Characterization of hole traps in MOVPE-grown p-type GaN layers using low-frequency capacitance deep-level transient spectroscopy

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Received November 9, 2018; accepted December 27, 2018; published online May 23, 2019

Traps in MOVPE-grown Mg-doped GaN samples composed of p+/p−/n+ structures were investigated using low-frequency capacitance deep-level transient spectroscopy (DLTS). A drop-off in capacitance with decreasing temperature was observed. This is caused by the longer RC time constant of the diode with lower temperature, which is due to a decrease in the number of ionized Mg acceptors (which have a high ionization energy). This limits the use of lower temperatures in DLTS measurements. To extend DLTS to a lower temperature (105 K), DLTS using a capacitance measurement frequency of 1 kHz was applied. Thus, we can quantitatively discuss concentrations of traps with shallow energy levels. We obtained a nearly one-to-one relation between Ha (Ev +0.29 eV) and Hd (Ev +0.88 eV) in the p-type layer, which strongly supports the theoretical calculation that a carbon on a nitrogen site forms donor-like (Ha) and acceptor-like (Hd) states.

1. Introduction

The growth technology of Mg-doped p-type GaN (p-GaN) has made a large contribution to the improvement of optical and power electric devices.1–16 In the case of power devices especially, a MOS structure on a p-GaN layer allows normally-off operation with an optimal threshold voltage by controlling the effective acceptor concentration.1–3 Then, hole traps involved in p-GaN layers can generally modify the threshold voltage due to compensating carriers4,5) and may cause instability during switching operation similar to bulk traps in high-mobility electron transistors.6,9,10 From this point of view, characterization of hole traps in p-GaN layers is crucial. Deep-level transient spectroscopy (DLTS) is generally used to characterize such hole traps. However, DLTS measurement for a p-GaN layer is more difficult than for n-type GaN (n-GaN). DLTS for n-GaN is usually performed using Schottky diode structures composed of Schottky and ohmic electrodes.10–12) To obtain a p-GaN-based Schottky diode, both electrodes are formed for a p-GaN layer because a p-GaN substrate has not been available until now; this reduces the testable doping range. Moreover, such diodes usually suffer from leakage current and/or series resistance,1,3–16) leading to quantitative inaccuracy. Reference 16 provided an answer to this problem by using a p+/p−/n+ structure grown by NH3-based molecular beam epitaxy. To achieve a similar device structure by metalorganic vapor phase epitaxy (MOVPE), commonly used in manufacturing, the growth technology of a p+ layer doped with 1016 to 1018 cm−3 Mg was required. Recently, we successfully demonstrated the control of low-Mg doping into GaN7,8) and fabricated a p+/p−/n+ structure.18)

However, there is another issue unique to capacitance DLTS measurement for a p-GaN layer. Although Mg is only an acceptor for GaN, the energy level is not shallow. The activation energy of around 0.2 eV leads to carrier freeze-out in the measurement at low temperature,19) where a p+ layer acts as a high-resistivity layer and is fully depleted. As a result, a significant capacitance drop occurs below 200 K in capacitance DLTS at 1 MHz, not allowing detection of traps near the valence band.18) The key to detect traps with a relatively shallow level is the choice of measurement frequency in the capacitance DLTS, considering the temperature-dependent resistance–capacitance (RC) time constant in a p+/p−/n+ structure. Actually, the capacitance DLTS at 1 kHz allows the detection of traps near the valence band.20)

In this study, considering the RC time constant of devices, we quantitatively discuss hole traps with relatively shallow energy levels detected in MOVPE-grown p-GaN layers by low-frequency (1 kHz) capacitance DLTS.

