Materials Science Forum Vols. 353-356 (2001) pp. 495-498

Donor Densities and Donor Energy Levels in 3C-SiC Determined by a New Method Based on Hall-Effect Measurements

H. Matsuura[1], Y. Masuda[2], Y. Chen[2] and S. Nishino[2]
[1] Osaka Electro-Communication University,
18-8 Hatsu-cho, Neyagawa, Osaka 572-8530, Japan
[2] Kyoto Institute of Technology,
Matsugasaki, Sakyo, Kyoto 606-8585, Japan

Keywords: Free carrier Concentration Spectroscopy (FCCS), Donor Energy Level, Donor Density, Hall-Effect Measurement, Temperature Dependence of Majority-Carrier Concentration, Graphical Peak Analysis, Hexamethyldisilane (HMDS),

Abstract Without any assumption of the number of donor species, the densities and energy levels of donors in undoped 3C-SiC grown from hexamethyldisilane (HMDS; $Si_2(CH_3)_6$) are precisely determined by a graphical peak analysis method proposed here, using the temperature dependence of the majority-carrier concentration obtained from Hall-effect measurements.

1. Introduction

Silicon carbide (SiC) has been regarded as a promising semiconductor for power electronic applications owing to its excellent physical properties. In order to use SiC wafers or epilayers for electronic devices, an accurate evaluation of densities and energy levels of electronically active impurities or defects is essential. Among these impurities and defects, the electronic properties of deep level impurities or defects can be accurately determined by deep level transient spectroscopy (DLTS) or isothermal capacitance transient spectroscopy (ICTS) [1,2].

The temperature dependence of the majority-carrier concentration $n(T)$ obtained from Hall-effect measurements includes important information on shallow level impurities in a semiconductor. However, it has been difficult to determine the energy levels and densities of shallow impurities from the experimentally obtained $n(T)$. A curve-fitting method seems unsuitable because of the uncertainty in the number of impurity species in the semiconductor.

In this article, we introduce a new graphical peak analysis method (free carrier concentration spectroscopy; FCCS) to analyze the free carrier concentration $n(T)$, and apply it to undoped cubic SiC (3C-SiC) grown on silicon (Si) from non-flammable hexamethyldisilane (HMDS). In addition, we investigate the dependence of the donor energy levels on the thickness of the 3C-SiC film.

2. Basic Concept of Free Carrier Concentration Spectroscopy

DLTS or ICTS can uniquely determine the densities and energy levels, because each peak in the signal corresponds one-to-one to an impurity or defect. 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. Since $S(t)$ is described as the sum of $N_i e_i t \exp(-e_i t)$, it has a peak value of $N_i e_i t_{\mathrm{peak}i} \exp(-1)$ at a peak time $t_{\mathrm{peak}i} = 1/e_i$. Here, N_i and e_i are the density and emission rate of the i-th energy level. Therefore, $N_i e_i t \exp(-e_i t)$ plays an important role in the analysis.

For the analysis of the free carrier concentration $n(T)$ with respect to impurities, we have introduced a function that is described as the sum of $N_i \exp(-\Delta E_i/kT)/kT$, where N_i and ΔE_i are the density and energy level of the i-th impurity, respectively, T is the measurement

temperature and k is the Boltzmann constant [3,4]. The function $N_i \exp(-\Delta E_i / kT)/kT$ has a peak at $T_{\text{peak}i} = \Delta E_i / k$, which is not for all impurities in the temperature range of the measurement. If we can introduce a function in which the peak appears at $T_{\text{peak}i} = (\Delta E_i - E_{\text{ref}})/k$, we can shift the peak temperature within the measurement temperature range by changing the parameter E_{ref}. This indicates that we can determine N_i and ΔE_i in a wide impurity-energy-level range. Therefore, a function to be evaluated should be described as the sum of $N_i \exp\left[-(\Delta E_i - E_{\text{ref}})/kT\right]/kT$, where N_i and ΔE_i determined by this method should be independent of E_{ref} [5,6]. In addition, we have avoided introducing a differential evaluation of $n(T)$, because the differential of experimental data results in an increase of observation errors.

