

Effect of structural parameters on 2DEG density and $C\sim V$ characteristics of $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{AlN}/\text{GaN}$ -based HEMT

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A new High Electron Mobility Transistor (HEMT) model is proposed in this paper by introducing a thin AlN layer in nanoscale range into the conventional $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}/\text{GaN}$ -based HEMT keeping the Al content of 30%. The AlN layer is very sensitive towards the development of polarization charges at the hetero interface and results into high 2DEG density (n_s). The role of AlN layer is essentially very much suitable in order to reduce various scattering exist at the hetero interface of the conventional GaN based devices. The change of various structural parameters such as Al mole fraction of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ from 0.25 to 0.45, thickness of AlGa_N cap layer, thickness of AlN channel layer, doping concentrations give rise to a significant change in the 2DEG transport and $C\sim V$ characteristics of the device and its detail discussion are presented in this paper. The 2DEG density with the variation of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ thickness and Al mole fraction (x) are in good agreement with the experimental results from the literature.

Keywords: HEMT, 2DEG, Heterostructure, Sheet resistance, Heterointerface, Nitride

I Introduction

Gallium nitride based semiconductors are very much suitable for high power and high frequency operation and is the preferred material of many research communities worldwide due to its superior material properties such as high band gap, large breakdown voltage, high electric field and high thermal conductivity¹. It has established itself as an extremely important material for next generation opto-electronics devices and its frequency ranges from green to ultra-violet opto-electronics spectrum. It has created new markets in green LED traffic signals and promises the next great advance in lighting systems¹⁻⁴. Alloy-based semiconductors (Al, Ga, In) nitride are expected to replace the present silicon and GaAs technologies in both microwave and millimeter wave power devices and in opto-electronics technology⁵⁻⁹.

However, due to existence of several scattering mechanisms, which play a major role in limiting the mobility of Two Dimensional Electron Gas (2DEG) in conventional² $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}/\text{GaN}$ -based HEMT. In addition to the traditional phonon scattering, interface roughness scattering, charged impurities scattering and alloy disorder scattering, dislocation scattering and dipole scattering are unique to GaN-based HEMTs, due to the large dislocation density and strong polarization effects in the GaN-based materials systems³⁻⁷.

In order to reduce the scattering in the 2DEG at the hetero interface of conventional $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}/\text{GaN}$ -HEMT, a novel $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}/\text{AlN}/\text{GaN}$ -based High Electron Mobility Transistor (HEMT) structure is proposed by inserting of a nanoscale AlN layer at the $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}/\text{GaN}$ heterointerface⁶⁻¹¹. AlN is a binary, direct high band gap semiconductor having very high polarization effect and is the main source of 2DEG density (n_s), formed at the interface. The dependence of this 2DEG density on various structural parameters such as thickness of AlGa_N cap layer, Al mole fraction, thickness of AlN layer has been studied and also compared with previous experimental results from the available literature.

To understand the frequency response of the device, it is very much essential to study the capacitance-voltage ($C\sim V$) characteristics of any device⁸⁻¹⁷. In this paper, the $C\sim V$ characteristics of the proposed HEMT have also been studied by changing its various structural parameters such as mole fraction, thickness of AlGa_N layer, thickness of AlN channel and doping concentrations.

2 Motivation of HEMT Design

In the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ HEMT structure, optical phonon scattering is the major contribution to scattering at room temperature. At low temperatures, since phonon scattering is largely suppressed, alloy disorder scattering and interface roughness scattering

become the two major dominating factors, depending upon the nature of the barrier. Alloy scattering dominates for $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barriers for all Al compositions^{5,6,12}.