2. Experimental methods

MOVPE was used to grow four samples with p+/p−/n+ structure on freestanding n-GaN substrates prepared by hydride VPE. Methylsilane gas and bis(cyclopentadienyl) magnesium were used as the n-type and p-type dopants, respectively, for GaN. The layered structure was composed of a 0.2-μm-thick n+ layer, a 0.7-μm-thick p+ layer and 0.1-μm-thick p++ layer, where the doping concentrations estimated by secondary ion mass spectroscopy (SIMS) were (6–8) × 1018, (0.3–2) × 1017 and 8 × 1016 cm−3, respectively. The carbon (C) concentrations in the p++ layers were varied in the range of (0.1–1.3) × 1016 cm−3 by controlling the growth temperature and pressure.15) The diodes were fabricated by the same procedure as in Ref. 16. The admissance measurements at zero bias were performed in parallel mode in the range of 1 kHz to 1 MHz to investigate the quantitative relation between measurement frequency and the capacitance drop-off at low temperature. Capacitance DLTS measurement was performed using a filling pulse of 0 V and a reverse bias of −2 V.18) In the measurement, a depletion layer was extended almost toward the p+ layer owing to a p+/n+ junction. Our conventional DLTS system using the Boonton 7200 capacitance meter only allows measurement at a frequency of 1 MHz. To change the measurement frequency, we prepared the capacitance measurement system equipped with a lock-in amplifier and a current preamplifier, which offers f = 0.5 MHz.
a sample doped with $2 \times 10^{17}$ cm$^{-3}$ Mg in the p$^+$ layer, where $\omega = 2\pi f$. A significant capacitance drop-off was seen in the temperature range from 100 to 150 K, corresponding to the peak $G_{\omega}$ at each measurement frequency. The peak $G_{\omega}$, denoted by $H_0$, was shifted to a lower temperature with the reduction of measurement frequency. We think that this shift is related to the temperature dependence of the RC time constants of p$^+/p^-/n^+$ diodes.

Figure 2 shows an equivalent circuit for p$^+/p^-/n^+$ diodes to explain the drop-off of the capacitance and the corresponding peak of $G_{\omega}$. $C_1$ is the depletion layer capacitance determined by ionized Mg acceptors. In the lower temperatures below the capacitance drop-off, Mg acceptors are un-ionized in the neutral region, which acts as an insulator layer characterized by the capacitance $C_2$. Then, an equivalent circuit is expressed by a series connection of $C_1$ and $C_2$, which is simply given by a plate capacitor with thickness $l$ and area $A$ of the p-GaN layer ($C_0 = \varepsilon A/l$). At temperatures sufficiently above the drop-off, the neutral region acts as the resistance ($R$) since Mg acceptors are ionized. When $1/\omega C_1 \gg R$, an equivalent circuit is expressed by the depletion layer capacitance $C_1$, which fulfills the condition for accurate performance of the capacitance DLTS measurement. In the intermediate temperature range, an equivalent circuit in the neutral region is the parallel connection of $C_2$ and $R$. When the equivalent circuit in Fig. 2 is transformed into the measured capacitance $C_m$ and conductance $G$ in the parallel mode, the magnitude of the capacitance drop-off is given by $C_1 - C_0$. Then, the peak of $G_{\omega}$ occurs under the condition where $1/\omega = R(C_1 + C_2)$ is met.

Based on an equivalent circuit for p$^+/p^-/n^+$ diodes, the value of $R$ in the neutral region is obtained from the temperature dependence of the capacitance and $G_{\omega}$ at each frequency. The value of $R$ is determined at each peak temperature of $G_{\omega}$ using the peak value of $G_{\omega}$, its corresponding value of $C_m$ and the peak condition of $1/\omega = R(C_1 + C_2)$. Then, the resistivity of the p-GaN layer is calculated assuming that the resistivity of the p$^+$ region is a factor of 400 lower than that of the p$^-$ region due to the doping ratio of between $8 \times 10^{17}$ and $2 \times 10^{17}$ cm$^{-3}$ for the respective p$^+$ and p$^-$ layers. The temperature dependence of the resistivity determined from 16 measurement frequencies, including four frequencies in Fig. 1, is shown in Fig. 3 and satisfies the Arrhenius relation. This indicates that the change in mobility has little influence on the temperature dependence of the resistivity in this limited temperature range.$^{20,22}$ The hole mobilities for samples having a similar Mg concentration were estimated to be around $100 \text{cm}^2\text{V}^{-1}\text{s}^{-1}$. Assuming this value, the hole concentrations calculated using the resistivity were found to coincide with those determined by Hall effect measurements (data not shown). This result verifies the equivalent circuit model in Fig. 2. From the Arrhenius plot of the resistivity in Fig. 3 the activation energy is estimated to be 0.21 eV, which corresponds to the previously reported ionization energy of Mg acceptors.$^{20,22,23}$ By seeing the drop-off temperatures in $C_m$ and the peak temperatures in $G_{\omega}$ in Fig. 1, we can properly select the measurement frequency for capacitance DLTS to avoid carrier freeze-out if the peak temperature of the focused trap is known.