3. Theoretical Consideration of FCCS

For the following theoretical considerations, we assume an n-type semiconductor with n different donor species (density $N_{\text{D}i}$ and energy level $\Delta E_{\text{D}i}$ of the i-th donor for $1 \le i \le n$) and one acceptor density (N_{A}). The donor energy levels $\Delta E_{\text{D}i}$ are measured from the bottom of the conduction band (E_{C}) with $\Delta E_{\text{D}i-1} < \Delta E_{\text{D}i}$. From the charge neutrality condition, the free electron concentration $n(T)$ can be derived as

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

where $f(\Delta E)$ is the Fermi-Dirac distribution function given by

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

ΔE_{F} is the Fermi level measured from E_{C}, and g_{D} is the degeneracy factor of donors.

On the other hand, using the effective density of states $N_{\text{C}}(T)$ in the conduction band, we can describe $n(T)$ as

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

where $N_{\text{C}}(T) = (kT)^{1.5} N_{\text{C0}}$, $N_{\text{C0}} = 2(2\pi m_{\text{n}}^* / h^2)^{1.5} M_{\text{C}}$, m_{n}^* is the electron effective mass, h is the Planck constant, and M_{C} is the number of equivalent minima in the conduction band.

From Eq. 1 and Eq. 3, we can introduce a favorable function to determine $N_{\text{D}i}$ and $\Delta E_{\text{D}i}$ as follows. We define the function to be evaluated as

$$H(T, E_{\text{ref}}) \equiv \frac{n(T)^2}{(kT)^{2.5}}\exp\left(\frac{E_{\text{ref}}}{kT}\right). \tag{4}$$

Substituting Eq. 1 for one of the $n(T)$ in Eq. 4 and substituting Eq. 3 for the other $n(T)$ in Eq. 4 give

$$H(T, E_{\text{ref}}) = \sum_{i=1}^{n} \frac{N_{\text{D}i}}{kT}\exp\left(-\frac{\Delta E_{\text{D}i} - E_{\text{ref}}}{kT}\right) I(\Delta E_{\text{D}i}) - N_{\text{A}}\frac{N_{\text{C0}}}{kT}\exp\left(\frac{E_{\text{ref}} - \Delta E_{\text{F}}}{kT}\right), \tag{5}$$

where

$$I(\Delta E_{\text{D}i}) = \frac{N_{C0}}{g_{\text{D}} + \exp\left(\frac{\Delta E_{\text{F}} - \Delta E_{\text{D}i}}{kT}\right)}. \tag{6}$$

Finally, using a personal computer, we take the temperature dependence of $I(\Delta E_{\text{D}i})$ into account,

and we can easily determine N_{Di} and ΔE_{Di} for each peak.

4. Experimental

3C-SiC epilayers with thicknesses (8 μm, 16 μm and 32 μm) were grown on (100) Si substrates by atmospheric pressure chemical vapor deposition. HMDS with a flow rate of 0.5 sccm and H_2 with a flow rate of 2.5 slm were introduced at 1350 °C. The growth rate was about 4.3 μm/h.

Each 3C-SiC was cut into pieces of 5x5 mm^2, and Si substrates were removed by chemical etching. The free electron concentration $n(T)$ was measured by the van der Pauw method at temperatures between 85 K and 500 K, at a magnetic field of 5 kG and a current of 1 mA.

5. Results and Discussions

Figure 1 shows the free electron concentration $n(T)$ (open circles) and the function $H(T,E_{ref})$ (solid line) for the 8-μm-thick 3C-SiC epilayer. $H(T,E_{ref})$ is calculated by interpolating $n(T)$ with a cubic spline function. From the peak, the density (N_{D2}) and energy level (ΔE_{D2}) can be determined to 1.7x10^{17} cm^{-3} and 46 meV, respectively.

As is clear from Eqs. 4 and 5, the function that is not influenced by this donor is introduced as

$$H2(T,E_{ref}) \equiv \frac{n(T)^2}{(kT)^{2.5}}\exp\left(\frac{E_{ref}}{kT}\right) - \frac{N_{D2}}{kT}\exp\left(-\frac{\Delta E_{D2}-E_{ref}}{kT}\right) I(\Delta E_{D2}), \quad (7)$$

which is shown by the solid line in Fig. 2. From the lower peak temperature and the lowest measurement temperature, N_{D1}, ΔE_{D1} and N_A are determined to be 1.1x10^{17} cm^{-3}, 10 meV and 1.3x10^{16} cm^{-3}, respectively.