There are two essential reasons for alloy disorder scattering in $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures: one is that the barrier is $\text{Al}_x\text{Ga}_{1-x}\text{N}$, which is a ternary material and has alloy disorder scattering. The second reason is that there is a wave function penetration into the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier, which is a quantum effect. To reduce or remove this effect, either a binary material is used for the barrier, or the penetration is suppressed. To suppress penetration, increasing the Al mole fraction of the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier can be helpful, since when the Al composition increases the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ has a larger conduction band discontinuity. This implies a larger barrier for the 2DEG, therefore, reducing the penetration. The higher the Al mole fraction, the smaller is the penetration. Due to the growth of $\text{Al}_x\text{Ga}_{1-x}\text{N}$, which is a ternary over GaN, the alloy disorder scattering is dominant due to variation of Al mole fraction and it limits the mobility. So in-order to reduce the scattering mechanism, many approaches are taken into consideration such as growth of high quality $\text{Al}_x\text{Ga}_{1-x}\text{N}$ and/or adopting novel epitaxial structures.

AlN is seen to be effective in removing the alloy disorder scattering, therefore, improving the 2DEG mobility in heterostructures. It is, therefore, useful to incorporate it into the conventional AlGaN/GaN-based HEMT, i.e. by inserting an AlN layer between the AlGaN and GaN to form a new hetero structure i.e. AlGaN/AlN/GaN-based HEMT and is shown in Fig. 1. Smorchkova *et al.*^{5,6,12} experimentally demonstrated the structure including effects of the

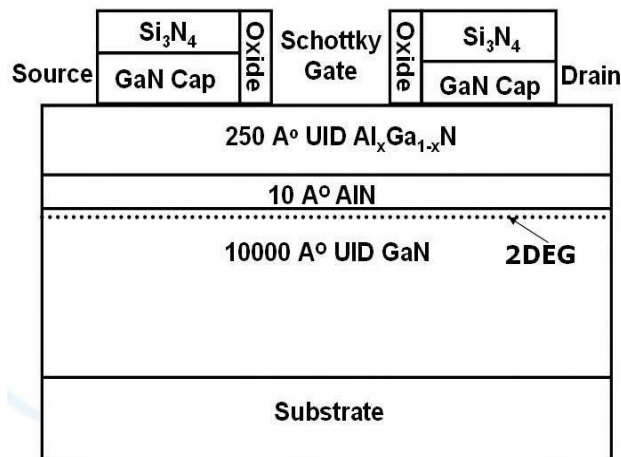


Fig. 1 — Epitaxial structure of $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{AlN}/\text{GaN}$ -based HEMT

polarization. The proposed device is shown in Fig. 1 which consists of several stacked layers grown over each other by Molecular Beam Epitaxy (MBE) technique¹¹. It includes growth of unintentionally doped (UID) GaN layer of thickness 10000Å over SiC semi insulating substrate for good thermal conductivity, to reduce self-heating and over which UID AlN binary layer is grown of thickness 10Å followed by another undoped barrier layer of $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}$ of thickness 250Å. Doped GaN layer of thickness 0.03 μm has been deployed for the cap layer of the device. To eliminate *dc* to *RF*-power level dispersion, insulated Si_3N_4 passivation layers of thickness 0.05 μm is deployed. The gate length (L_g) and width (W) of the device is taken as 0.25 μm and 1.6 μm , respectively. The Schottky gate turn-on voltage was approximately 0.6 V.

3 2 DEG Transport Properties

$\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}$ is a wide band gap semiconductor of energy gap, $E_g=4.24$ eV and GaN is having comparatively less band gap than AlGaN having energy gap, $E_g=3.4$ eV. The growth of wide band gap material over narrow band gap material creates a 2DEG at the hetero interface, so that confinement of electrons in the quantum well is possible, which leads to higher mobility and resulting into a high speed device³⁻⁸. The epitaxial structure of AlGaN/AlN/GaN gives rise to the formation of 2DEG at the hetero interface and is shown in Fig. 2(a).