To choose the measurement frequency for capacitance DLTS we need to know the energy levels of traps involved in the p-GaN layer as well as the peak temperatures of DLTS signals. Current DLTS measurements is another way to avoid carrier freeze-out, allowing the detection of relatively shallow
trap levels. However, current measurement essentially makes it difficult to estimate the trap concentrations because it does not give the capacitance of the depletion layer. In other words, the capacitance DLTS at a proper measurement frequency has the advantage for quantitative analyses of traps compared with current DLTS. Accordingly, we employed current DLTS only to investigate the trap levels and then determined the proper measurement frequency for capacitance DLTS. The quantitative discussion on trap concentrations was informed by using capacitance DLTS.

Figure 4 shows the current DLTS spectrum for the same sample as used in previous research when the emission time constant was 1.82 ms. The dashed line shows the DLTS signal enlarged 10 times. H0 is consistent with the Hb peak as indicated in Fig. 1(b).

Figure 4 shows the current DLTS spectrum for the same sample as used in Fig. 1 and in the previous work. The Arrhenius plot of time constants for a peak observed at the lowest temperature is consistent with that obtained from the H0 peaks of $G/\omega$ at different frequencies as shown in Fig. 1(b), although the estimated temperature ranges are different. That is why that peak in the current DLTS spectrum is labeled H0. We observed the Ha trap as the shallowest level around 160 K. Considering measurements at different time constants as well as different peak temperatures, we performed capacitance DLTS at 1 kHz, allowing detection above 105 K, based on Fig. 1. Figure 5 shows a comparison of capacitance DLTS spectra at measurement frequencies of 1 MHz (upper dashed line) and 1 kHz (bottom, solid line), where an emission time constant of 191 ms was used. As indicated by the arrow, the Hc and H0 traps are observed as a broad single peak in the 1 MHz DLTS. The energy level for each trap is noted in brackets in units of eV.

Figure 6 shows Arrhenius plots for hole traps detected in the p-GaN layer. The plot of the Hx trap was obtained from the $G/\omega$ spectra in Fig. 2(b) and those of the other traps were estimated by using the 1 kHz capacitance DLTS measurements. The energy level for each trap was noted in brackets in units of eV. The obtained trap parameters are summarized in Table I.
are the averaged values in the sample doped with Mg and C of $2 \times 10^{17}$ and $1.6 \times 10^{16}$ cm$^{-3}$, respectively. The energy levels and $\sigma$ values for the $H_x$ and $H_y$ traps are presented in Ref. 18.

Table I. All traps detected in p-GaN samples, where $\sigma$ is the capture cross-section of hole assuming an effective mass of 0.9$m_0$. The trap concentrations ($N_T$) are the averaged values in the sample doped with Mg and C of $2 \times 10^{17}$ and $1.6 \times 10^{16}$ cm$^{-3}$, respectively. The energy levels and $\sigma$ values for the $H_x$ and $H_y$ traps are presented in Ref. 18.

| Trap | Energy level (eV) | $\sigma$ (cm$^2$) | $N_T$ (cm$^{-3}$) | Remarks |
|------|-----------------|------------------|-----------------|---------|
| $H_x$ | $E_V + 0.29$ | $1.2 \times 10^{-14}$ | $9.0 \times 10^{15}$ | $C_N + 1/0$ |
| $H_y$ | $E_V + 0.33$ | $6.5 \times 10^{-15}$ | $3.7 \times 10^{15}$ | Observed in all samples |
| $H_x$ | $E_V + 0.46$ | $2.1 \times 10^{-15}$ | $1.6 \times 10^{15}$ | |
| $H_x$ | $E_V + 0.88$ | $7.5 \times 10^{-14}$ | $1.3 \times 10^{16}$ | $C_N 0/-1$ |
| $H_x$ | $E_V + 0.08$ | $6.6 \times 10^{-18}$ | | Unknown |

originates from $C_N$ but has a different charge state from the $H_d$ (or $H_1$) level.\(^{20}\)

