Determination of densities and energy levels of donors in free-standing undoped 3C-SiC epilayers with thicknesses of 80 μ m

Hideharu Matsuura^{a)}

Department of Electronic Engineering and Computer Science, Osaka Electro-Communication University, 18-8 Hatsu-cho, Neyagawa, Osaka 572-8530, Japan

Hiroyuki Nagasawa, Kuniaki Yagi, and Takamitsu Kawahara

Hoya Advanced Semiconductor Technologies Co., Ltd., 1-17-16 Tanashioda, Sagamihara, Kanagawa 229-1125, Japan

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The densities and energy levels of donors in free-standing undoped 3C-SiC epilayers with the thicknesses of ~80 μ m are investigated from the temperature dependence of the electron concentration n(T) obtained by Hall-effect measurements. Although in the analysis of n(T) many researchers usually assume that only one type of donor species is included in *n*-type 3C-SiC, no one knows whether this assumption is correct or not. In order to determine the densities and energy levels using n(T) without any assumptions regarding donor species, the graphical peak analysis method called free carrier concentration spectroscopy is applied. Three types of donor species are detected in these epilayers. These donor densities can be reduced to $<5 \times 10^{15}$ cm⁻³ by growing 3C-SiC epilayers on undulant Si substrate. Moreover, the dependence of each donor level on a total donor density is investigated, which is used in 3C-SiC device simulation. © 2004 American Institute of Physics. [DOI: 10.1063/1.1814805]

I. INTRODUCTION

Silicon carbide (SiC) is a semiconductor with a wide band gap, high electron mobility, high electron saturation drift velocity, and high thermal conductivity. It is also chemically and thermally stable and extremely hard. As a consequence, it is regarded as a promising semiconductor for the devices operating at high powers, high frequencies, and high temperatures. Among SiC polytypes (e.g., 3C-SiC, 4H-SiC, 6H-SiC), 3C-SiC is a promising polytype for metal-oxide-semiconductor field-effect transistors (MOSFETs), because the trap density below the conduction band of 3C-SiC at SiO₂/3C-SiC interfaces can be reduced due to its band gap narrower than band gaps of 4H-SiC and 6H-SiC.¹ In fact, electron channel mobilities in 3C-SiC MOSFETs reach 230 cm² V⁻¹ s⁻¹,² which is higher than by at least 2 than those in 4H-SiC or 6H-SiC MOSFETs.^{3,4} The epitaxial growth of 3C-SiC on silicon (Si) substrate is possible in spite of the 21% misfit between the Si and 3C-SiC system.⁵ Due to the large misfit, the density of defects in the early stage of the growth is very high, and the remaining density of defects at the uppermost part of the 3C-SiC epilayer is still high, indicating that 3C-SiC epilayers show poor electrical characteristics.

Recently, these defects have been eliminated by growing 3C-SiC epilayers on undulant Si substrate.^{6–8} This substrate has a wavy Si(001) surface with countered slopes oriented in the [110] and [$\overline{110}$] directions. Using this technique, free-standing 200 μ m thick 3C–SiC epilayers with a diameter of 6 in. can be grown. Since these undoped epilayers exhibit

n-type conduction, it is important to investigate the origins of donor species in them for growing well-controlled *p*-type or *n*-type 3C-SiC epilayers.

In many papers, ${}^{9-16}$ under the assumption that only one type of donor species existed in unintentionally doped 3C-SiC, the density and energy level of the donor as well as the acceptor (or compensating) density were determined by a curve-fitting method using the temperature dependence of the electron concentration n(T). Using those results, moreover, the donor level corresponding to substitutional nitrogen (N) was reported to decrease with an increase in the N donor density from ~50 meV to ~15 meV as measured from the bottom of the conduction band $E_{\rm C}$. However, no one knows whether only one type of donor species actually exists there.

In this study, the n(T) and the temperature-dependent electron mobility $\mu_n(T)$ are obtained from Hall-effect measurements for free-standing undoped *n*-type 3C–SiC epilayers with the thicknesses of ~80 μ m. In order to determine the densities and energy levels of donors using n(T) without any assumptions regarding donor species, the graphical peak analysis method called free carrier concentration spectroscopy (FCCS) (Refs. 17–24) is applied. Using these results, the number of donor species in undoped 3C–SiC is investigated, and the dependence of each donor level on a total donor density is discussed.

