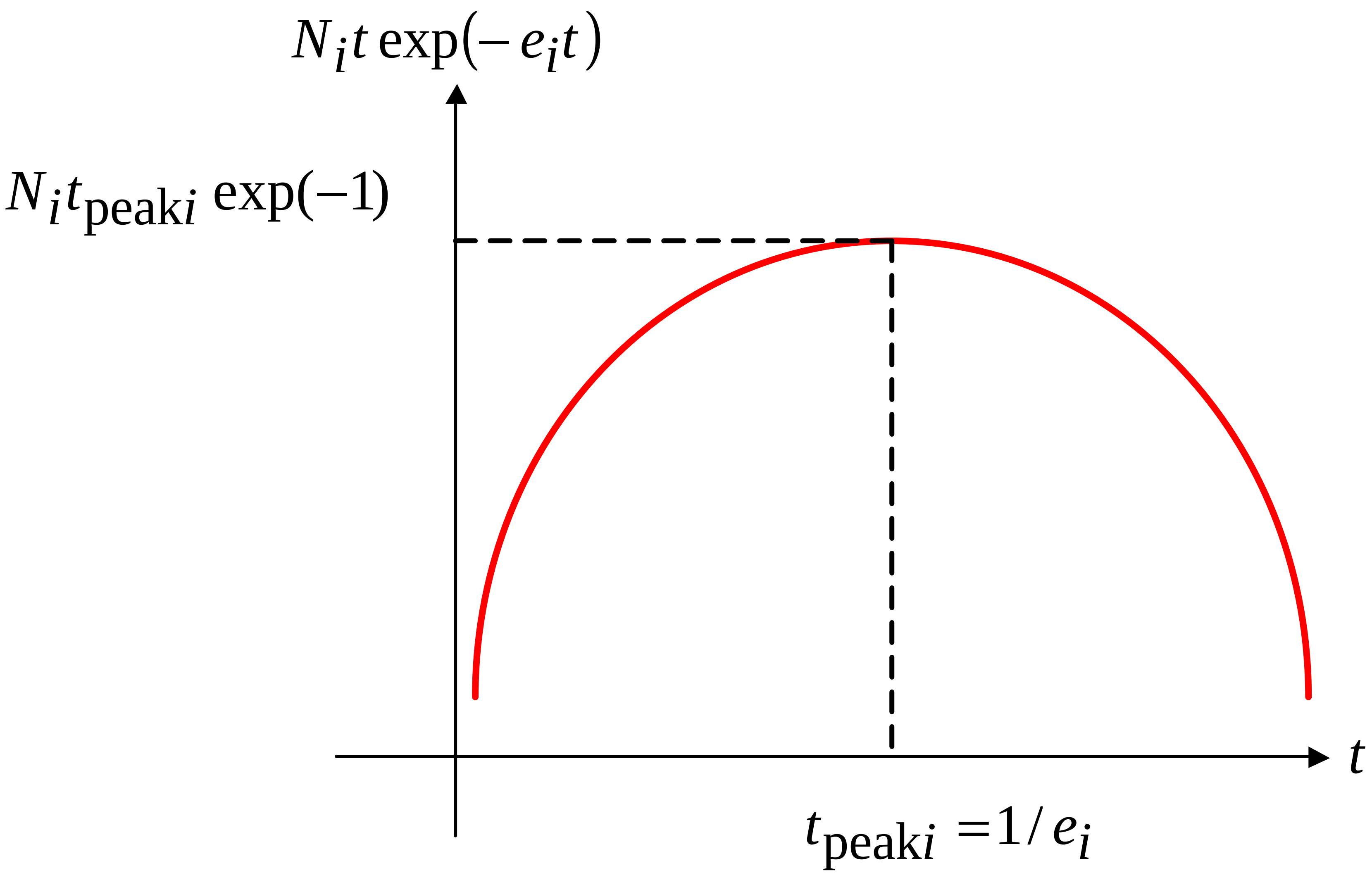
$$S(t) \equiv t \frac{\mathrm{d}C(t)^2}{\mathrm{d}t}. \qquad C(t): \text{ transient capacitance}$$

