Quantitative analysis of electrically active defects in Au/AlGaN/GaN HEMTs structure using capacitance–frequency and DLTS measurements

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Abstract

Electrical trap states in the AlGaN-based high-electron-mobility transistor (HEMT) structures limit the performances of devices. In this study, we present a comprehensive study of the electrical trap states in AlGaN/GaN HEMT structures and examine their influence on the device performance. We performed capacitance–frequency and conductance–frequency measurements to determine the time constant and the density of the interface states. The density of the interface states was calculated to be $2 \times 10^{10} \text{ cm}^{-2} \text{ eV}^{-1}$, and the time constant of the interface states was 1 μs. Deep-level transient spectroscopy showed the presence of one electron trap E1 (negative peak) and three hole-like traps P1, P2, and P3 (positive peaks). The thermal activation energies for E1, P1, P2, and P3 traps were calculated to be 1.19, 0.64, 0.95, and 1.32 eV, respectively. The electron trap E1 and the hole-like traps P1, P2 and P3 were observed to originate from the point defects or their complexes in the material. The hole-like traps reflected the changes created in the population of the surface states owing to the capture of the surface states; these traps originated from the point defects related to the nitrogen vacancy.

1. Introduction

Owing to their exceptional properties, AlGaN/GaN high-electron-mobility transistors (HEMTs) have evoked great interest among researchers for more than three decades for potential applications in high-frequency and high-power devices [1–5]. A new market is now emerging in telecommunications using HEMT structures; however, the main obstacle in developing device applications is the density of the interface states [6, 7]. Interface states induce frequency-dispersive effects, which compromise the reliability of AlGaN/GaN HEMT. This is one of the most critical challenges faced in developing a mature AlGaN/GaN HEMT technology [7].

The electrical trap states in the HEMT structures change the density of the two-dimensional electron gas (2DEG) in the quantum well (QW); this change limits the device performance in the operational mode [7, 8]. Furthermore, trapping/de-trapping processes also limit the performances of HEMTs at high frequencies [7]. Therefore, it is important to characterize the electrical trap states in the HEMT structures. The frequency-dependent capacitance and deep-level transient spectroscopy (DLTS) methods are sensitive techniques for investigating the following features: the position of the 2DEG channel; the density of the electrical trap states in the QW; and the relaxation times of the electrical trap states [7–10]. Usually, deep interface traps exist with long emission time constants in wide-bandgap semiconductors that do not follow the probing frequency; these traps generate excess capacitancies and conductance, which cannot be explained using the traditional trapping mechanism [10–12]. Therefore, frequency-dependent conductance methods have been widely used to evaluate...
the fast traps; current–voltage (I–V) measurements have also been used to evaluate the slow traps in AlGaN/GaN structures. In this study, we report I–V, capacitance–voltage (C–V), capacitance–frequency (C–f), and DLTS measurements for Al$_{0.25}$Ga$_{0.75}$N/GaN HEMT structures grown using the hot-wall metal organic chemical vapor deposition (MOCVD) method.

2. Materials and methods

The Al$_x$Ga$_{1-x}$N/GaN HEMT was grown using hot-wall MOCVD on a four-hexagonal silicon carbide substrate as shown in figure 1. The epitaxial structures comprised a 100-nm AlN buffer layer an undoped 2 $\mu$m GaN layer and an undoped 25 nm AlGaN barrier layer with 25% Al mole fraction. It is very common that the ohmic contact is placed on the backside of the semiconductor, but this requires a conductive substrate. All the samples in this study were grown on semi-insulating SiC substrates therefore a 150-nm thick Al ohmic contact was evaporated on the top layer of Al$_{0.25}$Ga$_{0.75}$N/GaN structure followed by annealing at 650 °C for 60 s in N$_2$. The Schottky contact was realized by evaporating 100 nm of Au on the Al$_{0.25}$Ga$_{0.75}$N structure. For the I–V, frequency-dependent capacitance/conductance, and DLTS measurements, we used Keithley 4200A-SCS, Agilent E4980A precision LCR meter, and DLS-80, respectively. The schematic diagram of the experimental setup and procedure are given elsewhere [13].

