Influence of Excited States of Deep Acceptors on Hole Concentration in SiC

Hideharu Matsuura

Department of Electronics,
Osaka Electro-Communication University
18-8 Hatsu-cho, Neyagawa, Osaka 572-8530, Japan

E-mail: matsuura@isc.osakac.ac.jp
Web site: http://www.osakac.ac.jp/labs/matsuura/

FCCS Windows Application Software can be freely downloaded from our web site.

Abstract

The influence of the excited states of acceptors on the hole concentration in p-type SiC is investigated theoretically and experimentally.

Using the temperature dependence of the hole concentration $p(T)$ in a p-type 6H-SiC wafer, a distribution function suitable for deep acceptors is examined.

From the discussion, it is found that we cannot ignore the influence of the excited states on $p(T)$ as well as the ensemble average of the ground and excited state levels of the acceptor when the acceptor level is deep.

1. Reported Distribution Function for Electrons

1.1 Fermi-Dirac distribution function, which does not include the influence of the excited states of the acceptor

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

1.2 Distribution function, which include the influence of the excited states

$$f_{\mathrm{con}}(\Delta E_{\mathrm{A}}) = \frac{1}{1 + 4\left[g_1 \exp\left(\dfrac{\Delta E_{\mathrm{A}} - \Delta E_{\mathrm{F}}}{kT}\right) + \sum\limits_{r=2} g_r \exp\left(\dfrac{\Delta E_r - \Delta E_{\mathrm{F}}}{kT}\right)\right]}$$

2. Acceptor Level and Excited State Levels

2.1 Excited state levels (hydrogenic dopant model)

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

2.2 Acceptor level

$$\Delta E_\mathrm{A} = \Delta E_1 + E_\mathrm{CCC}$$

E_CCC: the energy induced due to central cell correction

2.3 In the case of 6H-SiC

$$\Delta E_1 = 136 \text{ meV}$$

$$\Delta E_2 = 34.0 \text{ meV}, \; \Delta E_3 = 15.1 \text{ meV}, \; \Delta E_4 = 8.5 \text{ meV},$$

$$\Delta E_5 = 5.4 \text{ meV}, \quad \Delta E_6 = 3.8 \text{ meV}, \quad \Delta E_7 = 2.8 \text{ meV}$$

3. Theoretical Consideration of Distribution Function

3.1 Number of configurations in allowed bands or a band gap

A. In allowed bands

Multiplicity function $W_{\mathrm{B}i}$ for the $n_{\mathrm{h}}(\Delta E_i)$ holes arranged in the $D_{\mathrm{h}}(\Delta E_i)$ degenerate states at ΔE_i

$$W_{\mathrm{B}i} = \frac{D_{\mathrm{h}}(\Delta E_i)}{[D_{\mathrm{h}}(\Delta E_i) - n_{\mathrm{h}}(\Delta E_i)]! \cdot n_{\mathrm{h}}(\Delta E_i)!}$$

B. In a band gap

(1) Multiplicity function W_{A1} for the n_{A} holes arranged in the N_{A} acceptors

$$W_{\mathrm{A1}} = \frac{N_{\mathrm{A}}!}{(N_{\mathrm{A}} - n_{\mathrm{A}})! \cdot n_{\mathrm{A}}!}$$

(2) Multiplicity function W_{A2} for the ground state and the excited states of the acceptor

$$W_{A2} = \left[g_1 + \sum_{r=2} g_r \exp\left(-\frac{\Delta E_A - \Delta E_r}{kT} \right) \right]^{n_A}$$

(3) Multiplicity function W_{A3} for degenerate spin-up and spin-down states

$$W_{A3} = 2^{n_A}$$

(4) Multiplicity function W_{A4} for degenerate heavy and light hole valence bands

$$W_{A4} = 2^{n_A}$$

Multiplicity function for acceptors

$$W_A = W_{A1} W_{A2} W_{A3} W_{A4}$$

3.2 Ensemble average $\overline{E_{\mathrm{ex}}}$ of the ground and excited state levels of the acceptor

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

3.3 Average acceptor level

$$\overline{\Delta E_{\mathrm{A}}} = \Delta E_{\mathrm{A}} - \overline{E_{\mathrm{ex}}}$$