II. FREE CARRIER CONCENTRATION SPECTROSCOPY

A. Basic concept

Deep level transient spectroscopy,²⁵ isothermal capacitance transient spectroscopy (ICTS),²⁶ and other methods^{27,28} can uniquely determine the densities and energy levels of

^{a)}Electronic mail: matsuura@isc.osakac.ac.jp

traps in semiconductors or insulators, because each peak in the signal corresponds one-to-one to a trap. For example, the ICTS signal is defined as $S(t) \equiv t dC(t)^2/dt$, where C(t) is the transient capacitance after a reverse bias is applied for a *pn* diode or a Schottky barrier diode. Since S(t) is theoretically described as the sum of $N_i e_i t \exp(-e_i t)$, it has a peak value of $N_i \exp(-1)$ at a peak time of $t_{\text{peak}i} = 1/e_i$. Here, N_i and e_i are the density and emission rate of an *i*th trap. Therefore, the function $N_i e_i t \exp(-e_i t)$ plays an important role in the ICTS analysis.

In order to analyze n(T), the function theoretically described as the sum of $N_{\rm Di} \exp(-\Delta E_{\rm Di}/kT)/kT$ was introduced, 17,18 where T is the measured absolute temperature, k is the Boltzmann constant, N_{Di} and ΔE_{Di} are the density and energy level of an *i*th donor species, and ΔE_{Di} is measured from $E_{\rm C}$. The function $N_{\rm Di} \exp(-\Delta E_{\rm Di}/kT)/kT$ has a peak at $T_{\text{peak}i} = \Delta E_{\text{D}i}/k$, which does not apply to all the donor species in the temperature range of the measurement. If you can introduce a function in which the peak appears at $T_{\text{peak}i} = (\Delta E_{\text{D}i} - E_{\text{ref}})/k$, you can shift the peak temperature to the measurement temperature range by changing the parameter $E_{\rm ref}$. This indicates that you can determine $N_{\rm Di}$ and $\Delta E_{\rm Di}$ in a wide range of donor levels. Therefore, the function to be evaluated should be approximately described as the sum of $N_{\rm Di} \exp[-(\Delta E_{\rm Di} - E_{\rm ref})/kT]/kT$. It should be noted that $N_{\rm Di}$ and $\Delta E_{\mathrm{D}i}$ determined by this method are independent of E_{ref} . In addition, although Hoffmann proposed an interesting graphical peak analysis method,^{29,30} you should avoid introducing a differential evaluation of n(T) because the differential of the experimental data results in an increase in the observational errors.17,18,20

B. Theoretical consideration

In the following theoretical consideration, we assume an *n*-type semiconductor with *n* different donor species, and an acceptor density (N_A). From the charge neutrality condition, n(T) can be expressed as³¹

$$n(T) = \sum_{i=1}^{n} N_{\mathrm{D}i} [1 - f(\Delta E_{\mathrm{D}i})] - N_{\mathrm{A}}, \qquad (1)$$

where $f(\Delta E_{Di})$ is the Fermi-Dirac distribution function given by³¹

$$f(\Delta E_{\mathrm{D}i}) = \frac{1}{1 + \frac{1}{g_{\mathrm{D}}} \exp\left(\frac{\Delta E_{\mathrm{F}}(T) - \Delta E_{\mathrm{D}i}}{kT}\right)},\tag{2}$$

 $\Delta E_{\rm F}(T)$ is the Fermi level measured from $E_{\rm C}$ at T, and $g_{\rm D}$ is the degeneracy factor for donors. On the other hand, using the effective density of states $N_{\rm C}(T)$ in the conduction band, n(T) is written as³¹

$$n(T) = N_{\rm C}(T) \exp\left(-\frac{\Delta E_{\rm F}(T)}{kT}\right),\tag{3}$$

where

$$N_{\rm C}(T) = N_{\rm C0} k^{3/2} T^{3/2},\tag{4}$$

 m_n^* is the electron effective mass, M_c is the number of equivalent minima in the conduction band, and *h* is Planck's constant.

