Short Note

Evaluation of Densities and Energy Levels of Donors and Acceptors in Compensated Semiconductor from Temperature Dependence of Majority Carrier Concentration

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An accurate evaluation of densities and energy levels of donors and acceptors in a compensated semiconductor from the temperature dependence of the majority carrier concentration $n(T)$ is carried out by modifying the graphic method proposed in Jpn. J. Appl. Phys. **35** (1996) L555. The introduced function, $S(T, E_{\mathrm{ref}})$, is defined as $S(T, E_{\mathrm{ref}}) \equiv n(T) \exp(E_{\mathrm{ref}}/kT)/kT$, where k is the Boltzmann constant and E_{ref} is the newly introduced parameter. From the dependence of $S(T, E_{\mathrm{ref}})$ on the impurity density of minority carriers, the densities and energy levels of donors and acceptors can be determined accurately.

The majority carrier concentration $n(T)$ is sensitive to impurities (i.e., donors and/or acceptors) in a semiconductor. Since semiconductors usually include several kinds of impurities, evaluating the densities and energy levels of the impurities is very important. For example, 6H–SiC often includes both acceptors (Al and/or B)[1,2] and N atoms which act as donors with two sets of energy levels.[1] Therefore, methods for evaluating the densities and energy levels of impurities have been proposed.[3–5]

We have proposed a simple graphic method in which, from each peak in the curve representing the product of $1/kT$ and $n(T)$, the corresponding density and energy level can be evaluated.[5] Here, k is the Boltzmann constant and T is the temperature. However, using this method, it is difficult to evaluate the densities and energy levels of both donors and acceptors in a compensated semiconductor. Therefore, the author aims to evaluate the densities and energy levels of both donors and acceptors by modifying this graphic method.

To simplify the following arguments, the temperature dependence of the free electron concentration $n(T)$ in an n-type semiconductor is considered. Instead of $n(T)/kT$,[5] a new function is defined as

$$S(T, E_{\mathrm{ref}}) \equiv \frac{n(T) \exp\left(\dfrac{E_{\mathrm{ref}}}{kT}\right)}{kT}, \qquad (1)$$

where E_{ref} is the newly introduced parameter.

The value of $n(T)$ is theoretically expressed as[3]

$$n(T) = \sum_i N_{\mathrm{D}i} \left[1 - f(E_{\mathrm{D}i})\right] - \sum_j N_{\mathrm{A}j} f(E_{\mathrm{A}j}), \qquad (2)$$

where $f(E)$ is the Fermi-Dirac distribution function, $N_{\mathrm{D}i}$ and $E_{\mathrm{D}i}$ are the density of the i-th donor and the corresponding energy level, respectively, and $N_{\mathrm{A}j}$ and $E_{\mathrm{A}j}$ are the density of the j-th acceptor and the corresponding energy level, respectively. Since an n-type semiconductor is considered, all $f(E_{\mathrm{A}j})$ are nearly equal to 1. Therefore,

$$n(T) \simeq \sum_i N_{\mathrm{D}i} F_i(T) \exp\left(-\frac{\Delta E_{\mathrm{D}i}}{kT}\right) - N_{\mathrm{A}}, \qquad (3)$$

with

$$F_i(T) = \frac{\exp\left(\dfrac{\Delta E_{\mathrm{F}}}{kT}\right)}{g_{\mathrm{D}i} + \exp\left(\dfrac{\Delta E_{\mathrm{F}} - \Delta E_{\mathrm{D}i}}{kT}\right)} \qquad (4)$$

and

$$N_{\mathrm{A}} = \sum_j N_{\mathrm{A}j}, \qquad (5)$$

where ΔE_{F} and $\Delta E_{\mathrm{D}i}$ are the Fermi level and the i-th donor level measured from the conduction band edge, respectively, and $g_{\mathrm{D}i}$ is the degeneracy factor of the i-th donor. Thus, the function $S(T, E_{\mathrm{ref}})$ is written as

$$S(T, E_{\mathrm{ref}}) = \sum_i N_{\mathrm{D}i} D_i(T, E_{\mathrm{ref}}) - \frac{N_{\mathrm{A}}}{kT} \exp\left(\frac{E_{\mathrm{ref}}}{kT}\right), \qquad (6)$$

with

$$D_i(T, E_{\mathrm{ref}}) = \frac{1}{kT} F_i(T) \exp\left(-\frac{\Delta E_{\mathrm{D}i} - E_{\mathrm{ref}}}{kT}\right). \qquad (7)$$

Since the function of $\exp[-(\Delta E_{\mathrm{D}i} - E_{\mathrm{ref}})/kT]/kT$ in eq. (7) has a maximum at $T = (\Delta E_{\mathrm{D}i} - E_{\mathrm{ref}})/k$, the peak temperature of $D_i(T, E_{\mathrm{ref}})$ can be decreased by using a positive E_{ref}, although the peak temperature is not exactly equal to $(\Delta E_{\mathrm{D}i} - E_{\mathrm{ref}})/k$ due to the factor $F_i(T)$. By changing E_{ref}, therefore, we can change each peak temperature ($T_{\mathrm{peak}i}$) in the $S(T, E_{\mathrm{ref}})$ curve.

