Parameters required to simulate electric characteristics of SiC devices for *n*-type 4H–SiC

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In order to obtain some of the parameters required to simulate the electric characteristics of silicon carbide (SiC) power electronic devices in a wide temperature range from startup temperatures ($\leqslant$30 °C) to steady-operation temperatures ($\geqslant$200 °C), we discuss the dependence of the two donor levels on the total donor density (N_D) as well as the dependence of the electron mobility on the total impurity density (N_{imp}) and operating temperature (T) in the *n*-type 4H–SiC. The temperature-dependent electron concentration $n(T)$ and electron mobility $\mu_n(T)$ in the *n*-type 4H–SiC epilayers with several nitrogen-doping densities are obtained from the Hall-effect measurements. By the graphical peak analysis method (free carrier concentration spectroscopy: FCCS) without any assumptions regarding the donor species, the two types of donor species are detected from $n(T)$. Moreover, the energy level and density of each donor species are determined by the FCCS. Using these results, we obtain the parameters with which the dependence of each donor level on N_D can be simulated. Using $\mu_n(T)$ at $T>250$ K, moreover, we obtain the parameters with which the dependence of the electron mobility on N_{imp} and T can be simulated. © *2004 American Institute of Physics*. [DOI: 10.1063/1.1798399]

I. INTRODUCTION

Silicon carbide (SiC) is a semiconductor with a wide band gap, a high electron mobility, a high electron saturation drift velocity, and a high thermal conductivity. It is also chemically and thermally stable and extremely hard. As a result, it is regarded as a promising semiconductor for the devices operating at high powers, high frequencies, and high temperatures. In order to design the optimum device structures for these SiC devices, it is necessary to simulate their electric characteristics in a wide temperature range from startup temperatures ($\leqslant$30 °C) to steady-operation temperatures ($\geqslant$200 °C). Therefore, it is essential to determine the parameters required to carry out the device simulations for SiC devices over the previously mentioned temperature range.

In SiC power electronic devices, a metal-oxide-semiconductor field-effect transistor (MOSFET) is an appropriate device structure. In the power MOSFETs, the Poisson equation is used to simulate the band bending in *p* layers for the MOS structures as well as in n^--drift layers near *pn* junctions in the wide temperature range, suggesting that ionized dopant densities at a given temperature should be calculated for designed dopant densities. Therefore, the dependence of each dopant level on the designed dopant density has been actually required.

Since the resistivity in the n^--drift layer is proportional to the electron mobility besides the electron concentration, the dependence $\mu_n(T, N_{imp})$ of the electron mobility on the total impurity density N_{imp} as well as temperature T is required. Although the dependence of the electron mobility $\mu_n(300)$ at 300 K on the electron concentration $n(300)$ at 300 K were reported (Refs. 1–3), $\mu_n(T, N_{imp})$ is actually important in the device simulation for SiC. This is because the donors in an *n*-type SiC are partially ionized even at 300 K, although the donors in silicon (Si) are completely ionized at 300 K.

In this paper, the temperature-dependent electron concentration $n(T)$ and electron mobility $\mu_n(T)$ for the *n*-type 4H–SiC epilayers with several nitrogen (N) densities are obtained from the Hall-effect measurements. In order to determine the densities and energy levels of the donors without any assumptions regarding the donor species from $n(T)$, the graphical peak analysis method, called free carrier concentration spectroscopy (FCCS),[4–6] is applied. Using these results, the parameters required to simulate the dependence of each donor level on a total donor density N_D is determined. Using the experimental $\mu_n(T)$, moreover, the parameters in $\mu_n(T, N_{imp})$ are determined.

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II. FREE CARRIER CONCENTRATION SPECTROSCOPY

A. Basic concept

Deep-level transient spectroscopy,[7] isothermal capacitance transient spectroscopy (ICTS),[8] and other methods[9,10] can uniquely determine the densities and energy levels of the 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 $S(t) \equiv t\mathrm{d}C(t)^2/\mathrm{d}t$, 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 $t_{\mathrm{peak}i}=1/e_i$. Here, N_i and e_i are the density and the emission rate of an ith trap. Therefore, the function of $N_i e_i t \exp(-e_i t)$ plays an important role in the ICTS analysis.