The Fermi energy level is nearer to the conduction band and it represents the richness of electrons in the conduction band. The conduction band and valence band discontinuity with the position of Fermi Energy level is also shown in Fig. 2(a). Better modulation of the 2DEG density results into high current gain cut-off frequency^{3,8} (f_T). To reduce the wave propagation into the AlGaN barrier, AlN channel layer of 10Å thickness having energy band gap of 6.2eV, at the hetero interface of AlGaN/GaN epitaxial layer¹¹, is introduced. The effective mass approximation is used here to calculate the sub bands structure¹⁴ in the 2DEG, formed at the $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}/\text{GaN}$ hetero interface and is shown in Fig. 2(b). In order to obtain the sub bands structure, we have solved the Schrödinger equation and Poisson equation self-consistently incorporating both heavy hole and light holes in the simulation model^{11,14} and are given by :

$$-\frac{\hbar^2}{2} \frac{d}{dx} \left[\frac{1}{m^*} \frac{d\psi_i(x)}{dx} \right] + [V(x) - E_i] \psi_i(x) = 0 \quad \dots(1)$$

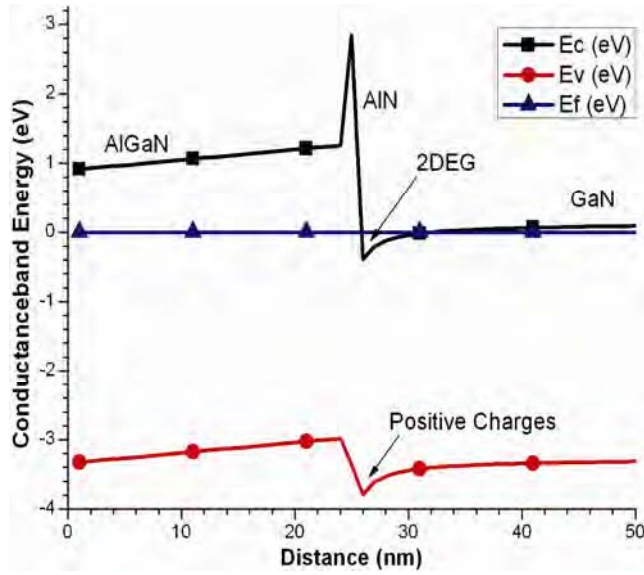


Fig. 2(a) Energy band Structure in AlGaN/AIN/GaN structure

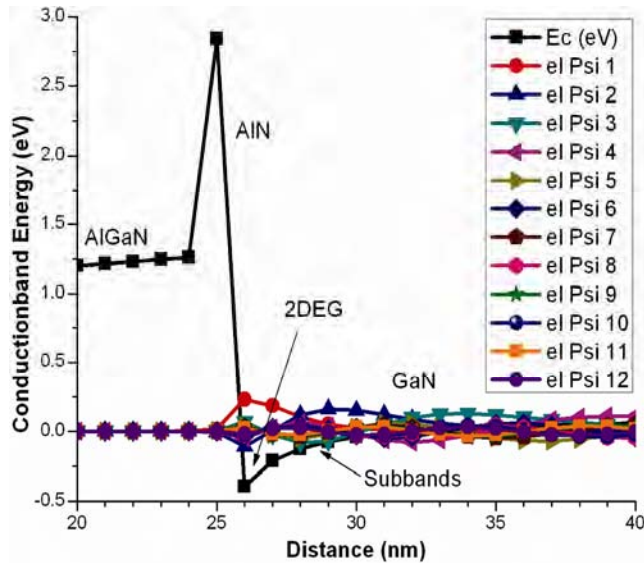


Fig. 2(b) — 2DEG formation with sub bands at the hetero interface of AlGaN/AIN/GaN-based HEMT

$$\left[-\frac{\hbar^2}{2m^*} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = E_i \psi(x) \quad \dots(2)$$

Now Eq. (2) can be reduced to $[H\psi(x) = E_i \psi(x)]$, then the Schrödinger equation with Hamiltonian operator H is solved^{11,14} as follows :

$$(H - I\lambda)\psi(x) = 0 \quad \dots(3)$$

where λ is the eigen value, that is the eigen energy E_i in Eq. (2). Because of the determinant of $|H - I\lambda| = 0$, this indicates that $\psi_i(x)$ may have infinite dependent

solutions and are shown in Figs 2(c) and 3(a). The Poisson equation gives the idea of charge distribution in the 2DEG and is given by:

$$\nabla^2 \cdot V_H(x) = -\frac{4\pi e^2}{\epsilon} [n(x) - N_d^+(x) + N_a^-(x)] \quad \dots(4)$$

where $V(x)$ is the potential due to the conduction band-offset which depends on the Al mole fraction, $V_H(x)$ is the Hartree potential due to the electrostatic interaction of electrons with themselves and impurity charges, ϵ , is the dielectric constant and N_d^+ and N_a^- are the ionized donor and acceptor densities, respectively.