3.4 Total number W of configurations of the system

$$W = W_{\mathrm{A}} \times \sum_i W_{\mathrm{B}i}$$

3.5 Thermal Equilibrium configuration of the system

The thermal equilibrium configuration of the system occurs when the entropy

$$S = k \ln W$$

is maximum under the conservation laws;

total number of holes; $n_{\mathrm{h,total}} = n_{\mathrm{A}} + \sum_i n_{\mathrm{h}}\left(\Delta E_i\right) = \mathrm{constant}$

total energy of holes; $E_{\mathrm{total}} = \overline{\Delta E_{\mathrm{A}}} n_{\mathrm{A}} + \sum_i \Delta E_i n_{\mathrm{h}}\left(\Delta E_i\right) = \mathrm{constant}$

3.6 Distribution function for electrons derived under these conditions

A. In the allowed bands

$$f\left(\Delta E_i\right)=1-\frac{n_{\mathrm{h}}(\Delta E_i)}{D(\Delta E_i)}$$

$$=\frac{1}{1+\exp\left(\frac{\Delta E_i-\Delta E_{\mathrm{F}}}{kT}\right)}$$

B. In the band gap

$$f\left(\Delta E_{\mathrm{A}}\right)=1-\frac{n_{\mathrm{A}}}{N_{\mathrm{A}}}$$

$$=\frac{1}{1+4\exp\left(-\frac{\overline{E}_{\mathrm{ex}}}{kT}\right)\cdot\left[g_1\exp\left(\frac{\Delta E_{\mathrm{A}}-\Delta E_{\mathrm{F}}}{kT}\right)+\sum_{r=2} g_r\exp\left(\frac{\Delta E_r-\Delta E_{\mathrm{F}}}{kT}\right)\right]}$$