The signal can be theoretically expressed as

$$S(t) \propto \sum_i N_i t \exp(-e_i t).$$

N_i : density of i-th trap

e_i : emission rate of i-th trap



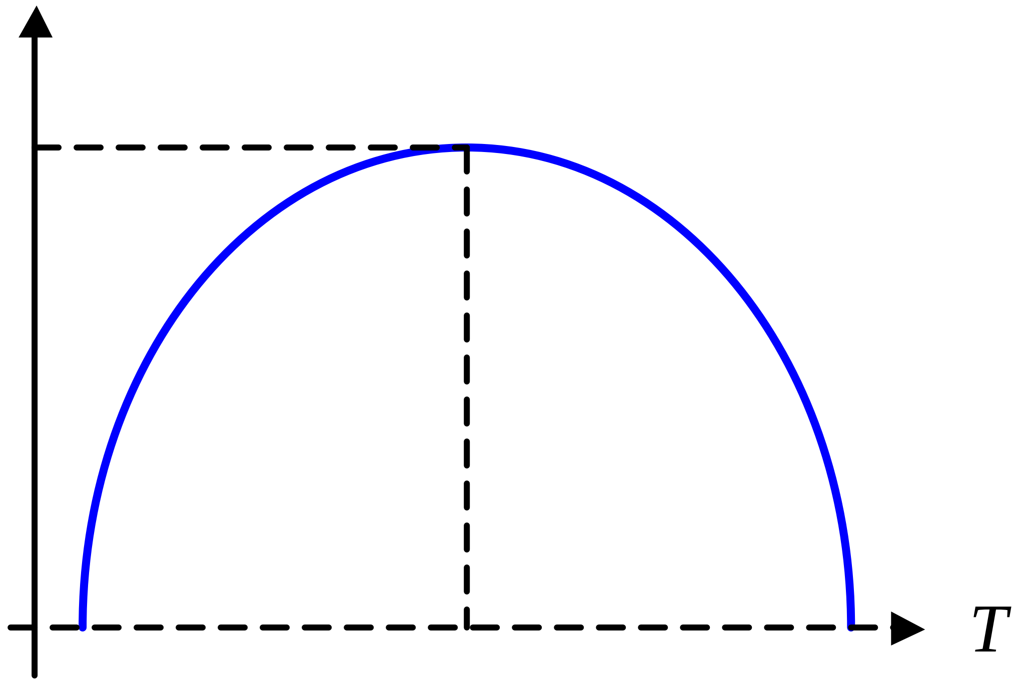
$N_i t \exp(-e_i t)$ plays an important role in the ICTS analysis.

Concept of New Graphical Method

Let us consider the following functions:

1. $\dfrac{N_i}{kT}\exp\left(-\dfrac{\Delta E_i}{kT}\right)$

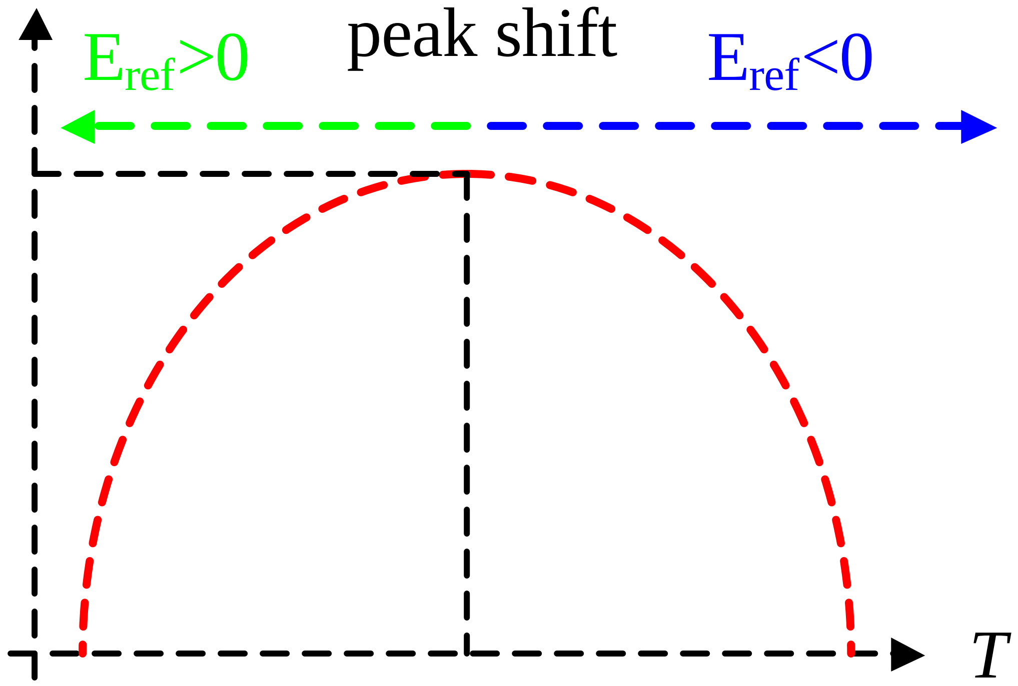
$$\frac{N_i}{kT_{\mathrm{peak}i}}\exp(-1)$$



