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Short Note

Evaluating Densities and Energy Levels of Impurities with Close Energy Levels in Semiconductor from Temperature Dependence of Majority-Carrier Concentration

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By modifying the graphic method proposed in Jpn. J. Appl. Phys. **35** (1996) L555, the author aims to evaluate the densities and energy levels of impurities with two kinds of close energy levels. Using the temperature dependence of the majority-carrier concentration $n(T)$, the function $n(T)\exp(E_{\rm ref}/kT)/kT$ is defined, where k is the Boltzmann constant and $E_{\rm ref}$ is a newly introduced parameter. The densities and energy levels of the impurities can be evaluated from the peaks of this function. Even in Si with two donors (Sb and P), it is found that the densities and energy levels of the two donors can be evaluated accurately.

KEYWORDS: evaluation of impurities, graphic method, impurity density, impurity level, temperature dependence of majority-carrier concentration

Semiconductors often include several impurities. Since the majority-carrier concentration (n or p) is very sensitive to impurities, evaluating the densities and energy levels of impurities in a semiconductor is important. Therefore methods for evaluating the densities and energy levels have been proposed.[1–3]

We have proposed a simple graphic method in which the product of $1/kT$ and n (or p) is calculated and the densities and energy levels of impurities are evaluated from the peaks in this curve.[3] Here, k is the Boltzmann constant and T is the measuring temperature. However, the smallest difference between the energy levels (i.e., the energy resolution) of two impurities, whose densities and energy levels can be determined accurately using this method, is about 0.05 eV. In this study, we aim to improve the energy resolution.

To simplify the following arguments, the temperature dependence of the free electron concentration $n(T)$ in an n-type semiconductor is considered. Instead of $n(T)/kT$,[3] the following function is defined:

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

where $E_{\rm ref}$ is the newly introduced parameter.

The peak temperature of this function can be changed by changing $E_{\rm ref}$. At low measuring temperatures, the donor with the shallowest donor level makes the dominant contribution to $n(T)$. Therefore, by moving the peak temperature to a lower temperature using a positive $E_{\rm ref}$, the density and energy level of the donor with the shallowest donor level can be evaluated accurately.

The free electron concentration $n(T)$ is theoretically given by

$$n(T) = \sum_i N_{{\rm D}i} \cdot \frac{1}{1 + g_{{\rm D}i}\exp\left(\dfrac{\Delta E_{{\rm D}i} - \Delta E_{\rm F}}{kT}\right)}, \tag{2}$$

where $N_{{\rm D}i}$ and $\Delta E_{{\rm D}i}$ are the density of the i-th donor and the corresponding energy level measured from the conduction band edge, respectively, $g_{{\rm D}i}$ is the degeneracy factor of the corresponding donor, and $\Delta E_{\rm F}$ is the energy at the Fermi level measured from the conduction band edge.[3] Thus, the function $S(T, E_{\rm ref})$ is theoretically given by

$$S(T, E_{\rm ref}) = \sum_i N_{{\rm D}i} D_i(T, E_{\rm ref}) \tag{3}$$

with

$$D_i(T, E_{\rm ref}) = \frac{1}{kT} \cdot \frac{\exp\left(\dfrac{E_{\rm ref}}{kT}\right)}{1 + g_{{\rm D}i}\exp\left(\dfrac{\Delta E_{{\rm D}i} - \Delta E_{\rm F}}{kT}\right)}. \tag{4}$$

In order to demonstrate the evaluation of $\Delta E_{{\rm D}i}$ and $N_{{\rm D}i}$ from $n(T)$, Si with two kinds of donors ($\Delta E_{\rm D1} = 0.039$ eV, $N_{\rm D1} = 1 \times 10^{16}$ cm^{-3}, $\Delta E_{\rm D2} = 0.054$ eV, and $N_{\rm D2} = 1 \times 10^{16}$ cm^{-3}) is considered. The energy levels of 0.039 eV and 0.054 eV correspond to those of Sb and As in Si, respectively.[1] The curve for $n(T)$ in the range $25\,{\rm K} \le T \le 230\,{\rm K}$ is shown in Fig. 1. Here, the value of $g_{{\rm D}i}$ used was 2.[1]