3.7 Assumptions used in the other distribution functions

A. Fermi-Dirac distribution function $f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$

$$r = 1, \quad g_1 = 1, \quad \overline{E_{\mathrm{ex}}} = 0$$

B. Reported distribution function $f_{\mathrm{con}}(\Delta E_{\mathrm{A}})$

$$\overline{E_{\mathrm{ex}}} = 0$$

4. Experimental

Sample: p-type 6H-SiC wafer

Resistivity ~1.4 Ωcm

Thickness 0.42 mm

Size 1×1 cm^2

Hall-effect measurement

Temperatures 100 K ~ 380 K

Magnetic field 1.4 T

5. Results and Discussion

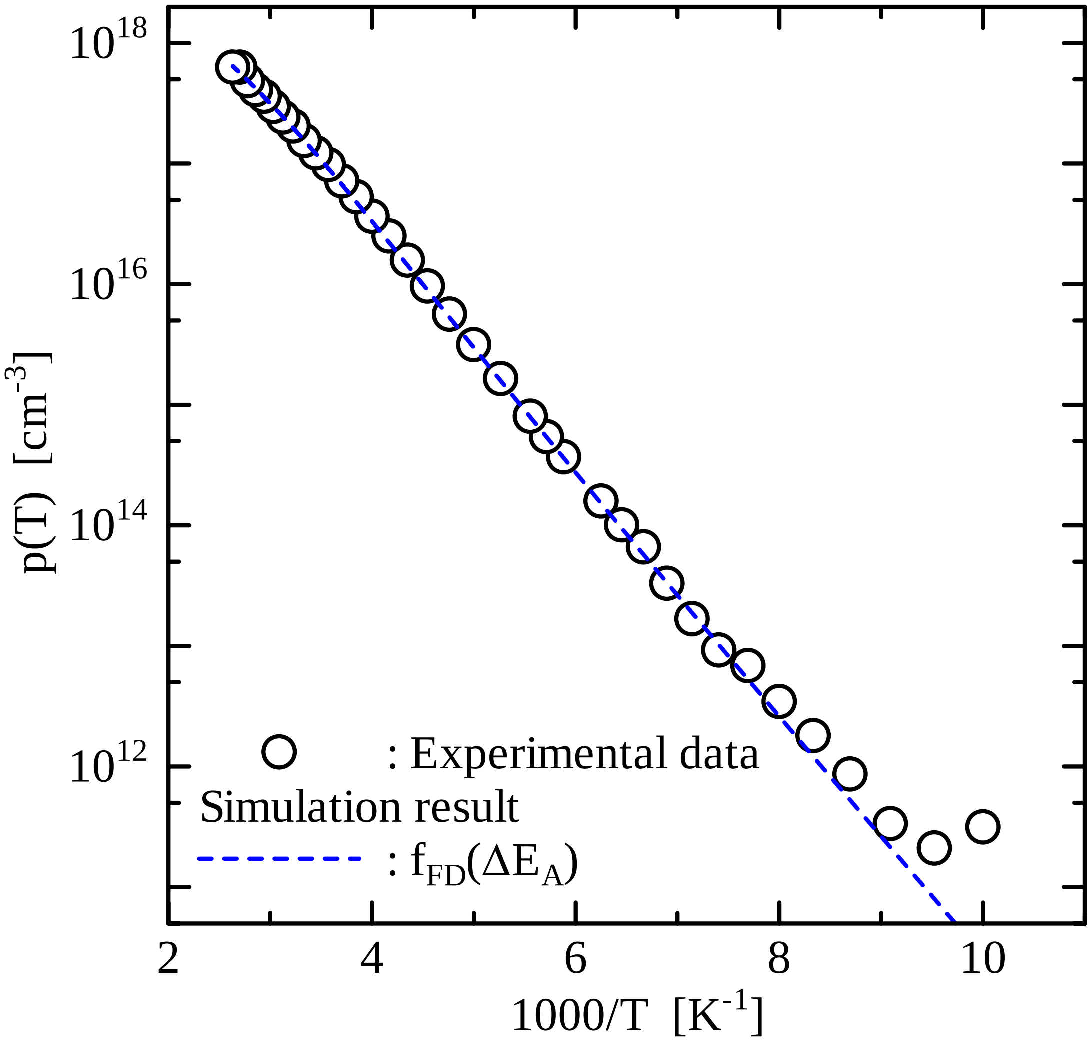

Fig. 1 Experimental and simulated $p(T)$

5.1 Least-squares fit of the neutral equation to $p(T)$

$$\Delta E_A = 182 \text{ meV}$$

$$N_A = 3.0\times 10^{19} \text{ cm}^{-3}$$

$$N_{com} = 8.4\times 10^{17} \text{ cm}^{-3}$$

5.2 Free Carrier Concentration Spectroscopy (FCCS)

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

From the peak of $H(T, E_{\mathrm{ref}})$, the values of ΔE_A, N_A and N_{com} can be determined.