From Eqs. (1) and (3), a favorable function to determine $N_{\text{D}i}$ and $\Delta E_{\text{D}i}$ can be introduced as follows. The function to be evaluated is defined as²¹⁻²⁴

$$H(T, E_{\rm ref}) \equiv \frac{n(T)^2}{(kT)^{5/2}} \exp\left(\frac{E_{\rm ref}}{kT}\right).$$
 (6)

Substituting Eq. (1) for one of the n(T) in Eq. (6) and substituting Eq. (3) for the other n(T) in Eq. (6) yield

$$H(T, E_{\rm ref}) = \sum_{i=1}^{n} \frac{N_{\rm Di}}{kT} \exp\left(-\frac{\Delta E_{\rm Di} - E_{\rm ref}}{kT}\right) I(\Delta E_{\rm Di}) - \frac{N_{\rm A} N_{\rm C0}}{kT} \exp\left(\frac{E_{\rm ref} - \Delta E_{\rm F}(T)}{kT}\right),$$
(7)

where

$$I(\Delta E_{\mathrm{D}i}) = \frac{N_{\mathrm{C}0}}{g_{\mathrm{D}} + \exp\left(\frac{\Delta E_{\mathrm{F}}(T) - \Delta E_{\mathrm{D}i}}{kT}\right)}.$$
(8)

The function

$$\frac{N_{\rm Di}}{kT} \exp\left(-\frac{\Delta E_{\rm Di} - E_{\rm ref}}{kT}\right) \tag{9}$$

in Eq. (7) has a peak value of $N_{\text{D}i} \exp(-1)/kT_{\text{peak}i}$ at a peak temperature

$$T_{\text{peak}i} = \frac{\Delta E_{\text{D}i} - E_{\text{ref}}}{k}.$$
 (10)

It is clear from Eq. (10) that E_{ref} can shift the peak of $H(T, E_{ref})$ within the temperature range of the measurement. Although the actual T_{peaki} of $H(T, E_{ref})$ is slightly different from T_{peaki} calculated by Eq. (10) due to the temperature dependence of $I(\Delta E_{Di})$, we can easily determine the accurate values of N_{Di} and ΔE_{Di} from the peak of the experimental $H(T, E_{ref})$, using a personal computer. The WINDOWS application software for FCCS can be freely downloaded at our web site (http://www.osakac.ac.jp/labs/matsuura/). This software can also evaluate them by using the curve-fitting method or the differential method.

III. EXPERIMENT

The entire surface of well-oriented Si(001) substrate was scratched with a diamond slurry paralleling the $[\bar{1}10]$ direction, which forms continuous undulant Si substrate with ridges roughly paralleling the $[\bar{1}10]$ direction. Then, sacrificial oxidation was carried out to remove crystal defects introduced by the scratching process.

A cold-wall low-pressure chemical vapor deposition system was used for 3C-SiC epitaxial growth. After the Si substrate was carbonized for 5 min using a mixture of C_2H_2 of 10 SCCM (SCCM—cubic centimeter per minute at STP)



FIG. 1. Temperature dependencies of electron concentration for two different undoped 3C-SiC epilayers.

and H₂ of 100 SCCM, a 3C–SiC epilayer was grown on the substrate at 1350°C at 100 mTorr using a mixture of SiH₂Cl₂ of 50 SCCM, C₂H₂ of 10 SCCM, and H₂ of 100 SCCM. The growth rate was \approx 40 μ m/h, which is comparable to that in the sublimation method.³² The details were reported in the previous papers.^{6–8,16}

Two 3C–SiC epilayers (sample number; 3C–SiC1, 3C–SiC2) were investigated. The epilayer thickness and resistivity at 300 K were 88 μ m and ~2 Ω cm for 3C–SiC1, and 74 μ m and ~0.6 Ω cm for 3C–SiC2. To fabricate freestanding 3C–SiC epilayers, the Si substrate was removed by chemical etching. The samples were cut to a 5×5 mm² size. Ohmic metal (Ni) was deposited at the four corners of the etched surface, and then the samples were annealed for 30 min at 500°C in a N₂ atmosphere. Hall-effect measurements were conducted in van der Pauw configuration at a current of 1 mA in a magnetic field of 0.53 T.

IV. RESULTS AND DISCUSSION

A. Determination of donor levels and donor densities

Figure 1 shows n(T) for two samples (open circles, 3C–SiC1; solid triangles, 3C–SiC2). Both epilayers show *n*-type conduction. Figure 2 depicts $\mu_n(T)$ for two samples (open circles, 3C–SiC1; solid triangles, 3C–SiC2). Judging



FIG. 2. Temperature dependencies of electron mobility for two different undoped 3C-SiC epilayers.