3. Results and discussion

Figure 2 illustrates the cross-sectional TEM image, which was captured from an area that seemed crack free in the optical microscope; the thickness of the three individual layers can be seen in this figure. Figure 3 shows the I–V characteristics of the Au Schottky diode on Al$_{0.25}$Ga$_{0.75}$N/GaN structures at room temperature. Using the thermionic emission model, the ideality factor and barrier height were determined to be 3 eV and 0.96 eV.
respectively. The room temperature capacitance of the AlGaN Schottky diode is shown in figure 4. The carrier concentration and barrier height were determined by plotting the $1/C^2$–$V$ graph using the following equations:

\[
\frac{1}{C^2} = \frac{2}{q\varepsilon_0 \varepsilon_r A^2 N_D} (V_{bi} - V),
\]

\[
\Phi_B = V_{bi} + \frac{kT}{q} \left( \frac{N_C}{N_D} \right)
\]

Here, $N_C = 2(2\pi m^* kT/h^2)^{3/2}$ is the effective density of the interface states, and the carrier concentration is $3.24 \times 10^{17} \text{ cm}^{-3}$. The barrier height is 0.95 eV, which is close to the theoretical value, i.e., 1 eV, obtained from the Schottky–Mott relationship ($\phi_B = \phi_m - q\chi$), wherein the work function of Au is 5.1 eV, and the electron affinity of GaN is 4.10 eV. The C–V measurement is an efficient method to attain the doping concentration and density of the interface states. In the C–V measurement, the device capacitance comprises the depletion capacitance and interface capacitance. At high frequencies, shallow donors usually contribute to the capacitance. However, at low frequencies, less shallow states also contribute to the trapping and de-trapping processes, which increases the capacitance. Hence, capacitance variations arise at different frequencies bowing to deep-level traps [10, 11]. Therefore, we performed C–V measurements at different frequencies to determine
the concentrations of net ionized impurities. Figure 5 shows the C–V measurements as a function of the frequency; the variations in the capacitance due to the dispersion effect can be clearly seen in the figure. The room temperature capacitance measurement as a function of frequency (C–f) is shown in figure 6. Figure 6 demonstrate the capacitance is frequency dependent to authorize this dependence the experimental data is compared with simulation (solid line) results obtained by exponential fitting procedure which also confirms that the capacitance has exponential dependence on frequency. This variation in capacitance is due to a typical dispersion effect that occurs when the interface states in equilibrium with the semiconductor do not contribute to the capacitance at sufficiently high frequencies because the charge at the interface states cannot follow the ac signal [12]. In this case, the capacitance of the Schottkey diode is the only space charge capacitance. Frequency-dependent capacitance and conductance analysis is an efficient method for interface analysis that helps us measure the equivalent parallel conductance \( G_p \) as a function of the frequency \( \omega \) [14–16]. The parallel capacitance and conductance are expressed as

\[
C_p = C_s + \frac{C_{it}}{1 + (\omega \tau)^2}
\]

(3)

Here, \( C_p \), \( C_s \), \( C_{it} \), and \( \tau \) are the parallel capacitance, semiconductor capacitance, interface trap capacitance, and trap time constant, respectively. The density of the interface states, \( D_{it} \), can be calculated using the relation \( D_{it} = C_{it}/q \). In addition, \( D_{it} \) can be obtained from the measured low- and high-frequency capacitance curves [15]. The time constant and density of the interface states may also be obtained from the \( G_p/\omega \) versus \( \omega \) plot. The \( G_p/\omega \) values calculated from the measured capacitance using equation (4) are shown in figure 7. Then, \( D_{it} \) is extracted by fitting the normalized conductance \( G_p/\omega \) as a function of \( \omega \) (see figure 7) using the following equation:

![Figure 5. C–V characteristics of the AlGaN/GaN HEMT structure at different frequencies.](image)

![Figure 6. The C–f characteristics of the AlGaN/GaN HEMT structure at zero bias.](image)

\[ J. \text{Phys. Commun.} \ 5 \ (2021) \ 125010 \ \text{N Bano et al} \]
The Dit and \( \tau \) values obtained were \( 2 \times 10^{10} \) \( \text{cm}^{-2} \text{eV}^{-1} \) and 1 \( \mu \)s, respectively. The experimental \( G_p/\omega \) versus \( \omega \) curves are generally broader than predicted by equation (4), which is attributed to interface trap as well as doping density [15]. Therefore this behavior of the curve can be explained by the presence of a continuous distribution of interface state traps. When the AC signal corresponds to time constant, the peak loss associated with the interface trap levels then occurs. If the frequency is slightly different to the time constant, then the losses are reduced because either the trap levels do not respond or the response occurs at a different frequency, and therefore a peak loss as a function of frequency is achieved [12].

The depth profile of the carrier concentration was extracted from the C–V characteristics, as shown in figure 8, which was then compared with the simulation results obtained using the Poisson–Schrodinger solver [16]. The simulated carrier density as a function of the depth is shown in figure 7 (see solid line). The experimental and simulated results agreed well with each other, and the peak position corresponded to the 2DEG position; the AlGaN thickness was 25 nm. Figure 8 clearly shows that all the carriers are present in the 2DEG channel at the interface of AlGaN and GaN. The band structure was also designed using the Poisson–Schrodinger solver, we used 25% Al contents in the top 25-nm thick AlGaN layer as in the fabricated HEMT.

\[
\frac{G_p}{\omega} = \frac{qD_{it}}{2\omega\tau} \ln \left[1 + (\omega\tau)^2\right]
\]  

(4)
Figure 9 shows the presence of the 2DEG channel in the AlGaN and GaN interface, and the bandgaps for Al$_{0.25}$Ga$_{0.75}$N and GaN were 3.96 eV and 3.4 eV, respectively.

Furthermore, we investigated the DLTS technique for the precise characterization of deep-level traps because DLTS is suitable for deep-level characterizations. Figure 10 shows the associated DLTS spectra of the AlGaN/GaN HEMT structure for temperatures ranging from 250 K to 450 K under constant conditions (i.e., $V_R = -4$, $t_p = 10$ ms, and rate window = 156 s$^{-1}$). The DLTS measurements revealed the presence of one electron trap (E1) and three hole-like traps (P1, P2, and P3). The emission-rate signatures of the observed traps were measured over the maximum possible temperature range. The obtained data was interpreted using the Arrhenius plot as shown in figure 11; the empty circles are the results for the positive peaks P2 and P3, and the filled circles are those for the negative peak E1. The thermal activation energies of P2, P3, and E1 obtained from the slope of the Arrhenius plot were 0.95 eV, 1.32 eV, and 1.19 eV, respectively. However, the activation energy $P1 = 0.64$ eV was calculated using D. V. Lang’s line shape formula [17]. The capture cross sections of the observed traps P2, P3, and E1 at the infinite temperature $\sigma(\infty)$ were obtained from the intercept of the Arrhenius plot and were found to be $1.4 \times 10^{-11}$ cm$^2$, $4.7 \times 10^{-9}$ cm$^2$, and $1.7 \times 10^{-9}$ cm$^2$, respectively. However, the captured cross section $2.5 \times 10^{-14}$ cm$^2$ of P1 was calculated using D. V. Lang’s line shape formula [17].
Arrhenius plot shown in figure 11 is used to describe the activation energy and the capture cross section. Arrhenius plots gives a straight line, the slope of the line determines the activation energy and the intercept gives the capture cross section. The Arrhenius plot with the steeper slope has a higher activation energy and the plot with the flatter slope has a smaller activation energy. This means that over the same temperature range, a reaction with a higher activation energy changes more rapidly than a reaction with a lower activation energy. The obtained data for the levels P1–P3 and E1 are listed in the table 1.