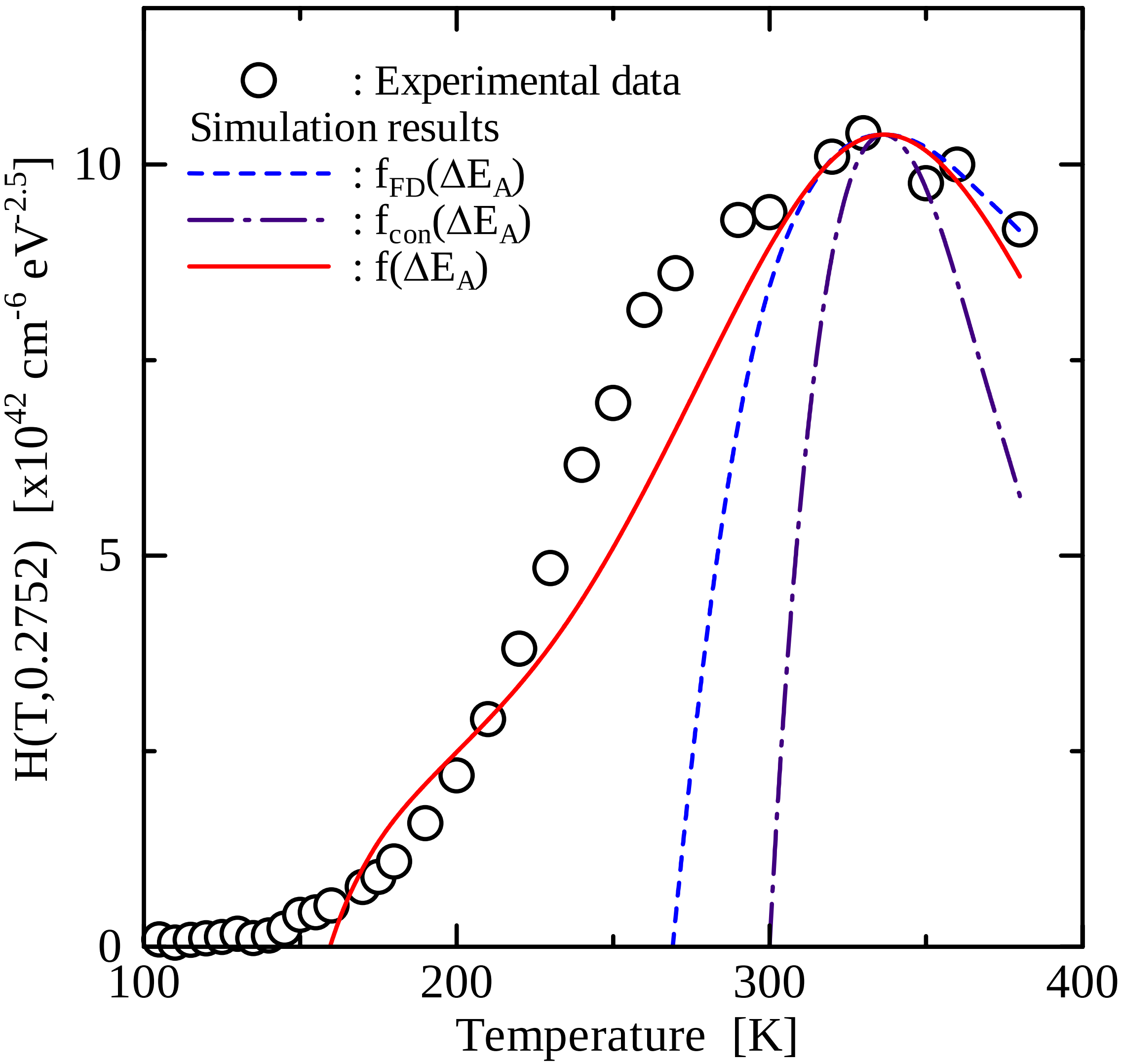

Fig. 2 Experimental and simulated $H(T, E_{\mathrm{ref}})$

5.3 Obtained results

	Fermi-Dirac $f_{FD}(\Delta E_A)$	Reported $f_{con}(\Delta E_A)$	Proposed $f(\Delta E_A)$
N_A [cm^{-3}]	3.0×10^{19}	2.2×10^{20}	1.9×10^{18}
ΔE_A [meV]	182	205	189
N_{com} [cm^{-3}]	8.4×10^{17}	2.7×10^{18}	3.4×10^{16}

The values of all the ΔE_A are considered to be reasonable.

The value of $(N_A - N_{com})$ to be expected is less than 5×10^{18} cm^{-3}.

↓

The proposed $f(\Delta E_A)$ is considered to be suitable for deep acceptors.

