Determination of Densities and Energy Levels of Impurities and Traps in Semiconductor by a New Method Based on Hall-Effect Measurements

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Abstract Without any assumptions of the number of impurity species and trap species in a semiconductor, we demonstrate that a graphical peak analysis method based on Hall-effect measurements, referred to as Free Carrier Concentration Spectroscopy (FCCS), can precisely determine their densities and energy levels. We experimentally determine accurate acceptor densities and acceptor levels in p-type undoped GaSb grown by MBE.

1. Introduction

In order to fabricate a device-quality n-type or p-type semiconductor, we should lower densities of impurities and defects that behave as a donor or an acceptor in an undoped semiconductor before we put dopants into the semiconductor. After that, we should search a dopant (donor or acceptor) with low ionization energy. Therefore, an accurate evaluation of the densities and energy levels of dopants in a semiconductor is essential.

In order to determine these densities and energy levels, the temperature dependence of the majority-carrier concentration $p(T)$ is usually measured. Although these values are usually determined using the $\ln p(T)-1/T$ curve, this analysis cannot be applied in the case of semiconductors with more than one dopant species or compensated semiconductors. Moreover, it is difficult to obtain reliable values by fitting a curve to the experimental data on $p(T)$, since too many curve-fitting parameters must be determined at the same time. Though Hoffmann [1] proposed a differential evaluation of $p(T)$, the differential of the experimental data results in an increase in observed errors. Therefore, one of the authors has proposed the precise determination without the differential of $p(T)$, referred to as Free Carrier Concentration Spectroscopy (FCCS), and has applied FCCS to Si irradiated with high energy protons or electrons, and SiC [2-6].

GaSb-based semiconductors have been regarded as a promising semiconductor for near and mid infrared laser diodes and photodiodes, which are used for monitoring CO_2, CO, NO_x and SO_x in atmosphere. In this paper, using FCCS, we attempt to determine acceptor densities and acceptor levels in p-type undoped GaSb grown by MBE (molecular beam epitaxy).

2. Basic Concept of Free Carrier Concentration Spectroscopy

Deep level transient spectroscopy (DLTS) or isothermal capacitance transient spectroscopy (ICTS) can uniquely determine the densities and energy levels, because each peak in the signal corresponds one-to-one to an impurity or a defect [7]. 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 $N_i \exp(-1)$ 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, respectively. 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 $p(T)$, we have introduced a function 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. The function $N_i \exp(-\Delta E_i/kT)/kT$ has a peak at $T_{\mathrm{peak}i} = \Delta E_i/k$, 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 $T_{\mathrm{peak}i} = (\Delta E_i - E_{\mathrm{ref}})/k$, 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 $N_i \exp\left[-\left(\Delta E_i - E_{\mathrm{ref}}\right)/kT\right]/kT$, where N_i and ΔE_i determined by this method is independent of E_{ref}. In addition, we have avoided introducing a differential evaluation of $p(T)$.

3. Theoretical Consideration of FCCS

For the following theoretical considerations, we assume a p-type semiconductor with n different acceptor species (density $N_{\mathrm{A}i}$ and energy level $\Delta E_{\mathrm{A}i}$ of the i-th acceptor for $1 \le i \le n$), one acceptor (density N_{A}) that is completely ionized at the measurement temperatures, and one donor (density N_{D}). The acceptor energy levels $\Delta E_{\mathrm{A}i}$ are measured from the top of the valence band (E_{V}). From the charge neutrality condition, the free hole concentration $p(T)$ can be described as

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

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

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

ΔE_{F} is the Fermi level measured from E_{V}, and g_{A} is the degeneracy factor of acceptors.

On the other hand, using the effective density of states $N_{\mathrm{V}}(T)$ in the valence band, we can describe $p(T)$ as

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

where $N_{\mathrm{V}}(T) = N_{\mathrm{V0}} k^{3/2} T^{3/2}$, $N_{\mathrm{V0}} = 2(2\pi m_h^* / h^2)^{1.5}$, m_{h}^* is the hole effective mass, and h is the Planck constant.

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

$$H1(T, E_{\mathrm{ref}}) \equiv \frac{p(T)^2}{(kT)^{2.5}} \exp\left(\frac{E_{\mathrm{ref}}}{kT}\right). \tag{4}$$

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

$$H1(T, E_{\mathrm{ref}}) = \sum_{i=1}^{n} \frac{N_{\mathrm{A}i}}{kT} \exp\left(-\frac{\Delta E_{\mathrm{A}i} - E_{\mathrm{ref}}}{kT}\right) I(\Delta E_{\mathrm{A}i}) - \frac{\left(N_{\mathrm{D}} - N_{\mathrm{A}}\right) N_{\mathrm{V0}}}{kT} \exp\left(\frac{E_{\mathrm{ref}} - \Delta E_{\mathrm{F}}}{kT}\right), \tag{5}$$

where

$$I(\Delta E_{\mathrm{A}i}) = \frac{N_{V0}}{g_{\mathrm{A}} + \exp\left(\dfrac{\Delta E_{\mathrm{F}} - \Delta E_{\mathrm{A}i}}{kT}\right)}. \tag{6}$$

Finally, using a personal computer, we take the temperature dependence of $I(\Delta E_{\mathrm{A}i})$ into account, and we can easily determine $N_{\mathrm{A}i}$ and $\Delta E_{\mathrm{A}i}$ for each peak.