In order to analyze $n(T)$, the function theoretically described as the sum of $N_{\mathrm{D}i}\exp(-\Delta E_{\mathrm{D}i}/kT)/kT$ was introduced,[11] where k is the Boltzmann constant, $N_{\mathrm{D}i}$ and $\Delta E_{\mathrm{D}i}$ are the density and the energy level of an ith donor species, and $\Delta E_{\mathrm{D}i}$ is measured from the bottom of the conduction band E_{C}. The function $N_{\mathrm{D}i}\exp(-\Delta E_{\mathrm{D}i}/kT)/kT$ has a peak at $T_{\mathrm{peak}i}=\Delta E_{\mathrm{D}i}/k$, which does not apply to all the donor species in the temperature range of the measurement. If you introduce a function in which a peak appears at $T_{\mathrm{peak}i}=(\Delta E_{\mathrm{D}i}-E_{\mathrm{ref}})/k$, you can shift the peak temperature to the measurement temperature range by changing the parameter E_{ref}. This indicates that you can determine $N_{\mathrm{D}i}$ and $\Delta E_{\mathrm{D}i}$ in a wide donor-level range. Therefore, the function to be evaluated should be approximately described as the sum of $N_{\mathrm{D}i}\exp[-(\Delta E_{\mathrm{D}i}-E_{\mathrm{ref}})/kT]/kT$. It should be noted that $N_{\mathrm{D}i}$ 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,[12,13] we should avoid introducing a differential evaluation of $n(T)$ because the differential of the experimental data results in an increase in the observational errors.

B. Theoretical considerations

In the following, we assume an *n*-type semiconductor with n different donor species and a total acceptor density N_{A}. From the charge neutrality condition, $n(T)$ can be expressed as[14]

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

where $f(\Delta E_{\mathrm{D}i})$ is the Fermi-Dirac distribution function given by[14]

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

$\Delta E_{\mathrm{F}}(T)$ is the Fermi level measured from E_{C} at T, and g_{D} is the degeneracy factor of the donors. On the other hand, using the effective density of states $N_{\mathrm{C}}(T)$ in the conduction band, $n(T)$ is written as[14]

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

where

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

$$N_{\mathrm{C0}}=2\left(\frac{2\pi m_n^*}{h^2}\right)^{3/2}M_{\mathrm{C}}, \tag{5}$$

m_{n}^* is the electron effective mass, M_{C} is the number of equivalent minima in the conduction band, and h is the Planck's constant.

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

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

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

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

where

$$I(\Delta E_{\mathrm{D}i})=\frac{N_{\mathrm{C0}}}{g_{\mathrm{D}}+\exp\left(\frac{\Delta E_{\mathrm{F}}(T)-\Delta E_{\mathrm{D}i}}{kT}\right)}. \tag{8}$$

The function

$$\frac{N_{\mathrm{D}i}}{kT}\exp\left(-\frac{\Delta E_{\mathrm{D}i}-E_{\mathrm{ref}}}{kT}\right) \tag{9}$$

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

$$T_{\mathrm{peak}i}=\frac{\Delta E_{\mathrm{D}i}-E_{\mathrm{ref}}}{k}. \tag{10}$$

It is clear from Eq. (10) that E_{ref} can shift the peak of $H(T,E_{\mathrm{ref}})$ within the temperature range of the measurement. Although the actual $T_{\mathrm{peak}i}$ of $H(T,E_{\mathrm{ref}})$ is slightly different from the $T_{\mathrm{peak}i}$ calculated by Eq. (10) due to the temperature dependence of $I(\Delta E_{\mathrm{D}i})$, we can easily determine the accurate values of $N_{\mathrm{D}i}$ and $\Delta E_{\mathrm{D}i}$ from the peak of the experimental $H(T,E_{\mathrm{ref}})$, using a personal computer. The WINDOWS application software for the 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

Three 10-μm-thick *n*-type 4H–SiC epilayers with different N-doping densities were grown on p^+-type 4H–SiC substrates,[15] and another three 10-μm-thick *n*-type 4H–SiC epilayers grown on p^+-type 4H–SiC substrates were pur-

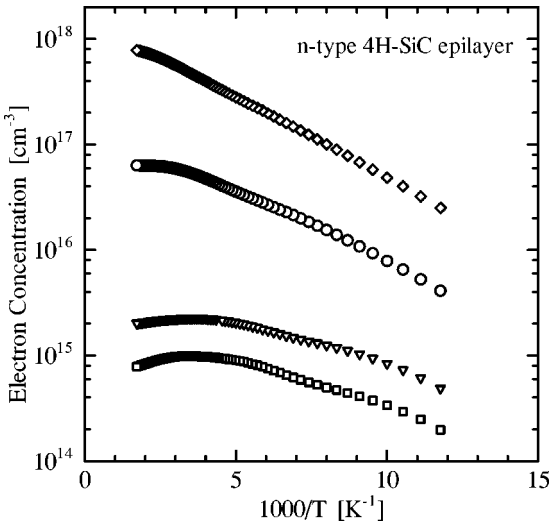

FIG. 1. Temperature dependence of electron concentrations for the four different *n*-type 4H–SiC epilayers.