$$T_{\mathrm{peak}i} = \Delta E_i / k$$

2. $\dfrac{N_i}{kT}\exp\left(-\dfrac{\Delta E_i - E_{\mathrm{ref}}}{kT}\right)$

$$\frac{N_i}{kT_{\mathrm{peak}i}}\exp(-1)$$



$$T_{\mathrm{peak}i} = (\Delta E_i - E_{\mathrm{ref}})/k$$

Introducing a parameter E_{ref}, we can change the peak condition.

Desirable Function to be evaluated

The temperature dependence of the electron concentration $n(T)$ in an n-type semiconductor is described as follows:

1. From the charge neutrality condition,

$$n(T) = \sum_i N_{Di}\left[1 - f(\Delta E_{Di})\right] - N_A \tag{1}$$

N_{Di}: i-th donor density

ΔE_{Di}: i-th donor level measured from E_C

$f(\Delta E_{Di})$: Fermi-Dirac distribution function

N_A : acceptor density

2. From the effective density of states $N_C(T)$,

$$n(T) = N_C(T)\exp\left(-\frac{\Delta E_F}{kT}\right) \tag{2}$$

ΔE_F: Fermi level measured from E_C

Using the two equations (1) and (2),
how shall we define a desirable function?

[The defined function should include the following terms.]

$$\sum_i \frac{N_{Di}}{kT}\exp\left(-\frac{\Delta E_{Di} - E_{ref}}{kT}\right)$$

Desirable Definition

When we define a function to be evaluated as

$$\boxed{H(T, E_{\mathrm{ref}}) \equiv \frac{n(T)^2}{(kT)^{2.5}} \exp\left(\frac{E_{\mathrm{ref}}}{kT}\right),}$$

the defined function can be expressed as

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

$$- N_{\mathrm{A}} \frac{N_{\mathrm{C0}}}{kT} \exp\left(\frac{E_{\mathrm{ref}} - \Delta E_{\mathrm{F}}}{kT}\right)$$

using eqs. (1) and (2), where $N_{\mathrm{C0}} = 2(2\pi m_{\mathrm{n}}^{*} / h^2)^{1.5}$.

Since $I(\Delta E_{\mathrm{D}i})$ is found to be almost independent of T,

$H(T, E_{\mathrm{ref}})$ can be approximately expressed as

the sum of $\underline{\dfrac{N_{\mathrm{D}i}}{kT} \exp\left(-\dfrac{\Delta E_{\mathrm{D}i} - E_{\mathrm{ref}}}{kT}\right)}$.

Good points of our method

1. Definition: $H(T, E_{\mathrm{ref}}) \equiv \dfrac{n(T)^2}{(kT)^{2.5}} \exp\left(\dfrac{E_{\mathrm{ref}}}{kT}\right)$

$H(T, E_{\mathrm{ref}})$ has peaks corresponding to each energy level.

i-th peak temperature $\longrightarrow$ energy level of i-th donor

i-th peak value $\longrightarrow$ density of i-th donor

2. Peak temperature: $T_{\mathrm{peak}i} \cong \dfrac{\Delta E_{\mathrm{D}i} - E_{\mathrm{ref}}}{k}$

Even when none of peaks of $H(T,0)$ appear within the measurement temperature range, the peak of $H(T, E_{\mathrm{ref}})$ can be shifted to the measurement temperature range by changing E_{ref}.

3. From the number of peaks in $H(T, E_{\mathrm{ref}})$,

we can know the number of types of donors.

4. We can determine the compensating density

(i.e., acceptor density).