4. Experimental

2- μm-thick undoped GaSb epilayers were grown on semi-insulator (100) GaAs at 470 ℃

by the water-cooled MBE with three different Sb/Ga flux ratios of 6, 8 and 10. The growth rate was about 500 nm/h.

Each undoped GaSb was cut into pieces of 7x7 mm^2. The free hole concentration $p(T)$ was measured by the van der Pauw method at temperatures between 80 K and 420 K, at a magnetic field of 1.4 T and a current of 0.1 mA. In addition, 0.5-mm-thick undoped GaSb wafer was cut into 10x10 mm^2, and the $p(T)$ was measured.

5. Results and Discussions

Figure 1 shows three $p(T)$ of undoped GaSb epilayers for different Sb/Ga flux ratios of 6, 8 and 10. The concentration for Sb/Ga=8 is lowest, and it for Sb/Ga=6 is highest. Let us discuss the number of acceptor species, acceptor densities, and acceptor levels.

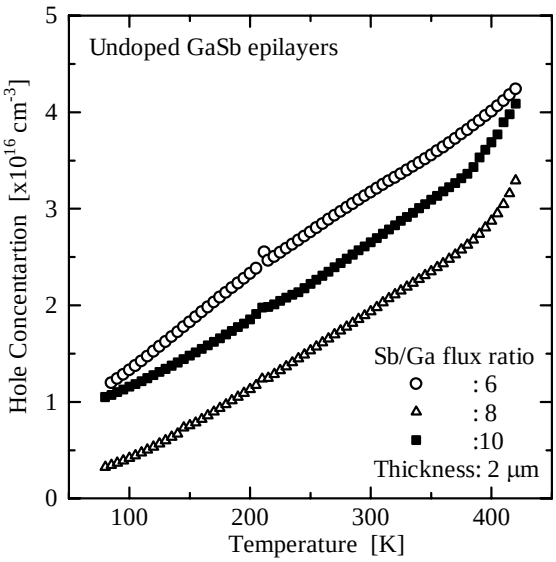

Fig. 1 Temperature dependence of hole concentartions.

Figure 2 show the $H1(T,E_{\mathrm{ref}})$ of the undoped GaSb epilayer for Sb/Ga=10. The $H1(T,E_{\mathrm{ref}})$ is calculated by interpolating $p(T)$ with a cubic spline function. Since one peak and two shoulders appear in the figure, it is found that at least three acceptor species are included in this undoped GaSb epilayer. From the peak, the density (N_{A1}) and energy level (ΔE_{A1}) are determined to 3.8x10^{15} cm^{-3} and 28 meV, respectively, and also the value of $N_{\mathrm{A}}-N_{\mathrm{D}}$ are evaluated to be 9.2x10^{15} cm^{-3}.

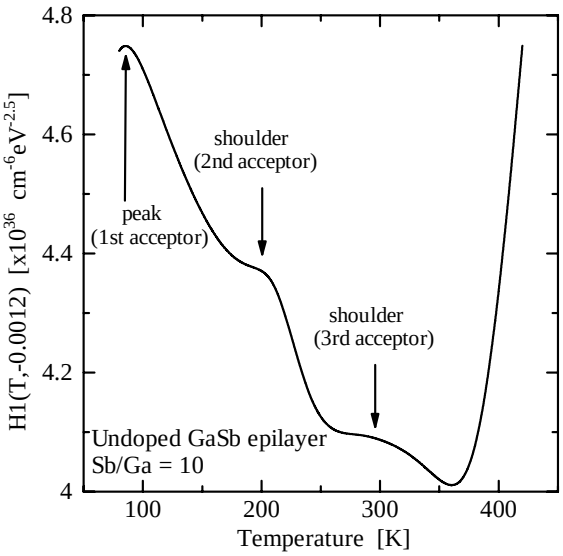

Fig. 2 H1(T,E_{ref}) with E_{ref}=-0.0012 eV.

As is clear from Eqs. 4 and 5, the function, which is not influenced by the acceptors obtained above, is introduced as

$$H2(T,E_{\mathrm{ref}}) \equiv H1(T,E_{\mathrm{ref}}) - \frac{N_{\mathrm{A1}}}{kT}\exp\left(-\frac{\Delta E_{\mathrm{A1}}-E_{\mathrm{ref}}}{kT}\right) I(\Delta E_{\mathrm{A1}}) - \frac{(N_{\mathrm{A}}-N_{\mathrm{D}})N_{\mathrm{V0}}}{kT}\exp\left(\frac{E_{\mathrm{ref}}-\Delta E_{\mathrm{F}}}{kT}\right), \tag{7}$$

which is shown by the solid line in Fig. 3. From the peak, N_{A2} and ΔE_{A2} are determined to be 1.2x10^{16} cm^{-3} and 75 meV, respectively.