FIG. 3. FCCS signal of $H(T, E_{ref})$.

from the magnitude of $\mu_n(T)$, the band conduction of electrons is dominant over the measurement temperature range. Therefore, n(T) obtained from Hall-effect measurements is the electron concentration in the conduction band.

Using FCCS, the densities and energy levels of donors are determined from n(T). Figure 3 shows H(T,0) calculated by Eq. (6) for 3C-SiC1. This solid line is calculated by interpolating n(T) with a cubic smoothing natural spline function. The values of $\Delta E_F(T)$, which is used in the following evaluation, are also calculated by interpolating n(T) with the same spline function using

$$\Delta E_{\rm F}(T) = kT \, \ln \left[\frac{N_{\rm C}(T)}{n(T)} \right]. \tag{11}$$

The peak temperature and peak value of H(T,0) are 135.7 K and $2.22 \times 10^{36} \text{cm}^{-6} \text{eV}^{-2.5}$. From this peak, the energy level ΔE_{D2} and density N_{D2} of the corresponding donor species are determined as 68.7 meV and $4.59 \times 10^{15} \text{cm}^{-3}$.

In order to investigate another donor species included in this epilayer, the FCCS signal of $H2(T, E_{ref})$, in which the influence of the above determined donor species is removed, is calculated using the following equation. It is clear from Eq. (7) that



FIG. 4. FCCS signal of $H2(T, E_{ref})$, in which the influence of the determined donor species is removed.



FIG. 5. FCCS signal of $H3(T, E_{ref})$, in which the influence of the two determined donor species is removed.

$$H2(T, E_{\rm ref}) = \frac{n(T)^2}{(kT)^{5/2}} \exp\left(\frac{E_{\rm ref}}{kT}\right) - \frac{N_{\rm D2}}{kT} \exp\left(-\frac{\Delta E_{\rm D2} - E_{\rm ref}}{kT}\right) I(\Delta E_{\rm D2})$$
(12)

is not influenced by the donor species with ΔE_{D2} . Figure 4 depicts H2(T, 0.0138). Since a peak appears in this figure, another donor species is included in this epilayer. Using the peak temperature of 89.7 K and the peak value of 6.14 $\times 10^{36}$ cm⁻⁶ eV^{-2.5}, donor level ΔE_{D1} and the donor density N_{D1} are determined as 41.3 meV and 3.70×10^{15} cm⁻³. Since this donor level is considered to be shallowest in the measurement temperature range, N_A is determined to be 1.17 $\times 10^{14}$ cm⁻³ from the value of the signal at the lowest temperature.

The FCCS signal of $H3(T, E_{ref})$, in which the influences of two donor species above determined are removed, is calculated using

$$H3(T, E_{\rm ref}) = \frac{n(T)^2}{(kT)^{5/2}} \exp\left(\frac{E_{\rm ref}}{kT}\right)$$
$$-\sum_{i=1}^2 \frac{N_{\rm Di}}{kT} \exp\left(-\frac{\Delta E_{\rm Di} - E_{\rm ref}}{kT}\right) I(\Delta E_{\rm Di})$$
$$+ \frac{N_{\rm A}N_{\rm C0}}{kT} \exp\left(\frac{E_{\rm ref} - \Delta E_{\rm F}(T)}{kT}\right).$$
(13)

Figure 5 shows H3(T,0). Since third peak appears in this figure, third donor species is included in this epilayer. Using the peak temperature of 339.4 K and the peak value of $1.55 \times 10^{34} \text{cm}^{-6} \text{ eV}^{-2.5}$, the donor level ΔE_{D3} and the donor density N_{D3} are determined as 154.1 meV and 7.28 $\times 10^{14} \text{cm}^{-3}$.



FIG. 6. Experimental and simulated n(T).