In the $n - 1/T$ characteristics, the donor density is equal to $n(T)$ in the saturation region.[1] The energy level can be determined from the slope of the $\ln n - 1/T$ curve in the freeze-out region, because $n(T)$ in this region is approximately proportional to[1]

$$\exp\left(-\frac{\Delta E_{{\rm D}i}}{2kT}\right). \tag{5}$$

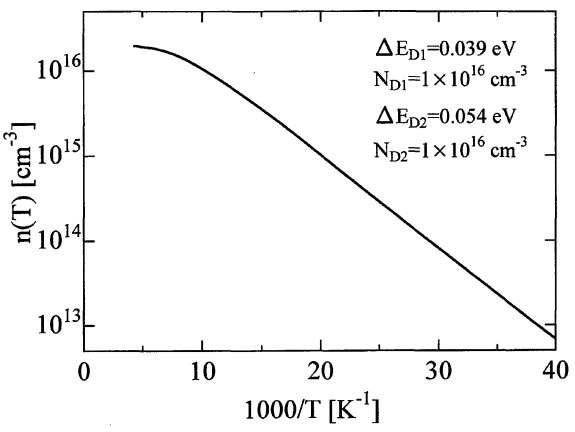

Fig. 1. Temperature dependence of majority-carrier concentration.

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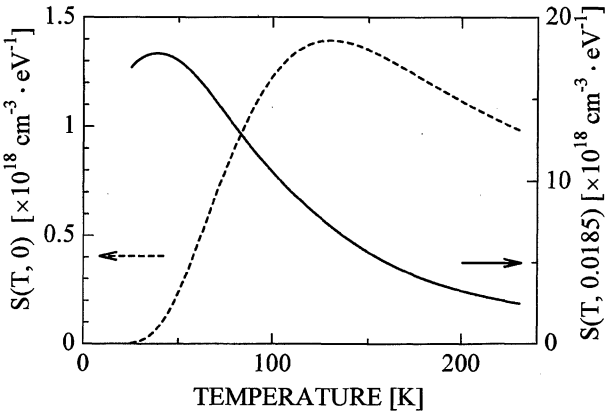

Fig. 2. $S(T,\ 0)$ (broken line) and $S(T,\ 0.0185)$ (solid line) calculated using eq. (1).

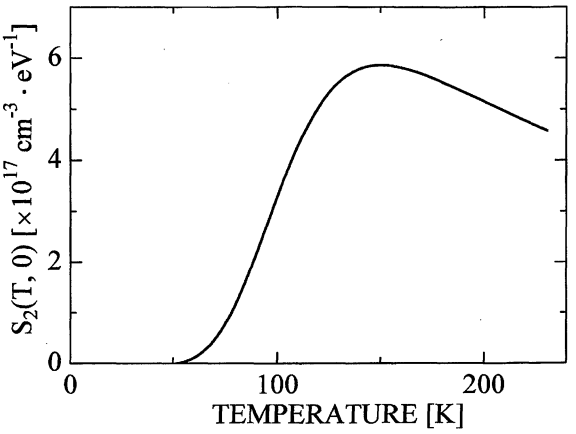

Fig. 3. $S_2(T,\ 0)$ calculated using eq. (7) with $N_{D1} = 1.06 \times 10^{16}$ cm^{-3} and $\Delta E_{D1} = 0.0392$ eV.

From Fig. 1, it is found that only one kind of donor exists and that ΔE_{D1} and N_{D1} are 0.0435 eV and about 2×10^{16} cm^{-3}, respectively. It is found using Hoffmann's method[2] that ΔE_{D1} and N_{D1} are 0.0511 eV and 1.45×10^{16} cm^{-3}, respectively, and that there are no other donor levels. However, these results are completely inaccurate.