Undoped 3C-SiC

Growth condition

(Atmospheric pressure chemical vapor deposition)

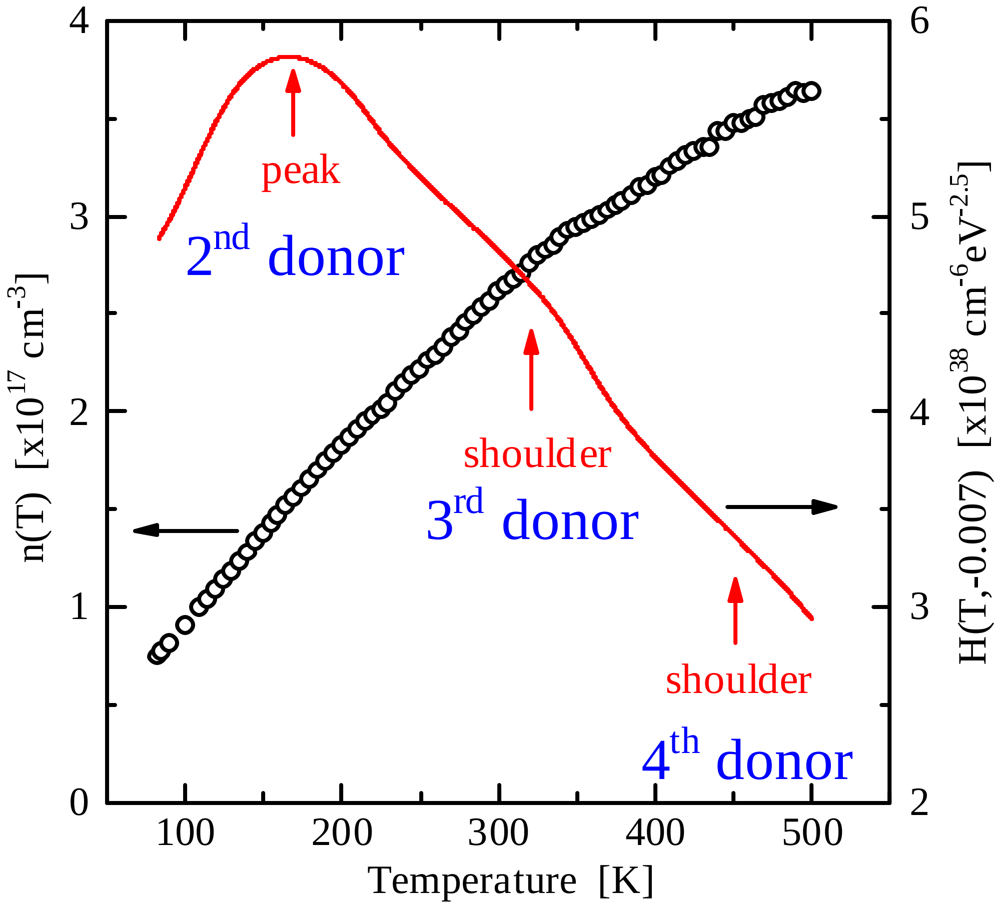
1. Cleaning of (100) n-type Si substrate
   (Etching of Si surface)
   1175 ℃, 11 min.
   HCl: 63 sccm, H_2: 1.5 slm
2. Formation of buffer layer on Si substrate
   (Carbonization of Si surface)
   1350 ℃, 3 min.
   C_3H_8: 1 sccm, H_2: 1 slm
3. Growth of undoped 3C-SiC
   1350 ℃
   $Si_2(CH_3)_6$: 0.5 sccm, H_2: 2.5 slm
   growth rate: 4.3 μm/h

Conditions of Hall-effect measurement

Removal of Si substrate (chemical etching)
Thicknesses: 8 μm, 16 μm, 32 μm
Size: 5×5 mm^2
Magnetic field: 5 kG
Temperature range: 85 K~500 K

Electron Concentration and Fermi Level

$$H(T, E_{\mathrm{ref}}) \equiv \frac{n(T)^2}{(kT)^{2.5}} \exp\left(\frac{E_{\mathrm{ref}}}{kT}\right)$$