The one-dimensional electron concentration $n(x)$ is related by the wave function and number of electrons per unit area for each energy state and is given by:

$$n(x) = \sum_i N_i |\psi_i(x)|^2 \quad \dots(5)$$

where N_i is the number of electrons per unit area for each energy state E_i and wave function ψ_i of the i^{th} state. The presentation of energy states in AIN-based HEMTs are shown in Fig. 3(a). N_i can be found by integrating the density of states function $g(E)$ and the Fermi-Dirac probability function^{11,14} $f(E)$:

$$N_i = \int_{E_i}^{\infty} g(E) f(E) dE \quad \dots(6)$$

For a 2DEG, the density of states (DOS) is given by $g(E) = m^* / \pi \hbar^2$, where m^* is the effective mass of the electron in GaN. Now substituting the DOS, Eq. (4) can be written^{11,14} as:

$$N_i = \frac{m^*}{\pi \hbar^2} \int_{E_i}^{\infty} f(E) dE \quad \dots(7)$$

$$N_i = \frac{m^*}{\pi \hbar^2} \int_{E_i}^{\infty} \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)} dE$$

$$N_i = \frac{m^* kT}{\pi \hbar^2} \ln \left[1 + \exp\left(\frac{E_F(x) - E_i}{kT}\right) \right] \quad \dots(8)$$

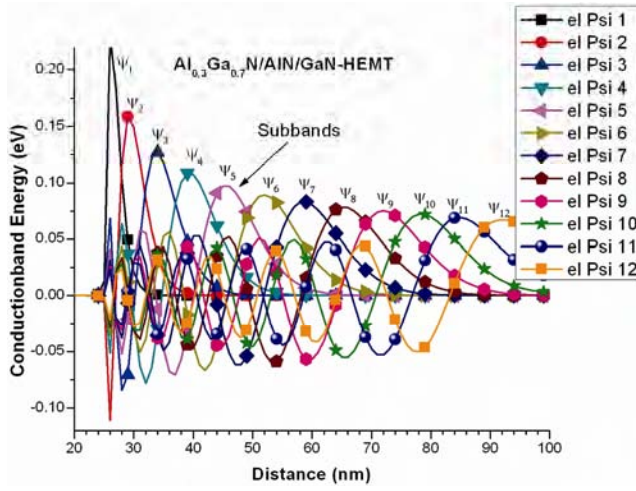


Fig. 3(a) — Sub bands at the heterointerface of $\text{AlGaN}/\text{AlN}/\text{GaN}$ structure

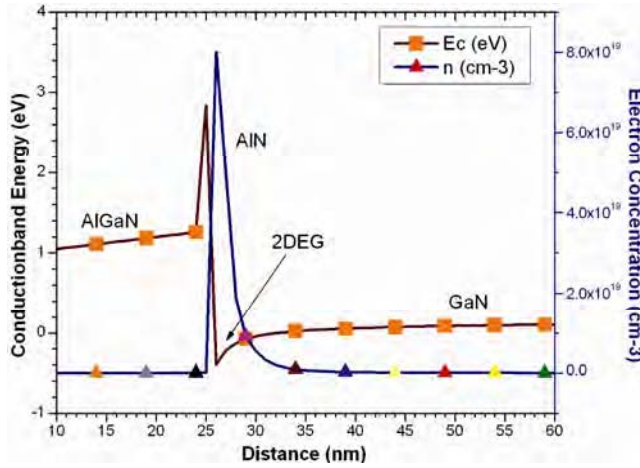


Fig. 3(b) — Electron concentration in the 2DEG of $\text{AlGaN}/\text{AlN}/\text{GaN}$ structure

It can be realized from Fig. 3 that the 2DEG is formed at a distance of 250\AA from the surface. The 2DEG is filled with abundant number of electrons at the hetero interface and the various sub bands from ψ_1 to ψ_{12} are available at the 2DEG, is shown in Fig. 3(a). Figure 3(b) shows that the electrons concentration (n) reaches to its peak value ($8 \times 10^{19} \text{ cm}^{-3}$) at the hetero interface only i.e. at a depth of 250\AA from the surface.