The broken curve for $S(T,\ 0)$ in Fig. 2 is calculated using eq. (1) and $n(T)$ shown in Fig. 1. The peak temperature (130 K) in the broken curve is much higher than the lowest measuring temperature. In order to accurately determine the density and energy level of the shallowest donor, the peak temperature should be reduced by using a positive E_{ref}.

The solid curve in Fig. 2 represents $S(T,\ 0.0185)$ calculated using $n(T)$ in Fig. 1. From this figure, T_{peak1} and $S(T_{peak1},\ 0.0185)$ are 38.8 K and 1.78×10^{19} cm$^{-3}\cdot$eV^{-1}, respectively.

The value of ΔE_{D1}, which maximizes $D_1(T, E_{ref})$ at T_{peak1}, is calculated numerically. Using $T_{peak1} = 38.8$ K, ΔE_{D1} is found to be 0.0392 eV, which is close to the actual value.

The value of N_{D1} is given by

$$N_{D1} = \frac{S(T_{peak1}, E_{ref})}{D_1(T_{peak1}, E_{ref})}, \tag{6}$$

since $S(T_{peak1}, E_{ref})$ with $E_{ref} = 0.0185$ eV is considered to be $N_{D1}D_1(T_{peak1}, E_{ref})$. Using the values obtained above, N_{D1} is estimated to be 1.06×10^{16} cm^{-3}, which is close to the actual value.

In order to estimate ΔE_{D2} and N_{D2}, the function

$$S_2(T,\ E_{ref}) \equiv S(T,\ E_{ref}) - N_{D1}D_1(T, E_{ref}) \tag{7}$$

is defined. The curve for $S_2(T,\ 0)$, which is calculated using eq. (7) with $\Delta E_{D1} = 0.0392$ eV and $N_{D1} = 1.06 \times 10^{16}$ cm^{-3}, is shown in Fig. 3. At high temperature, the contribution of the donor with ΔE_{D2} to $n(T)$ becomes large. The peak value $S_2(T_{peak2},\ 0)$ and the corresponding temperature T_{peak2} are 5.86×10^{17} cm$^{-3}\cdot$eV^{-1} and 150 K, respectively.

For $\Delta E_{D2} = 0.0547$ eV, $D_2(T, E_{ref})$ is a maximum at $T_{peak2} = 150$ K. This value of ΔE_{D2} is close to the actual value.

The value of N_{D2} is given by

$$N_{D2} = \frac{S_2(T_{peak2}, E_{ref})}{D_2(T_{peak2}, E_{ref})}, \tag{8}$$

since $S_2(T_{peak2}, E_{ref})$ with $E_{ref} = 0$ eV is considered to be $N_{D2}D_2(T_{peak2}, E_{ref})$. Using the obtained values, N_{D2} is estimated to be 9.41×10^{15} cm^{-3}, which is close to the actual value.

The limitations of this modified method are discussed in the following. When $\Delta E_{D1} = 0.039$ eV and $\Delta E_{D2} = 0.054$ eV, the densities and energy levels of the two donors can be determined in the range $4 \times 10^{-2} \leq N_{D1}/N_{D2} \leq 20$, which is the same as the range for the method proposed previously.[3] For Si with Sb ($\Delta E_{D1} = 0.039$ eV, $N_{D1} = 1 \times 10^{16}$ cm^{-3}) and P ($\Delta E_{D2} = 0.045$ eV, $N_{D2} = 1 \times 10^{16}$ cm^{-3}), the calculated values of ΔE_{D1}, N_{D1}, ΔE_{D2} and N_{D2} are 0.0395 eV, 1.33×10^{16} cm^{-3}, 0.0468 eV and 6.71×10^{15} cm^{-3}, respectively. Therefore, the energy resolution is about 0.006 eV. By modifying the previously proposed method,[3] the energy resolution is improved from about 0.05 eV to about 0.006 eV. Therefore, this modified method gives more accurate values of the densities and energy levels of impurities, estimated from $n(T)$, than other methods.[1-3]

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2) H. J. Hoffmann: Appl. Phys. **19** (1979) 307.
3) H. Matsuura and K. Sonoi: Jpn. J. Appl. Phys. **35** (1996) L555.