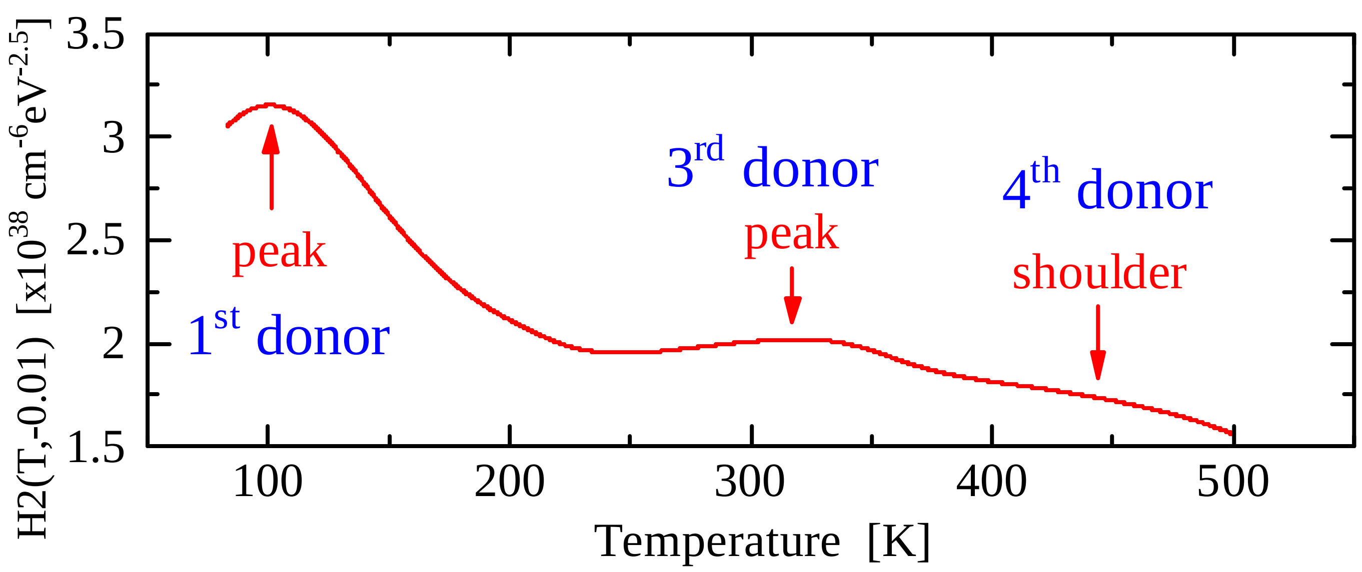


peak
166 K
$5.8\mathrm{x}10^{38}$ cm^{-6}eV$^{-2.5}$

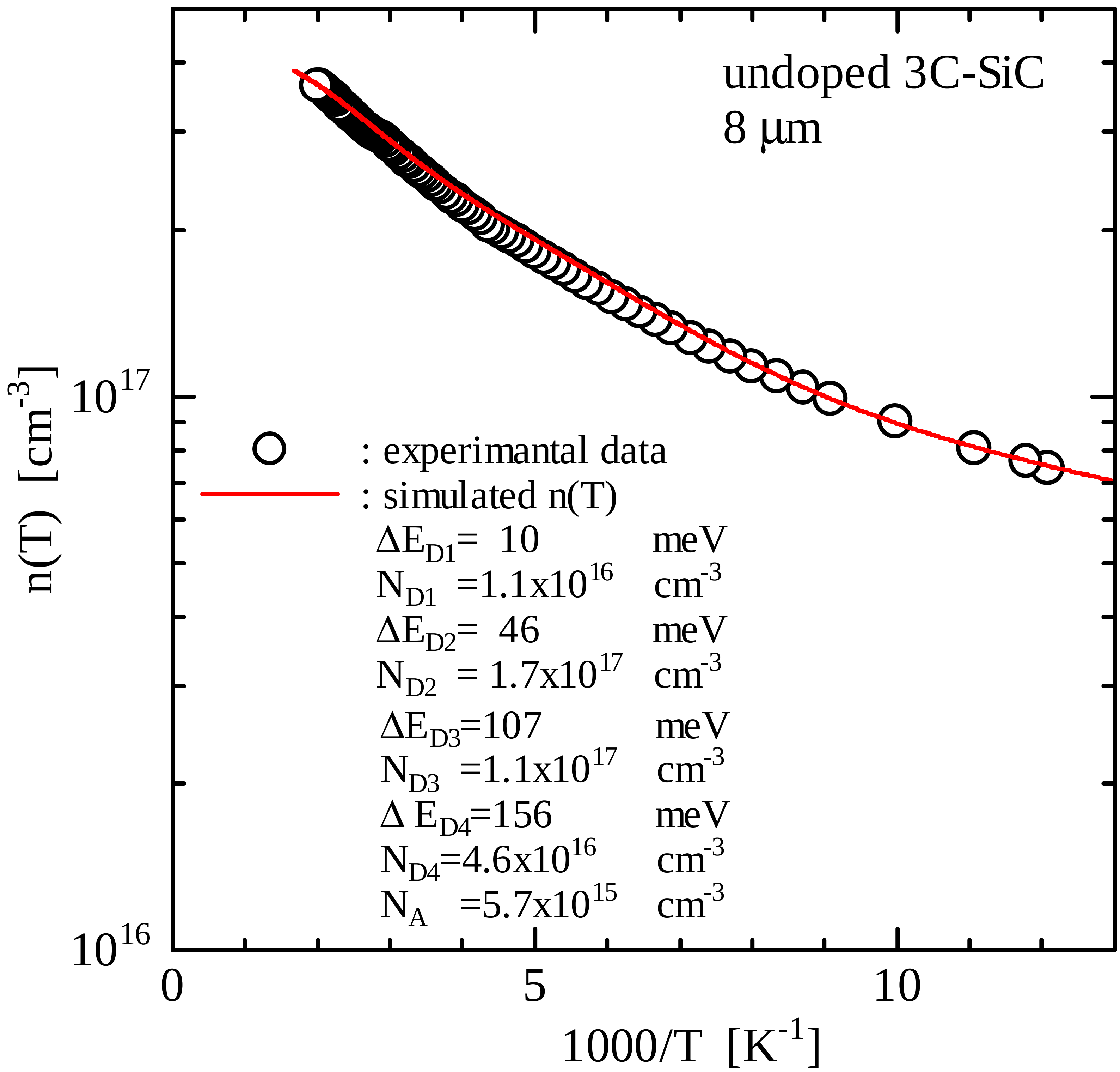
2nd donor level
ΔE_{D2} =46 meV
2nd donor density
N_{D2} =$1.7\mathrm{x}10^{17}$ cm^{-3}