The FCCS signal of $H4(T, E_{ref})$, in which the influences of three donor species above determined are removed, is calculated. However, $H4(T, E_{ref})$ is nearly zero, indicating that this epilayer includes three types of donor species, which is consistent with the previous report.²² The results obtained by FCCS are listed in Table I. These donor densities can be reduced to $<5 \times 10^{15}$ cm⁻³ by using undulant Si substrate, while those reported in free-standing undoped 3C–SiC epilayers were $>5 \times 10^{16}$ cm⁻³.²²

In order to verify the values obtained by FCCS, n(T) is simulated using Eqs. (1) and (3). The open circles in Fig. 6 represent the experimental n(T), and the solid line represents the n(T) simulation. The solid line is in good agreement with the experimental n(T), indicating that the values determined by FCCS are reliable.

In the same way as illustrated for 3C–SiC1, the donor levels and densities for 3C–SiC2 are determined, and are listed in Table I. Since a pace of decrease in p(T) drops down at 1000/T>14 K⁻¹ in the solid triangles of Fig. 6 (i.e., very low temperatures), N_A becomes negative, indicating that another very shallow donor with a slight density might still exist. The solid triangles in Fig. 6 represent the experimental n(T) for 3C–SiC2, and the broken line represents the n(T)simulation for 3C–SiC2. The broken line is in good agreement with the experimental n(T), indicating that the values determined by FCCS are reliable.

In many papers,^{9–16} under the assumption that only one type of donor species existed in unintentionally doped 3C-SiC, the density N_D and energy level ΔE_D of the donor as well as N_A were determined by the curve-fitting method using n(T). Figure 7 shows the n(T) simulations under the assumption of one donor species. The open circles and solid triangles represent the experimental n(T) for 3C-SiC1 and 3C-SiC2. The solid line represent the n(T) simulation with $N_D=1.3 \times 10^{16}$ cm⁻³, $\Delta E_D=60$ meV, and $N_A=4 \times 10^{15}$ cm⁻³ for 3C-SiC1, while the broken line is the n(T) simulation

TABLE I. Results obtained by FCCS.

Sample	$E_{\rm D1}({\rm meV})$	$N_{\rm D1}({\rm cm}^{-3})$	$E_{\rm D2}({\rm meV})$	$N_{\rm D2}({\rm cm}^{-3})$	$E_{\rm D3}({\rm meV})$	$N_{\rm D3}({\rm cm}^{-3})$	$N_{\rm A}({\rm cm}^{-3})$
3C–SiC1 3C–SiC2	41.3 33.7	3.70×10^{15} 1.36×10^{15}	68.7 57.1	$\begin{array}{c} 4.59 \times 10^{15} \\ 1.74 \times 10^{16} \end{array}$	154.1 110.1	$\begin{array}{c} 7.28 \times 10^{14} \\ 1.89 \times 10^{15} \end{array}$	1.17×10^{14} -3.69 × 10 ¹⁴



FIG. 7. Experimental and simulated n(T) under the assumption of one donor species.

with $N_{\rm D}=3 \times 10^{16}$ cm⁻³, $\Delta E_{\rm D}=57$ meV, and $N_{\rm A}=9 \times 10^{15}$ cm⁻³ for 3C–SiC2. Since the n(T) simulation is not in agreement with the corresponding experimental n(T) at low temperatures, it seems difficult to assume that only one type of donor species is included in these 3C–SiC epilayers.

B. Dependencies of donor levels on total donor density

Figure 8 depicts the dependence of each donor level on a total donor density ($N_{D,total} \equiv N_{D1} + N_{D2} + N_{D3}$). The other results reported in free-standing undoped 3C–SiC epilayers²² are inserted in this figure. The open squares, solid diamonds, and crosses represent ΔE_{D1} , ΔE_{D2} , and ΔE_{D3} , respectively. On the other hand, the dependence of one dopant level on one dopant density was discussed in Si (Ref. 33) or 3C–SiC,^{11,13} where the semiconductor was assumed to include only one type of dopant species.