At low temperature, the contribution of donors with high $\Delta E_{\mathrm{D}i}$ to $n(T)$ is very small. Therefore, after reducing $T_{\mathrm{peak}1}$ by using a positive E_{ref}, the values of N_{A}, $N_{\mathrm{D}1}$ and $\Delta E_{\mathrm{D}1}$ can be evaluated accurately from this peak.

In order to demonstrate how to evaluate $\Delta E_{\mathrm{D}1}$, $N_{\mathrm{D}1}$ and N_{A} from $n(T)$, 6H–SiC with one kind of donor ($\Delta E_{\mathrm{D}1} = 0.1$ eV, $N_{\mathrm{D}1} = 1 \times 10^{16}$ cm^{-3}) and one kind of acceptor ($\Delta E_{\mathrm{A}1} = 0.25$ eV, $N_{\mathrm{A}1} = 1 \times 10^{15}$ cm^{-3}) is considered. Here, $\Delta E_{\mathrm{A}1}$ is the acceptor level measured from the valence band edge, and N_{A} in eq. (5) is equal to $N_{\mathrm{A}1}$, since one kind of acceptor only is considered. The value $\Delta E_{\mathrm{D}1} = 0.1$ eV corresponds to N inserted into the hexagonal site of 6H–SiC,[1] and the value $\Delta E_{\mathrm{A}1} = 0.25$ eV corresponds to Al in 6H–SiC.[1] The $n(T)$ curve is shown in Fig. 1. Here, $g_{\mathrm{D}1}$ was assumed to be 2.[3]

In the $n(T)$–$1/T$ characteristics, the impurity density is equal to $n(T)$ in the saturation region.[3] The energy level is evaluated from the slope of the $\ln n(T)$–$1/T$ curve
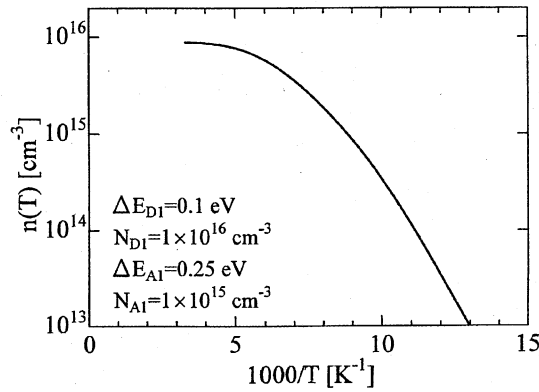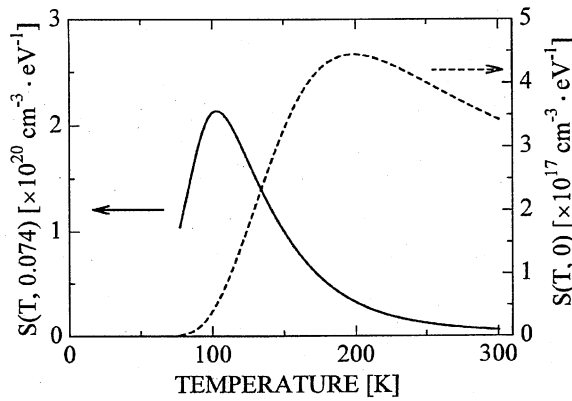
Fig. 1.   Temperature dependence of free electron concentration.

Fig. 2. $S(T, 0)$ signal (broken line) and $S(T, 0.074)$ signal (solid line) calculated using eq. (1) and $n(T)$ in Fig. 1.

in the freeze-out region, because $n(T)$ in this region is approximately proportional to[3]

$$\exp\left(-\frac{\Delta E_{Di}}{2kT}\right). \tag{8}$$

From Fig. 1, it is found that ΔE_{D1} and N_{D1} are 0.205 eV in the region $10\,\mathrm{K}^{-1} \leq 1000/T \leq 13\,\mathrm{K}^{-1}$, and about $9 \times 10^{15}\,\mathrm{cm}^{-3}$, respectively, indicating that the actual values cannot be obtained using this method. It is found using the Hoffmann's method[4] that ΔE_{D1} and N_{D1} are 0.104 eV and $9.14 \times 10^{15}\,\mathrm{cm}^{-3}$, respectively, and that the acceptor density cannot be evaluated. The author aims to obtain the densities and energy levels of donors and the acceptor density from $n(T)$ more accurately.