The function that is not influenced by the first donor, or the second donor, or the acceptor is introduced as

$$H3(T,E_{ref}) \equiv \frac{n(T)^2}{(kT)^{2.5}}\exp\left(\frac{E_{ref}}{kT}\right) - \sum_{i=1}^{2}\frac{N_{Di}}{kT}\exp\left(-\frac{\Delta E_{Di}-E_{ref}}{kT}\right) I(\Delta E_{Di}) + N_A\frac{N_{C0}}{kT}\exp\left(\frac{E_{ref}-\Delta E_F}{kT}\right), \quad (8)$$

which is shown by the broken line in Fig. 2. From the lower peak temperature, N_{D3} and ΔE_{D3} are determined to be 1.1x10^{17} cm^{-3} and 107 meV, respectively. In the same matter, N_{D4} and ΔE_{D4} are determined to be 4.6x10^{16} cm^{-3} and 156 meV, respectively.

Figure 3 shows the free electron concentration simulated using the values determined here (solid

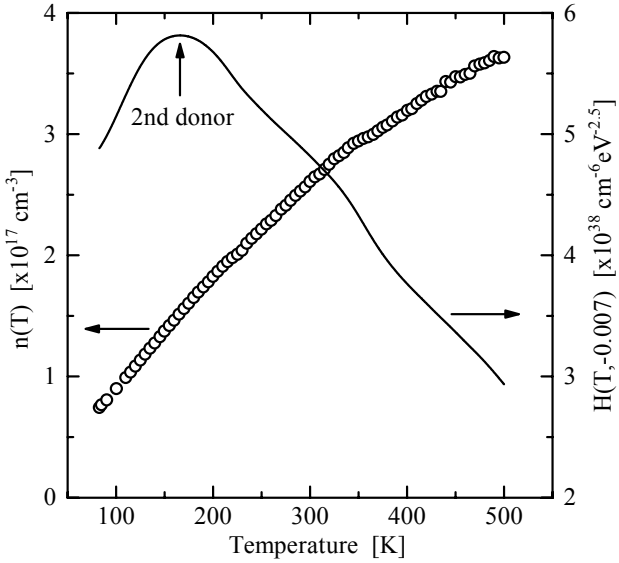

Fig. 1 n(T) and H(T,-0.007) for 8-μm-thick 3C-SiC

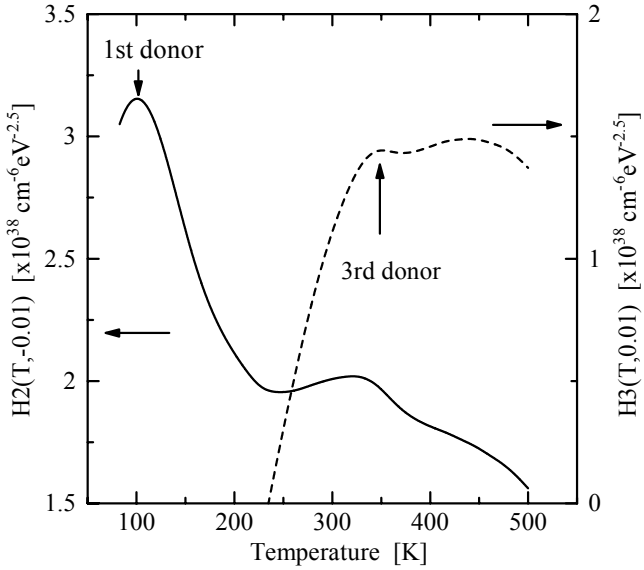

Fig. 2 H2(T,-0.01) and H3(T,0.01) for 8-μm-thick 3C-SiC

line). The open circles represent the experimentally obtained $n(T)$. The simulated free electron concentration is quantitatively in good agreement with the experimentally obtained $n(T)$, indicating that the values determined here are reliable.

In the same way as illustrated for the 8-μm-thick epilayer, the densities and energy levels of donors in the 16-μm-thick and 32-μm-thick 3C-SiC epilayers are determined, and are listed in Table 1.

In undoped 3C-SiC grown from a mixture of SiH_4 and C_3H_8, only the ~15 meV donor with a concentration higher than 10^{18} cm^{-3} was reported with the compensation ratio higher than 0.9 [7]. In high-purity 3C-SiC crystals, on the other hand, a ~50 meV donor was reported [8]. From those reports, Segall *et al.* [7] concluded that both the ~15 meV and ~50 meV donors resulted from substitutional nitrogen (N) atom, and that a high degree of compensation and a large N concentration induced the reduction of the N donor energy level.