chased from Cree Inc. They were cut into a 3×3-mm^2 size. The 100-nm-thick ohmic metal (Ni) was deposited on four corners of the surface of the sample, and then the sample was annealed at 1000 °C in an Ar atmosphere. $n(T)$ and $\mu_n(T)$ were measured in the van der Pauw arrangement in a temperature range from 85 to 580 K and in a magnetic field of 1.4 T using a modified MMR Technologies' Hall system.

IV. RESULTS AND DISCUSSION

A. Determination of donor levels and donor densities

Figures 1 and 2 show $n(T)$ and $\mu_n(T)$ for the four selected samples. Judging from the magnitude of $\mu_n(T)$, the band conduction of electrons is dominant over the measurement temperature range. Therefore, the $n(T)$ obtained from the Hall-effect measurements is the electron concentration in the conduction band.

Using the FCCS, the densities and energy levels of donors are determined from $n(T)$. Figure 3 shows $H(T,0)$, calculated by Eq. (6), using the data denoted by circles in Fig. 1. The peak temperature and the peak value of $H(T,0)$ are 228 K and 3.38×10^{37} cm^{-6} eV$^{-2.5}$. The donor level ΔE_{D2} and donor density N_{D2} corresponding to this peak are determined as 99.1 meV and 3.42×10^{16} cm^{-3}.

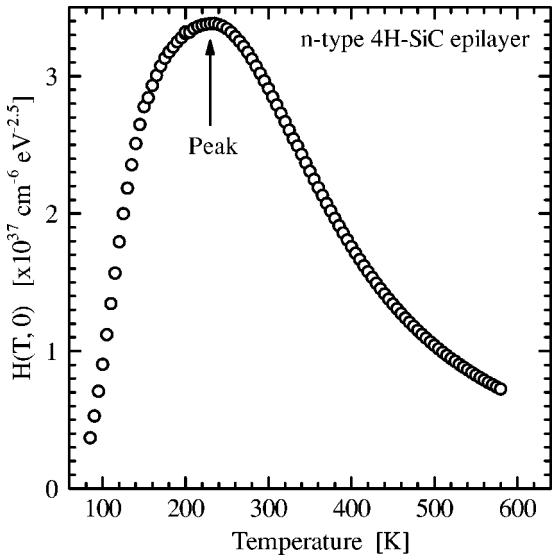

FIG. 3. FCCS signal of $H(T,E_{ref})$ with $E_{ref}=0$ eV.

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

$$H2(T,E_{ref}) = \frac{n(T)^2}{(kT)^{5/2}}\exp\left(\frac{E_{ref}}{kT}\right) - \frac{N_{D2}}{kT}\exp\left(-\frac{\Delta E_{D2}-E_{ref}}{kT}\right)I(\Delta E_{D2}) \qquad (11)$$

is not influenced by the donor species with ΔE_{D2}. Figure 4 depicts $H2(T,0.017)$. Since a peak appears in this figure,

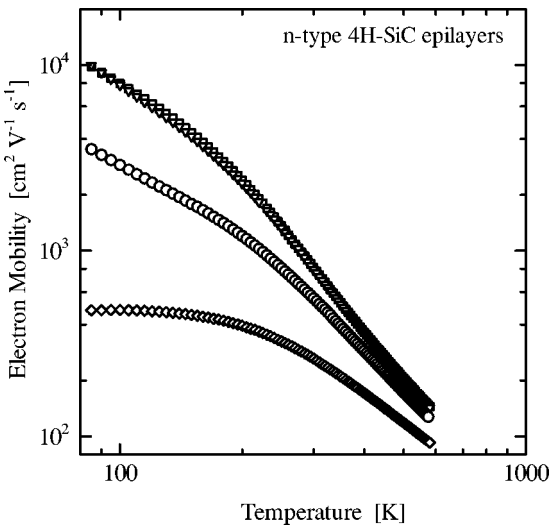

FIG. 2. Temperature dependence of electron mobilities for the four *n*-type 4H–SiC epilayers corresponding to Fig. 1.