An ideal donor level $\Delta E_{\text{D}i}(0)$ is the energy required to emit one electron from the donor site into infinity on E_{C} . However, since an *n*-type semiconductor is electrically neutral, each positively charged donor is shielded by one electron on E_{C} . This shielding electron is assumed to be located within half (\bar{r}) of an average distance $(1/\sqrt[3]{N_{\text{D,total}}})$ of the donors, indicating that the donor level should be lowered by the energy higher than $q/(4\pi\epsilon_{s}\epsilon_{0}\bar{r})$ due to Coulomb's attraction.³⁴ Therefore,

$$\Delta E_{\mathrm{D}i}(N_{\mathrm{D,total}}) = \Delta E_{\mathrm{D}i}(0) - \alpha_{\mathrm{D}i} \sqrt[3]{N_{\mathrm{D,total}}}$$
(14)

and

$$\alpha_{\mathrm{D}i} \ge \frac{q}{8\pi\epsilon_{\mathrm{s}}\epsilon_{\mathrm{0}}} = 2.44 \times 10^{-5} \mathrm{ meV cm}, \tag{15}$$

where q is the electron charge, ϵ_0 is the free space permittivity, and ϵ_s is the dielectric constant for 3C–SiC. The fitting parameters obtained by a least-squares fit of Eq. (14) to

TABLE II. Parameters for donor levels in 3C-SiC.



FIG. 8. Dependence of each donor level on the total donor density.

data in Fig. 8 are listed in Table II. The $\Delta E_{\text{D}i}(N_{\text{D,total}})$ simulations are denoted by the solid lines in Fig. 8. Since these $\alpha_{\text{D}i}$ are satisfied with Eq. (15), they are considered to be reasonable.

C. Reported donor levels in 3C-SiC

From photoluminescence (PL) measurements, Freitas *et al.*³⁵ and Kaplan *et al.*³⁶ insisted that the substitutional N donor level was ~54 meV. Moreover, Freitas *et al.*³⁵ concluded that the ~15 meV donor species, which dominated the electrical properties of *n*-type films, could not be ascribed to isolated, substitutional N. If N is associated with the ~15 meV donor species, it can only be in inhomogeneities in the films where N is incorporated at much higher concentrations or indirectly in the formation of other defects such as defect-impurity complexes or nonstoichiometric defects. Dean *et al.*³⁷ reported that in small high-purity crystals, the substitutional N donor level was ~54 meV. On the other hand, Choyke and Patrick³⁸ suggested that the N donor level was 118 meV.

Also from PL measurements, Padlasov and Mokhov³⁹ found that doping of 3C–SiC with P gave rise to a donor center with $\Delta E_{\rm D} \simeq 95$ meV.

From Fourier-transform infrared (FT-IR) spectroscopy in 3C-SiC, Moore *et al.*⁴⁰ reported that the binding energy of the ground state for substitutional N was 54.2 meV and that the binding energies of some excited states for substitutional N were 15.2 meV, 10.4 meV, and 7.0 meV.

From Hall-effect measurements, $\Delta E_{\rm D}$ and $N_{\rm D}$ in 3C–SiC were determined under the assumption of only one type of donor species in the following reports. Aivazova *et al.*⁴¹ reported that in high-purity crystals, $\Delta E_{\rm D}$ was ~50 meV, ~40 meV, and ~30 meV at $N_{\rm D} \approx 10^{15}$ cm⁻³, $N_{\rm D} \approx 10^{16}$ cm⁻³, and $N_{\rm D} \approx 10^{17}$ cm⁻³, respectively. They suggested that this donor was attributed to N by means of electron spin resonance. On the other hand, Segall *et al.*^{11,13} re-

$E_{D1}(0)(meV)$	$\alpha_{\rm D1}$ (meV cm)	$E_{\rm D2}(0)({\rm meV})$	$\alpha_{\rm D2}$ (meV cm)	$E_{\rm D3}(0)({\rm meV})$	$\alpha_{\rm D3}$ (meV cm)
51.9	5.97×10^{-5}	71.8	3.38×10^{-5}	$\sim \! 180$	$\sim 9.8 \times 10^{-5}$

ported that in unintentionally doped epilayers grown from a mixture of SiH₄ and C₃H₈, the values of $\Delta E_{\rm D}$, $N_{\rm D}$, and $N_{\rm A}/N_{\rm D}$ were ~15 meV, ~2×10¹⁸cm⁻³, and >0.9, respectively. Similar results were reported.^{10,12,14,15} However, Sasaki *et al.*⁹ reported that $\Delta E_{\rm D}$ was 40–50 meV on the assumption that $N_{\rm A}$ =0 cm⁻³. Segall *et al.*^{11,13} concluded that the ~15 meV donor spe-

Segall *et al.*^{11,13} concluded that the ~15 meV donor species resulted from the substitutional N donor, and that a high degree of compensation and a large concentration induced the reduction of the N donor depth. On the other hand, Suzuki *et al.*¹⁰ insisted that $\Delta E_{\rm D}$ for substitutional N donors was determined to be ~35 meV from the study of N-doped 3C–SiC, and that the ~15 meV donor species came from nonstoichiometric defects in unintentionally doped films.