$H2(T, E_{\mathrm{ref}})$ that is not influenced by the 2nd donor:

$$H2(T, E_{\mathrm{ref}}) \equiv \frac{n(T)^2}{(kT)^{2.5}} \exp\left(\frac{E_{\mathrm{ref}}}{kT}\right) - \frac{N_{\mathrm{D2}}}{kT} \exp\left(-\frac{\Delta E_{\mathrm{D2}} - E_{\mathrm{ref}}}{kT}\right) I(\Delta E_{\mathrm{D2}})$$



Comparison of the experimental $n(T)$ with the $n(T)$ simulated with the values determined by $H(T, E_{ref})$



The simulated $n(T)$ is quantitatively in good agreement with the experimental $n(T)$.

↓

The values determined by $H(T, E_{ref})$ are reasonable.

Thickness Dependence of Donor Densities and Donor Levels

3C-SiC thickness [μm]	8	16	32
ΔE_{D1} [meV]	10	7	14
N_{D1} [$\times 10^{16}$ cm^{-3}]	11	8.1	4.7
ΔE_{D2} [meV]	46	46	54
N_{D2} [$\times 10^{16}$ cm^{-3}]	17	20	8.1
ΔE_{D3} [meV]	107	97	120
N_{D3} [$\times 10^{16}$ cm^{-3}]	11	13	10
ΔE_{D4} [meV]	156	-----	-----
N_{D4} [$\times 10^{16}$ cm^{-3}]	4.6	-----	-----
N_A [$\times 10^{16}$ cm^{-3}]	1.3	0.99	0.57

Origin of donors

7-14 meV donor

defect-impurity complex or nonstoichiometric defect ?

(this donor was reported from Hall-effect measurements in undoped 3C-SiC grown from a mixture of SiH_4 and C_3H_8, where the donor density was higher than 10^{18} cm^{-3} and the compensation ratio was higher than 0.9)

46-54 meV donor

substitutional nitrogen atom

(this donor was reported from photoluminescence)

97-120 meV donor

156 meV donor

→ **not reported yet**

Conclusions

Using $n(T)$ obtained by Hall-effect measurements, we have attempted to precisely determine the densities and energy levels of shallow electrically active impurities and defects.

When we define a function to be evaluated as

$$\boxed{H(T, E_{\mathrm{ref}}) \equiv \frac{n(T)^2}{(kT)^{2.5}} \exp\left(\frac{E_{\mathrm{ref}}}{kT}\right),}$$

using peaks of $H(T, E_{\mathrm{ref}})$

1. we can determine the number of types of shallow impurities or defects in a semiconductor,
2. we can precisely determine the density and energy level of each impurity or defect,
3. we can determine the compensating density, and
4. we can easily verify the obtained values.

References

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More information is in our web site (http://www.osakac.ac.jp/labs/matsuura).

Free application software of this method for Windows OS is to appear in our web site by the end of this year.