5.4 Comparison

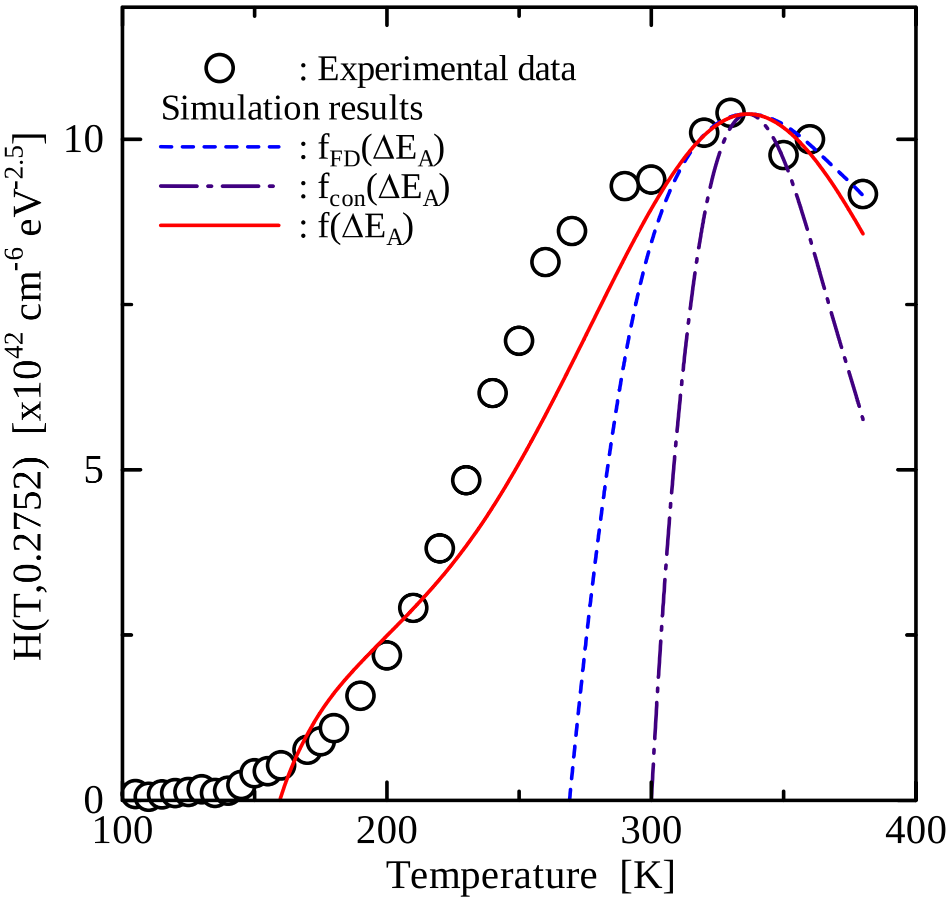

Fig. 3 Experimental and simulated $H(T, E_{\mathrm{ref}})$

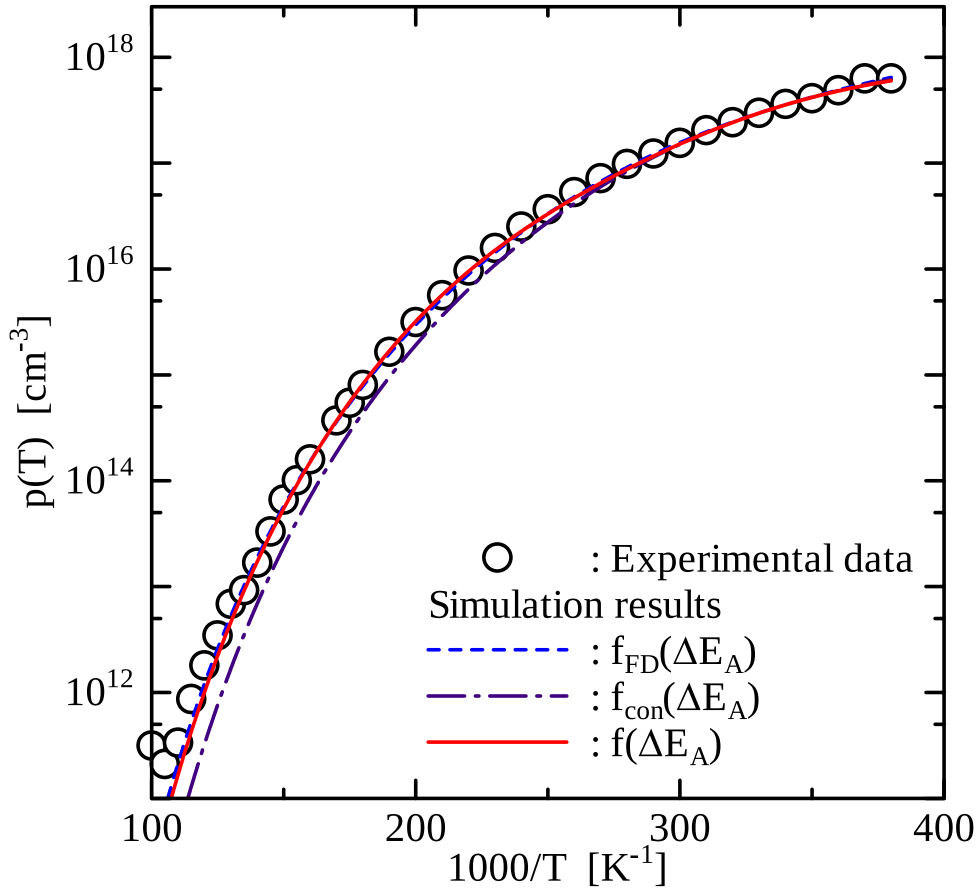

Fig.4 Experimental and simulated $p(T)$

The proposed $f(\Delta E_{\mathrm{A}})$ is considered to be suitable for deep acceptors.