The hole-like trap P1 had the activation energy of 0.64 eV, which was comparable to the activation energy of 0.63 eV reported by Masca et al [18] and 0.68 eV reported by [19]. P1 had a capture cross section of $3.5 \times 10^{-14}$ cm$^2$, which was comparable to the $2.5 \times 10^{-12}$ cm$^2$ value reported by Okino et al [19]. The hole-like trap P2 was similar to the defect level of 0.9 eV–1.0 eV reported by Fang et al [20]. The hole-like trap P3, which had the activation energy of 1.32 eV and a capture cross section of $4.7 \times 10^{-9}$ cm$^2$, was analogous to the 1.3-eV level [9] related to the extended defects. Hole-like traps were repeatedly observed in AlGaN HEMT structures. These positive peaks did not originate from the changes in the hole trap population in the channel; they probably reflected the changes in the population of the surface states in the HEMT access regions, which modulated the 2DEG density in the channel [21–28]. The changes in the population of the surface states originated from the point defects related to the nitrogen vacancy [29]. Moreover, such peaks could also be explained by the electron capture/emission at the surface states [30]. The electron trap E1 was similar to the electron traps reported by Wang et al [31] and Okino et al [19], which had activation energy values of 0.98 eV and 1.1 eV, respectively. Polyakov et al [32] reported similar electron traps with the activation energy of 0.9 eV; they reported that the activation energy of the trap increased from 0.45 eV to 0.9 eV when the Al mole fraction increased from $x = 0.15$ to $x = 0.25$. The electron traps could be detected close to the GaN layer whereas the hole-like traps could be detected in the AlGaN/GaN interface region [8].

Figure 12 shows a comparison of the emission-rate signatures of the observed levels with the reported values. In figure 12, the solid lines specify the commonly observed point defects related to the deep-level traps in the MOCVD-grown n-GaN [8, 33, 34], which were obtained by using the capacitance DLTS measurements; the dotted lines are the results obtained by the frequency dispersion in AlGaN/GaN HEMTs [35, 36]. The peaks E1, P2, and P3 almost coincide with the solid lines. This suggests that these levels are the commonly observed traps that originate from the point defects or their complexes in GaN.

### Table 1. List of energy traps in the AlGaN/GaN HEMT structure.

| Traps       | $E$ (eV) | $\sigma$ (cm$^2$) |
|-------------|---------|------------------|
| P1 (hole-like trap) | 0.64    | $2.5 \times 10^{-14}$ |
| P2 (hole-like trap) | 0.95    | $1.0 \times 10^{-11}$ |
| P3 (hole-like trap) | 1.32    | $1.2 \times 10^{-8}$  |
| E1 (electron trap) | 1.19    | $1.7 \times 10^{-9}$  |
4. Conclusions

In summary, the long-term reliability of the AlGaN/GaN HEMT devices is a major cause of concern because of the deep-level traps and interface surface states; therefore, the I–V, C–V, C–f, and DLTS measurement techniques were employed to identify the defects in HEMT structures. Using the conductance–frequency method, the density of the interface states and the trap time constant were calculated to be $2 \times 10^{10}$ cm$^{-2}$ eV$^{-1}$ and 1 $\mu$s, respectively. The DLTS measurements revealed the presence of one electron trap E1 (a negative peak) and three hole-like traps P1–P3 (positive peaks). The thermal activation energies for the E1, P1, P2, and P3 traps were calculated to be 1.19, 0.64, 0.95, and 1.32 eV, respectively. We discussed the identification of these traps and extracted their signatures using the Arrhenius plot and simulations.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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