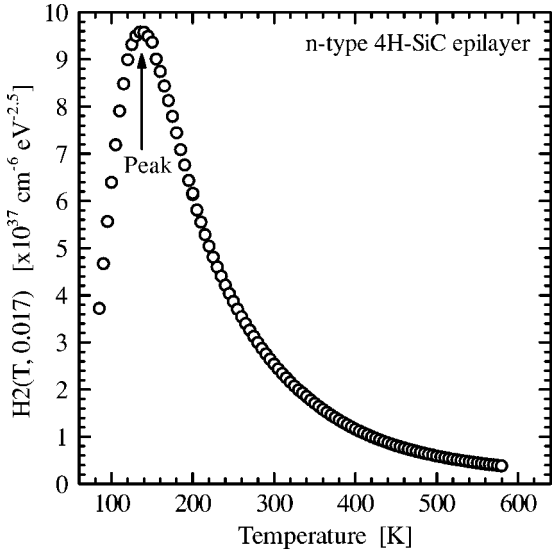

FIG. 4. FCCS signal of $H2(T,E_{ref})$ with $E_{ref}=1.7\times10^{-2}$ eV, in which the influence of the determined donor species is removed.

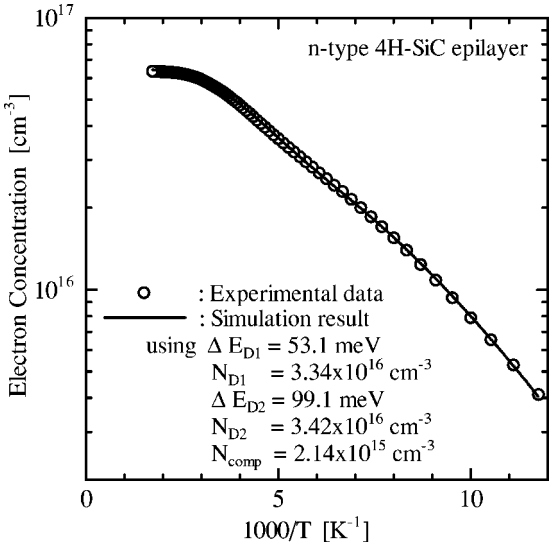

FIG. 5. Experimental and simulated $n(T)$.

another donor species is included in this epilayer. From the peak temperature of 142.3 K and the peak value of 9.51 $\times 10^{37}$ cm^{-6} eV$^{-2.5}$, the donor level ΔE_{D1} and donor density N_{D1} are determined as 53.1 meV and 3.34×10^{16} cm^{-3}. As a consequence, the ratio of N_{D1} to N_{D2} is 0.98.

The FCCS signal of $H3(T,E_{ref})$, in which the influences of the two donor species previously determined are removed, is calculated. However, $H3(T,E_{ref})$ is nearly zero, indicating that this epilayer includes only two types of donor species. Finally, N_A is determined to be 2.14×10^{15} cm^{-3}.

In order to verify the values obtained by the FCCS, $n(T)$ is simulated using Eqs. (1) and (3) with these values. The open circles in Fig. 5 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 the FCCS are reliable.

According to literature (Refs. 16 and 17), ΔE_{D1} and ΔE_{D2} correspond to the energy levels of the isolated, substitutional N donors at hexagonal and cubic lattice sites in 4H–SiC, respectively. Because the ratio of the number of the hexagonal lattice sites to the number of the cubic lattice sites in 4H–SiC is unit, the probability for the N atoms being put into each lattice site is found to be half.

TABLE I. Parameters for donor levels.

$E_{D1}(0)$ (meV)	α_{D1} (meV cm)	$E_{D2}(0)$ (meV)	α_{D2} (meV cm)
70.9	3.38×10^{-5}	123.7	4.65×10^{-5}

B. Dependence of each donor level on total donor density

In the same way as illustrated for the previously mentioned sample, the donor levels and densities for the other samples are determined. In all the epilayers, only two types of donor species are detected. Figure 6 shows the dependence of the donor levels on the total donor density ($N_D \equiv N_{D1}+N_{D2}$). The open and solid circles represent ΔE_{D1} and ΔE_{D2}. The dependence of each donor level on N_D is investigated here, whereas the dependence of one dopant level on one dopant density was discussed in Si that included only one type of dopant species.[18]