The broken curve $S(T, 0)$ in Fig. 2 is obtained using eq. (1) and $n(T)$ in Fig. 1. As is clear from eqs. (2) and (3), the number of electrons emitted from donors is small at low temperature, although the number of electrons captured by acceptors is constant over the whole temperature range, indicating that the effect of acceptors on $n(T)$ is large at low temperature. Thus, the acceptor density can be evaluated accurately from a low

T_{peak1}. In order to reduce T_{peak1}, a positive value of E_{ref}, 0.074 eV, was used. The solid curve in Fig. 2 is the curve for $S(T, 0.074)$ obtained using $n(T)$ in Fig. 1.

From the figure, T_{peak1} and $S(T_{\mathrm{peak1}}, 0.074)$ are 103 K and $2.14 \times 10^{20}\,\mathrm{cm}^{-3} \cdot \mathrm{eV}^{-1}$, respectively. We define T_R as the lower temperature at which $S(T, E_{\mathrm{ref}})/S(T_{\mathrm{peak1}}, E_{\mathrm{ref}})$ has a value of R (i.e., $0 < R < 1$). The values of $T_{0.5}$ and $S(T_{0.5}, 0.074)$ are 77.5 K and $1.07 \times 10^{20}\,\mathrm{cm}^{-3} \cdot \mathrm{eV}^{-1}$, respectively.

In order to determine the values of ΔE_{D1} and N_A/N_{D1} from two temperatures (T_{peak1} and $T_{0.5}$),

$$Y_1(T, E_{\mathrm{ref}}) \equiv \frac{S(T, E_{\mathrm{ref}})}{N_{D1}} \tag{9}$$

is defined. Since electrons emitted from the first donor make a dominant contribution to $n(T)$ at low temperature, $Y_1(T, E_{\mathrm{ref}})$ is approximately expressed as

$$Y_1(T, E_{\mathrm{ref}}) \simeq D_1(T, E_{\mathrm{ref}}) - \frac{N_A}{N_{D1}} \cdot \frac{1}{kT} \exp\left(\frac{E_{\mathrm{ref}}}{kT}\right). \tag{10}$$

The values of ΔE_{D1} and N_A/N_{D1}, which make $Y_1(T, 0.074)$ maximum at $T_{\mathrm{peak1}} = 103\,\mathrm{K}$ and make $Y_1(T, 0.074)$ half of the maximum value at $T_{0.5} = 77.5\,\mathrm{K}$, are 0.100 eV and 0.100, respectively, which are equal to the actual values. In the evaluation, $\exp(\Delta E_F/kT)$ included in $D_1(T, E_{\mathrm{ref}})$ is calculated from $N_C(T)/n(T)$, where $n(T)$ is shown in Fig. 1 and $N_C(T)$ for 6H–SiC is assumed to be $1.16 \times 10^{16} T^{1.5}\,\mathrm{cm}^{-3}$.

As is clear from eq. (9), N_{D1} can be estimated from

$$N_{D1} = \frac{S(T_{\mathrm{peak1}}, E_{\mathrm{ref}})}{Y_1(T_{\mathrm{peak1}}, E_{\mathrm{ref}})}. \tag{11}$$

Using $S(103, 0.074) = 2.14 \times 10^{20}\,\mathrm{cm}^{-3} \cdot \mathrm{eV}^{-1}$ and the value of $Y_1(103, 0.074)$ calculated using eq. (10) with $\Delta E_{D1} = 0.100$ eV and $N_A/N_{D1} = 0.100$, N_{D1} is found to be $9.99 \times 10^{15}\,\mathrm{cm}^{-3}$. Since $N_A/N_{D1} = 0.100$, N_A is estimated to be $9.99 \times 10^{14}\,\mathrm{cm}^{-3}$. These values are very close to the actual values.

Although a semiconductor with only the impurities (N_{D1} and N_{A1}) is considered here, this method can be applied to a semiconductor with several kinds of donors and acceptors. In principle, this method can be used for $N_A/N_{D1} < 1$. The application of this method to experimental data is currently in progress.

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