5.5 Temperature dependences of $\exp\left(-\frac{\overline{E_{\rm ex}}}{kT}\right)$ and $\overline{\Delta E_{\rm A}}$

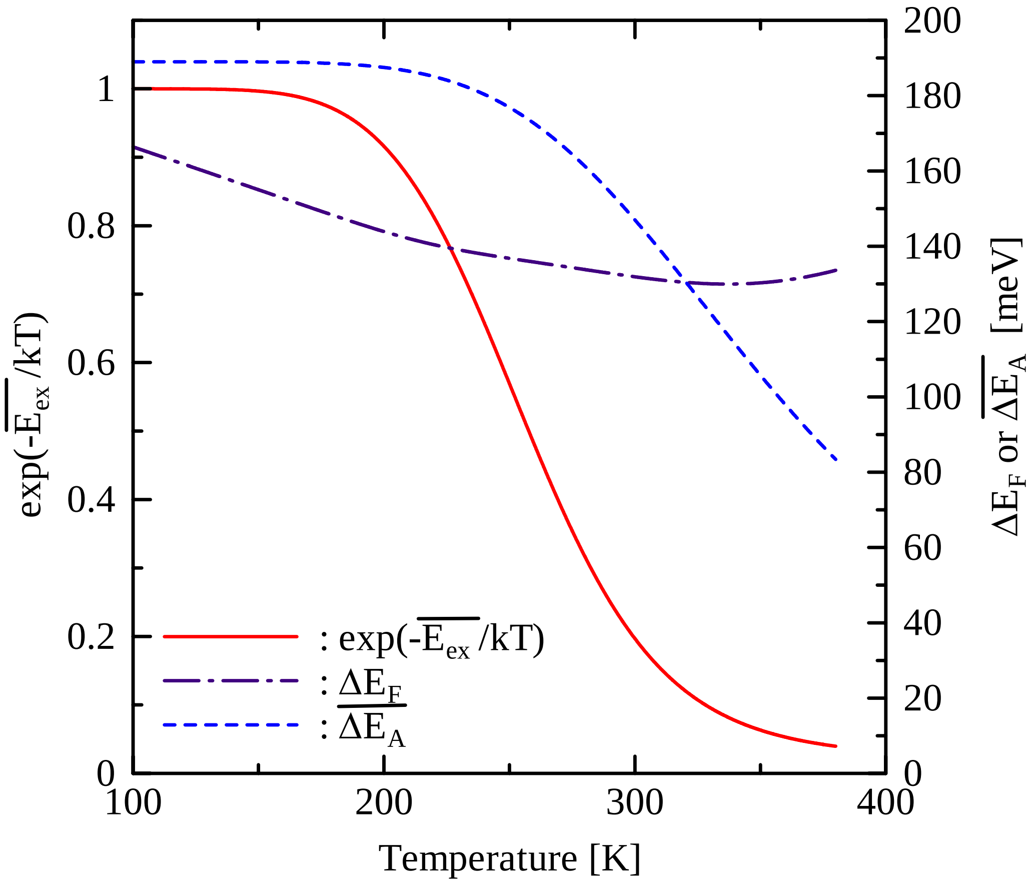

Fig. 5 Temperature dependences of $\exp(-\overline{E_{\rm ex}}/kT)$, $\Delta E_{\rm F}$ and $\overline{\Delta E_{\rm A}}$.

The average acceptor level $\overline{\Delta E_{\rm A}}$ decreases with T.

Since $\exp\left(-\frac{\overline{E_{\rm ex}}}{kT}\right)$ decreases with T rapidly, the acceptors are apt to be negatively ionized at moderate temperatures.

↓

The reliable $N_{\rm A}$ is obtained.

6. Summary

We theoretically derived the distribution function $f(\Delta E_{\mathrm{A}})$ considering the influence of the excited states on $p(T)$, in which the ensemble average $\overline{E_{\mathrm{ex}}}$ of the ground and excited state levels of the acceptor was introduced.

Using three kinds of distribution functions [$f_{\mathrm{FD}}(\Delta E_{\mathrm{A}})$, $f_{\mathrm{con}}(\Delta E_{\mathrm{A}})$, $f(\Delta E_{\mathrm{A}})$], we analyzed $p(T)$ in p-type 6H-SiC experimentally obtained by Hall-effect measurements.

It is found that FCCS is more suitable for investigating the influence of the excited states of the acceptor in SiC than the least-squares fit of the neutrality equation to $p(T)$.

Moreover, it is considered that the proposed distribution function $f(\Delta E_{\mathrm{A}})$ is suitable for deep acceptors.