An ideal donor level $\Delta E_{Di}(0)$ 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 ($\overline{r}$) of an average distance ($1/\sqrt[3]{N_D}$) of the donors, indicating that the donor level is lowered by the energy higher than $q/(4\pi\epsilon_s\epsilon_0\overline{r})$ due to Coulomb's attraction.[19] Therefore,

$$\Delta E_{Di}(N_D) = \Delta E_{Di}(0) - \alpha_{Di}\sqrt[3]{N_D}, \tag{12}$$

where

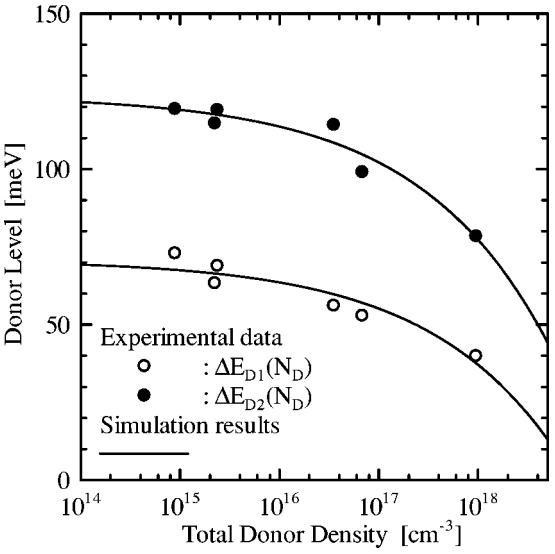

FIG. 6. Dependence of each donor level on the total donor density.

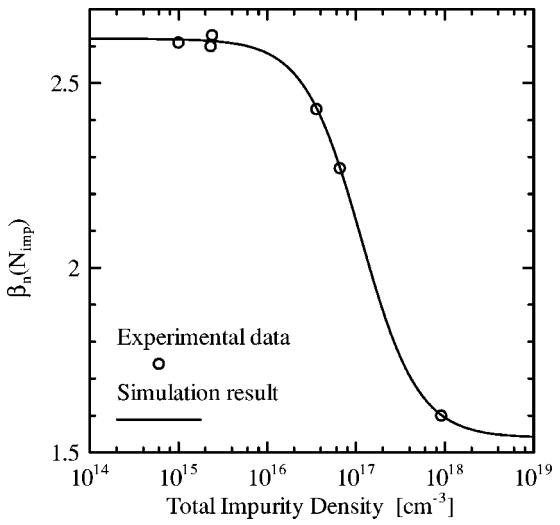

FIG. 7. $\beta_n(N_{imp})$ in $\mu_n(T,N_{imp}) \propto T^{\beta_n}(N_{imp})$.

TABLE II. Parameters for $\beta(N_{\mathrm{imp}})$.

$\beta_{\mathrm{n}}^{\mathrm{min}}$	$\beta_{\mathrm{n}}^{\mathrm{max}}$	N_{n}^{β} (cm^{-3})	$\gamma_{\mathrm{n}}^{\beta}$
1.54	2.62	1.14×10^{17}	1.35

$$\alpha_{\mathrm{D}i} \geqslant \frac{q}{8\pi\epsilon_{\mathrm{s}}\epsilon_0} = 2.44\times10^{-5}\ \mathrm{meV\ cm}, \tag{13}$$

q is the electron charge, ϵ_0 is the free space permittivity, and ϵ_{s} is the dielectric constant for 4H–SiC. By a least-squares fit of Eq. (12) to the data in Fig. 6, the fitting parameters are obtained and listed in Table I.

C. Dependence of electron mobility on temperature and total impurity density

As is clear from Fig. 2, the electron mobility at >250 K can be expressed as

$$\mu_{\mathrm{n}}(T,N_{\mathrm{imp}}) = \mu_{\mathrm{n}}(300,N_{\mathrm{imp}})\left(\frac{T}{300}\right)^{-\beta_{\mathrm{n}}(N_{\mathrm{imp}})}, \tag{14}$$

where $N_{\mathrm{imp}}=N_{\mathrm{D1}}+N_{\mathrm{D2}}+N_{\mathrm{A}}$.[20] Therefore, $\mu_{\mathrm{n}}(300,N_{\mathrm{imp}})$ and $\beta_{\mathrm{n}}(N_{\mathrm{imp}})$ can be evaluated individually.