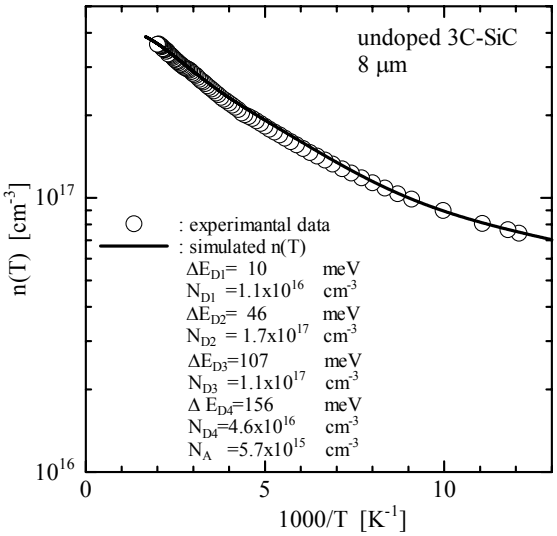

Fig. 3 Experiemtal and simulated n(T)

Table 1 Values determined by FCCS

Thickness [μm]	8	16	32
ΔE_{D1} [meV]	10	7	14
N_{D1} [x10^{16} cm^{-3}]	11	8.1	4.7
ΔE_{D2} [meV]	46	46	54
N_{D2} [x10^{16} cm^{-3}]	17	20	8.1
ΔE_{D3} [meV]	107	97	120
N_{D3} [x10^{16} cm^{-3}]	11	13	10
ΔE_{D4} [meV]	156	-----	-----
N_{D4} [x10^{16} cm^{-3}]	4.6	-----	-----
N_A [x10^{16} cm^{-3}]	1.3	0.99	0.57

In the 3C-SiC investigated here, both the ~15 meV and ~50 meV donors coexist. The density of the ~15 meV donor is sensitive to the crystallinity of the epilayer, as shown in Table 1, because the crystallinity of our epilayers was enhanced as the thickness increased. Moreover, the substitutional N donor energy level was reported to be 54 meV from photoluminescence measurements [9]. Therefore, the ~50 meV donor may be ascribed to a substitutional N atom, while the ~15 meV donor may be attributed to some defect-N complex or nonstoichiometric defect, which Freitas *et al.* [9] and Suzuki *et al.* [10] suggested.

6. Conclusion

Even if we do not know the number of impurity species included in a semiconductor, we have found that FCCS can determine the densities and energy levels of shallow impurities accurately. In undoped 3C-SiC grown from HMDS, we detected four types of donors whose energy levels are 7-14 meV, 46-54 meV, 97-120 meV and 156 meV.

References

[1] T. Dalibor, G. Pensl, H. Matsunami, T. Kimoto, W. J. Choyke, A. Schöner and N. Nordell, phys. stat. sol. 162 (1997) p. 199.
[2] H. Okushi, Philos. Mag. B 52 (1985), p. 33.
[3] H. Matsuura, Y. Uchida, T. Hisamatsu and S. Matsuda, Jpn. J. Appl. Phys. 37 (1998), p. 6034.
[4] H. Matsuura, T. Kimoto and H. Matsunami, Jpn. J. Appl. Phys. 38 (1999), p. 4013.
[5] H. Matsuura, Y. Uchida, N. Nagai, T. Hisamatsu, T. Aburaya and S. Matsuda, Appl. Phys. Lett. 76 (2000), p. 2092.
[6] H. Matsuura, Y. Masuda, Y. Chen and S. Nishino, Jpn. J. Appl. Phys. 39 (2000), to be published in September.
[7] B. Segall, S. A. Alterovitz, E. J. Haugland and L. G. Matus, Appl. Phys. Lett. 49 (1987), p. 584.
[8] L. S. Aivazova, S. N. Gorin, V. G. Sidyakin and I. M. Shvarts, Sov. Phys. Semicond. 11 (1977), p. 1067.
[9] J. A. Freitas, Jr., S. G. Bishop, P. E. R. Nordquist, Jr. and M. L. Gipe, Appl. Phys. Lett. 52 (1988), p. 1695.
[10] A. Suzuki, A. Uemoto, M. Shigeta, K. Furukawa and S. Nakajima, Appl. Phys. Lett. 49 819869, p. 350.