The function, which is not influenced by the acceptor obtained above, is introduced as

$$H3(T,E_{\mathrm{ref}}) \equiv H2(T,E_{\mathrm{ref}}) - \frac{N_{\mathrm{A2}}}{kT}\exp\left(-\frac{\Delta E_{\mathrm{A2}}-E_{\mathrm{ref}}}{kT}\right) I(\Delta E_{\mathrm{A2}}), \tag{8}$$

which is shown by the broken line in Fig. 2. From the peak, N_{A3} and ΔE_{A3} are determined to be 2.4x10^{16} cm^{-3} and 164 meV, respectively.

Figure 4 shows the free hole concentration simulated using the values determined here (solid line). The open circles represent the experimentally obtained $p(T)$. The simulated free hole concentration is quantitatively in good agreement with the experimentally obtained $p(T)$, indicating that the values determined here are reliable.

In the same way as illustrated for the undoped GaSb epilayer for Sb/Ga=10, the densities and energy levels of accepters in the undoped GaSb epilayers for Sb/Ga of 6 and 8 and also in the 0.5-mm-thick undoped GaSb wafer are determined, and are listed in Table 1.

According to the double acceptor model [8], a vacancy (V_{Sb}) or Ga (Ga_{Sb}) at a Sb site behaves as a singly ionized acceptor (20~40 meV) and a doubly ionized acceptor (60~100 meV). In this case, the density of the 20~40 meV acceptor should be equal to that of the 60~100 meV acceptor. However, since our experimental results are not the case, the double acceptor model is considered not to be reasonable.

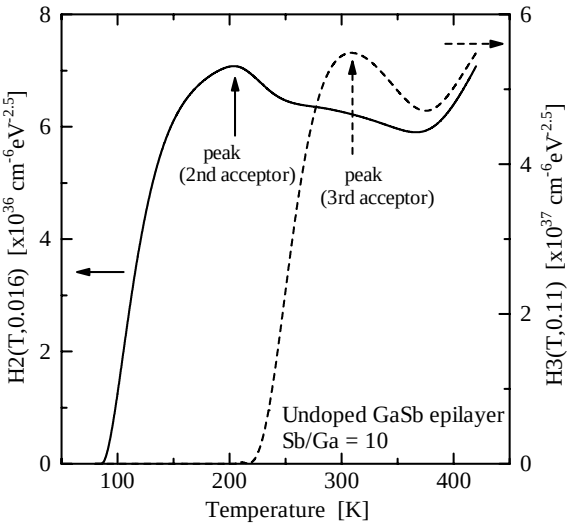

Fig. 3 $H2(T,E_{ref})$ and $H3(T,E_{ref})$.

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 GaSb epilayers grown by MBE, we detected one acceptor that is already ionized below 80 K, and four types of acceptors whose energy levels are 28~41 meV, 75~99 meV, 164~181 meV and 259 meV. On the other hand, in the thick undoped GaSb wafer, we detected two acceptor species whose energy levels are 21 meV and 83 meV.

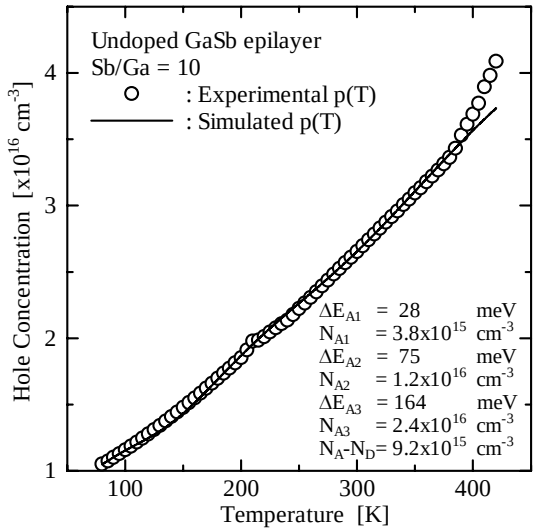

Fig. 4 Comparison of simulated p(T) with experimental p(T).

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Table 1 Obtained results

		Sb/Ga flux ratio			wafer
		6	8	10	
$N_A - N_D$	Density [cm^{-3}]	$1.1x10^{16}$	$7.2x10^{15}$	$9.2x10^{15}$	
Acceptor 1	Energy Level [meV]	41	-----	28	21
	Density [cm^{-3}]	$1.1x10^{16}$	-----	$3.8x10^{15}$	$2.5x10^{17}$
Acceptor 2	Energy Level [meV]	99	94	75	83
	Density [cm^{-3}]	$1.8x10^{16}$	$1.3x10^{16}$	$1.2x10^{16}$	$7.2x10^{16}$
Acceptor 3	Energy Level [meV]	-----	181	164	-----
	Density [cm^{-3}]	-----	$2.4x10^{16}$	$2.4x10^{16}$	-----
Acceptor 4	Energy Level [meV]	259	-----	-----	-----
	Density [cm^{-3}]	$9.2x10^{16}$	-----	-----	-----
$N_D - N_A$	Density [cm^{-3}]				$1.8x10^{16}$