The open circles in Fig. 7 represent $\beta_{\mathrm{n}}(N_{\mathrm{imp}})$. Since the acoustic phonon scattering and intervalley scattering are considered to mainly affect the electron mobility in SiC at $T>250$ K (Refs. 2, 3, 21, and 22), $\beta_{\mathrm{n}}(N_{\mathrm{imp}})$ is assumed to be

$$\beta_{\mathrm{n}}(N_{\mathrm{imp}}) = \beta_{\mathrm{n}}^{\mathrm{min}} + \frac{\beta_{\mathrm{n}}^{\mathrm{max}} - \beta_{\mathrm{n}}^{\mathrm{min}}}{1+\left(\dfrac{N_{\mathrm{imp}}}{N_{\mathrm{n}}^{\beta}}\right)^{\gamma_{\mathrm{n}}^{\beta}}}, \tag{15}$$

where $\beta_{\mathrm{n}}^{\mathrm{min}}$, $\beta_{\mathrm{n}}^{\mathrm{max}}$, N_{n}^{β}, and $\gamma_{\mathrm{n}}^{\beta}$ are the fitting parameters. By a least-squares fit of Eq. (15) to $\beta_{\mathrm{n}}(N_{\mathrm{imp}})$ in Fig. 7, these fitting parameters are obtained and listed in Table II. Since the values of $\beta_{\mathrm{n}}(N_{\mathrm{imp}})$ for the acoustic phonon scattering and the intervalley scattering are 1.5 and 2.6,[2,3,21,22] respectively, the obtained parameters are considered to be reasonable.

The solid circles in Fig. 8 represent $\mu_{\mathrm{n}}(300,N_{\mathrm{imp}})$. In this figure, the reported data are also inserted.[1–3,17,23–25] According to literature,[1,15,26] $\mu_{\mathrm{n}}(300,N_{\mathrm{imp}})$ is assumed to be

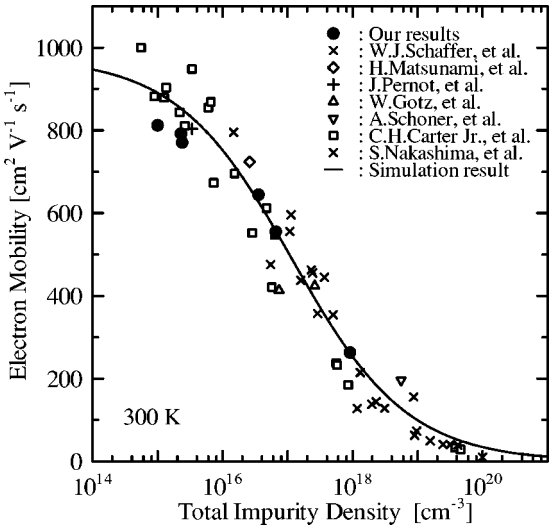

FIG. 8. Dependence of electron mobility at 300 K on the total impurity density.

TABLE III. Parameters for $\mu(300,N_{\mathrm{imp}})$.

$\mu_{\mathrm{n}}^{\mathrm{min}}$ [$\mathrm{cm}^2/(\mathrm{V\ s})$]	$\mu_{\mathrm{n}}^{\mathrm{max}}$ [$\mathrm{cm}^2/(\mathrm{V\ s})$]	N_{n}^{μ} (cm^{-3})	$\gamma_{\mathrm{n}}^{\mu}$
0	977	1.17×10^{17}	0.49

$$\mu_{\mathrm{n}}(300,N_{\mathrm{imp}}) = \mu_{\mathrm{n}}^{\mathrm{min}}(300) + \frac{\mu_{\mathrm{n}}^{\mathrm{max}}(300) - \mu_{\mathrm{n}}^{\mathrm{min}}(300)}{1+\left(\dfrac{N_{\mathrm{imp}}}{N_{\mathrm{n}}^{\mu}}\right)^{\gamma_{\mathrm{n}}^{\mu}}}, \tag{16}$$

where $\mu_{\mathrm{n}}^{\mathrm{min}}(300)$, $\mu_{\mathrm{n}}^{\mathrm{max}}(300)$, N_{n}^{μ}, and $\gamma_{\mathrm{n}}^{\mu}$ are the fitting parameters. By a least-squares fit of Eq. (16) to $\mu_{\mathrm{n}}(300)$ in Fig. 8, the fitting parameters are obtained and listed in Table III. Since all the parameters in Eqs. (15) and (16) are determined here, we can calculate the electron mobility for any N_{imp} at $T>250$ K.

V. CONCLUSION

In order to obtain some of the parameters required in the device simulation for 4H–SiC power electric devices, the Hall-effect measurements were conducted for the *n*-type 4H–SiC epilayers with several N-doping densities. We determined the parameters required to simulate the dependence of the two donor levels on the total donor density. Moreover, we determined the parameters with which the electron mobility could be simulated at $T>250$ K.

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