D. Comparison of our results with others

Judging from reported results concerning with PL and FT-IR measurements, the ~50 meV donor species corresponds to substitutional N. It is clear from Table I that the donor species with ΔE_{D2} is dominant. These indicate that the donor species with ΔE_{D2} is assigned to substitutional N.

donor species with ΔE_{D2} is assigned to substitutional N. According to Freitas *et al.*³⁵ and Suzuki *et al.*,¹⁰ the shallowest donor species is attributed to some defect-impurity complex or some nonstoichiometric defect. Therefore, the donor with ΔE_{D1} might be these defects. On the other hand, the origin of the donor species with ΔE_{D3} is uncertain, although it might be P according to Padlasov and Mokhov³⁹ or it might be N according to Choyke and Patrick.³⁸

V. CONCLUSION

The densities and energy levels of donors in freestanding undoped 3C–SiC epilayers with the thicknesses of ~80 μ m were determined using the graphical peak analysis method without any assumptions regarding donor species, called FCCS. Although many researchers insisted that only one type of donor species should exist in unintentionally doped 3C–SiC, three types of donor species were detected. According to literature, two of them are considered to be related with substitutional N and a complex of N and some defect, while the other is not assigned. These donor densities could be reduced to $<5 \times 10^{15}$ cm⁻³ by growing 3C–SiC epilayers on undulant Si substrate. Since it was found that each donor level was dependent on the sum of donor densities, these fitting parameters were determined in order to use in 3C–SiC device simulation.

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- ¹G. Pensl, M. Bassler, F. Ciobanu, V. Afanas'ev, H. Yano, T. Kimoto, and
- H. Matsunami, Mater. Res. Soc. Symp. Proc. 640, H3.2 (2001).
- ²T. Ohshima *et al.*, Mater. Sci. Forum **457–460**, 1405 (2004).
- ³H. Yano, T. Hirao, T. Kimoto, H. Matsunami, K. Asano, and Y. Sugawara,