To directly confirm this, we examined in the present work the quantitative relation between the $H_x$ and $H_y$ traps at the same sample position. Figure 7(a) shows the correlation of concentrations between the $H_x$ and $H_y$ traps, where samples with different C concentrations were examined. The trap concentration of $H_x$ was determined using the saturated value of the isothermal DLTS peak height with a pulse width of 10 s, while a pulse width of 10 ms was long enough to saturate the DLTS peak height for $H_y$. The result exhibited a nearly one-to-one relation for both traps, strongly supporting the picture originating from the same $C_N$ with the different +1/0 and 0/–1 charged states.\(^{20,25,26}\) The detection of the same concentration is not surprising considering the different emission time constants in the different ranges of temperature. When applying filling pulse, a $C_N^+$ can capture two holes and be charged with the +1 state. At a low temperature around 150 K, one hole is emitted from the $C_N$ and becomes neutral (i.e. $C_N^+ \rightarrow C_N^0 + h^+$). Then, emission of the second hole does not occur in the measurement time window because the emission time of the $H_d$ level is too long. At around 350 K, the first hole emission ($C_N^+ \rightarrow C_N^0 + h^+$) can occur before measurement of the capacitance transient. As a result, the capacitance transient due to only the second hole emission ($C_N^0 \rightarrow C_N^- + h^+$) was reasonably observed in the time window. Therefore, the nearly one-to-one correlation between $H_x$ and the $H_y$ traps provides direct evidence for the identification.

Next, we focus on the $H_y$ trap located at $E_V + 0.33$ eV. The capture cross-section was estimated to be $6.5 \times 10^{-15}$ cm$^2$. This trap was commonly observed in four samples with the different C concentrations used in this study. We previously reported that the trap having the nearest energy level in n-GaN is the $H_2$ trap located at $E_V + 0.25$ eV.\(^{24,27}\) Their Arrhenius plots were not in complete agreement (not shown), although this leaves room for investigation. To our knowledge there are few reports on such shallow hole traps detected by DLTS, although some traps with energy levels above 0.4 eV and shallow traps detected by admittance spectra have been reported.\(^{28}\) The $H_y$ trap concentrations were varied in the range of $(0.1–1.3) \times 10^{16}$ cm$^{-3}$. In the sample with the highest $H_y$ concentration, the concentration was comparable to the $H_x$ and $H_y$ ones. The $H_y$ concentration had no correlation to that of C, indicating that the $H_y$ trap does not originate from C, as shown in Fig. 7(b). Further investigations using different growth conditions are needed to assign its origin.

Finally, we discuss another capacitance step in the temperature above the capacitance drop-off as shown in Fig. 1(a). This was seen as another peak of $G_{ho}$ in Fig. 1(b). We mark this peak as $H_x$ in Fig. 6. Also, two such capacitance steps or two peaks in $G_{ho}$ have often been observed in p-GaN Schottky diodes.\(^{14,29–32}\) Since the peaks corresponding to $H_x$ are observed irrespective of growth methods, it is possible that $H_x$ is related to the presence of Mg in the p-GaN layer. As shown in Fig. 6, the Arrhenius plot of the $H_x$ level gave a small energy level of 0.08 eV despite the higher peak temperature than $H_0$. Therefore, the capture cross-section of $H_x$ is expected to be small. In fact, the hole capture cross-section of $H_x$ was estimated to be about $6.5 \times 10^{-18}$ cm$^2$. $H_x$ cannot be detected by capacitance DLTS because the peak temperature in the measurement time window is estimated to be below 70 K. Previous studies pointed out that such a small capacitance cross-section is due to the repulsive barrier associated with Mg.\(^{33}\) According to
first-principles calculation, however, a simple Mg on a Ga site only forms a 0/1 acceptor level within the bandgap, which presumably gives an attraction force to a hole. One possible explanation is an energy level due to the Mg–H complex which has its +1/0 transition level located at 0.13 eV above the valence band, as predicted in Ref. 34. Although the H concentration in this sample was below the detection limit of SIMS, the detection limit around 10¹⁶ cm⁻³ might hide small numbers of Mg–H complexes. The other Mg-related complexes allow the possibility of H₂ association and therefore the assignment of the origin requires further investigations.

4. Conclusions

Trap characterization of epitaxial p-GaN samples grown on freestanding GaN substrates was performed using DLTS measurements. We carefully discussed the relation between measurable temperature and measurement frequency based on the equivalent circuit model. The comparison of capacitance DLTS at 1 kHz and 1 MHz showed that a proper measurement frequency (1 kHz) is significant for the detection of relatively shallow traps. Thus by using the carefully determined measurement condition, a nearly one-to-one correlation between the H₂ and H₃ traps was presented, strongly supporting the theoretical calculation that a C on a N site forms donor-like (H₂) and acceptor-like (H₃) states.

Acknowledgments

This work was supported by MEXT “Program for research and development of next-generation semiconductor to realize energy-saving society”.

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