- IEEE Electron Device Lett. 20, 611 (1999).
- ⁴J. Senzaki, K. Kojima, S. Harada, R. Kosugi, S. Suzuki, T. Suzuki, and K. Fukuda, IEEE Electron Device Lett. 23, 13 (2002).
- ⁵S. Nishino, J. A. Powell, and H. A. Will, Appl. Phys. Lett. **42**, 460 (1983).
 ⁶H. Nagasawa, K. Yaga, and T. Kawahara, J. Cryst. Growth **237–239**, 1244 (2002).
- ⁷H. Nagasawa, T. Kawahara, and K. Yagi, Mater. Sci. Forum **389–393**, 319 (2002).
- ⁸H. Nagasawa, K. Yagi, T. Kawahara, and N. Hatta, Mater. Sci. Forum 433–436, 3 (2003).
- ⁹K. Sasaki, E. Sakuma, S. Misawa, S. Yoshida, and S. Gonda, Appl. Phys. Lett. 45, 72 (1984).
- ¹⁰A. Suzuki, A. Uemoto, M. Shigeta, K. Furukawa, and S. Nakajima, Appl. Phys. Lett. **49**, 450 (1986).
- ¹¹B. Segall, S. A. Alterovitz, E. J. Haugland, and L. G. Matus, Appl. Phys. Lett. **49**, 584 (1986).
- ¹²M. Yamanaka, H. Daimon, E. Sakuma, S. Misawa, and S. Yoshida, J. Appl. Phys. **61**, 599 (1987).
- ¹³B. Segall, S. A. Alterovitz, E. J. Haugland, and L. G. Matus, Appl. Phys. Lett. **50**, 1533 (1987).
- ¹⁴M. Shinohara, M. Yamanaka, H. Daimon, E. Sakuma, H. Okumura, S. Misawa, K. Endo, and S. Yoshida, Jpn. J. Appl. Phys., Part 2 27, L434 (1988).
- ¹⁵T. Tachibana, H. S. Kong, Y. C. Wang, and R. F. Davis, J. Appl. Phys. 67, 6375 (1990).
- ¹⁶H. Nagasawa, K. Yagi, T. Kawahara, N. Hatta, G. Pensl, in *Silicon Carbide*, edited by W. J. Choyke, H. Matsunami, and G. Pensl (Springer, Berlin, 2004), p. 209.
- ¹⁷H. Matsuura and K. Sonoi, Jpn. J. Appl. Phys., Part 2 35, L555 (1996).
- ¹⁸H. Matsuura, Jpn. J. Appl. Phys., Part 1 **36**, 3541 (1997).
- ¹⁹H. Matsuura, Y. Uchida, T. Hisamatsu, and S. Matsuda, Jpn. J. Appl. Phys., Part 1 **37**, 6034 (1998).
- ²⁰H. Matsuura, T. Kimoto, and H. Matsunami, Jpn. J. Appl. Phys., Part 1 38, 4013 (1999).
- ²¹H. Matsuura, Y. Uchida, N. Nagai, T. Hisamatsu, T. Aburaya, and S. Matsuda, Appl. Phys. Lett. **76**, 2092 (2000).
- ²²H. Matsuura, Y. Masuda, Y. Chen, and S. Nishino, Jpn. J. Appl. Phys., Part 1 **39**, 5069 (2000).
- ²³H. Matsuura, K. Morita, K. Nishikawa, T. Mizukoshi, M. Segawa, and W. Susaki, Jpn. J. Appl. Phys., Part 1 **41**, 496 (2002).
- ²⁴H. Matsuura, K. Sugiyama, K. Nishikawa, T. Nagata, and N. Fukunaga, J. Appl. Phys. **94**, 2234 (2003).
- ²⁵D. V. Lang, J. Appl. Phys. **45**, 3023 (1974).
- ²⁶H. Okushi, Philos. Mag. B **52**, 33 (1985).
- ²⁷H. Matsuura, J. Appl. Phys. **64**, 1964 (1988).
- ²⁸H. Matsuura, T. Hase, Y. Sekimoto, M. Uchida, and M. Simizu, J. Appl. Phys. **91**, 2085 (2002).
- ²⁹H. J. Hoffmann, Appl. Phys. **19**, 307 (1979).
- ³⁰H. J. Hoffmann, H. Nakayama, T. Nishino, and H. Hamakawa, Appl. Phys. A: Solids Surf. **33**, 47 (1984).
- ³¹S. M. Sze, *Physics of Semiconductor Devices*, 2nd ed. (Wiley, New York, 1981), Chap. 1.
- ³²V. B. Shields, K. Fekade, and M. G. Spencer, Appl. Phys. Lett. **62**, 1919 (1993).
- ³³G. L. Pearson and J. Bardeen, Phys. Rev. **75**, 865 (1949).
- ³⁴Due to Coulomb's repulsion by negatively charged acceptors, $N_{\text{D,total}}$ may be described as $N_{\text{D,total}} \approx \Sigma N_{\text{D}i} - N_{\text{A}}$. However, since N_{A} is much lower than the sum of the donor densities in the epilayers studied here, N_{A} is neglected in this article.
- ³⁵J. A. Freitas, Jr., S. G. Bishop, P. E. R. Nordquist, Jr., and M. L. Gipe, Appl. Phys. Lett. **52**, 1695 (1988).
- ³⁶R. Kaplan, R. J. Wagner, H. J. Kim, and R. F. Davis, Solid State Commun. 26, 67 (1985).
- ³⁷P. J. Dean, W. J. Choyke, and L. Patrick, J. Lumin. **15**, 299 (1977).
- $^{38}W\!$ J. Choyke and L. Patrick, Phys. Rev. B ~2,~4959~(1970).
- ³⁹S. A. Padlasov and V. G. Mokhov, Sov. Phys. Semicond. **20**, 462 (1986).
 ⁴⁰W. J. Moore, J. A. Freitas, Jr., Yu. M. Altaiskii, V. L. Zuev, and L. M. Ivanova, Inst. Phys. Conf. Ser. **137**, 185 (1994).
- ⁴¹L. S. Aivazova, S. N. Gorin, V. G. Sidyakin, and I. M. Shvarts, Sov. Phys. Semicond. **11**, 1069 (1977).