4 Results and Discussion

4.1 2DEG Density

The 2DEG density (n_s) is a function of thickness of AlGaN cap layer, AlN channel layer, mole fraction, polarization charges, conduction band offset. The 2DEG density in the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{AlN}/\text{GaN}$ structure can be obtained^{5,6,12,16} by:

$$n_s = \frac{\sigma_{\text{AlGaN}} \cdot t_{\text{AlGaN}} + \sigma_{\text{AlN}} \cdot t_{\text{AlN}} - \frac{\epsilon \epsilon_0}{q} \left(\phi_B - \frac{\Delta E_{c,\text{AlGaN}}}{q} \right)}{t_{\text{AlGaN}} + t_{\text{AlN}} + d_0}$$

$$= \frac{\sigma_{\text{AlGaN}} \cdot t_{\text{AlGaN}} - \frac{\epsilon \epsilon_0}{q} \phi_B + \frac{\epsilon \epsilon_0}{q^2} (\Delta E'_{c,\text{eff}})}{t_{\text{AlGaN}} + t_{\text{AlN}} + d_0} \quad \dots(9)$$

where

$$\Delta E'_{c,\text{eff}} = \Delta E_{c,\text{AlGaN}} + \left(\frac{q^2}{\epsilon \epsilon_0} \right) \sigma_{\text{AlN}} \cdot t_{\text{AlN}} \quad \dots(10)$$

The larger $\Delta E'_{c,\text{eff}}$ also affects the 2DEG density. The change of the energy band slope in AlGaN cap layer in Fig. 3(b), i.e. the electric field, already implies a change in the carrier density. The behaviour of 2DEG in the proposed structure can be attributed to the larger $\Delta E'_{c,\text{eff}}$ (or $\Delta E_{c,\text{eff}}$) which is caused by the insertion of the thin AlN layer. Because the AlN layer is very thin (1 nm), the effect of $\Delta E'_{c,\text{eff}}$ to the 2DEG density is still limited, compared with the term $\sigma_{\text{AlGaN}} t_{\text{AlGaN}}$, when the AlGaN is thick. For the proposed device, the charge increase caused by the insertion of the AlN layer^{5,6,12,16} is about 10-25%. This increase can also be explained by considering the band diagram in Fig. 2(a and b). The larger $\Delta E'_{c,\text{eff}}$ results in a decrease of the electric field in the AlGaN layer and the decrease can only be implemented, when the 2DEG density increases. The theoretical concepts are also supported by the experimental results from the literature^{5,6,12,16}.

Figure 4(a and b) shows both experimental and simulated curves of the 2DEG density as a function of AlGaN thickness and Al mole fraction. It is noted that the charge density is still a strong function of AlGaN thickness, similar to standard AlGaN/GaN -HEMTs. When the Al composition was varied from 0.2 to 0.45, the 2DEG density increased from $1.2 \times 10^{13} \text{ cm}^{-2}$ to $2.7 \times 10^{13} \text{ cm}^{-2}$. In fact, from Eq. (9), one could find that the dependence is almost identical to the standard structure. Simulations performed by 1D Poisson Solver, agreed with the experimental data from the literature very well^{5,6,12,16}.

However, it is difficult to grow thick AlN as compared to Molecular Beam Epitaxy (MBE), it is more difficult to grow thick AlN by Metal Organic Chemical Vapour Deposition (MOCVD) technique^{5,6,12,16}. Therefore, in this work the results of a series of simulations with different AlN thickness

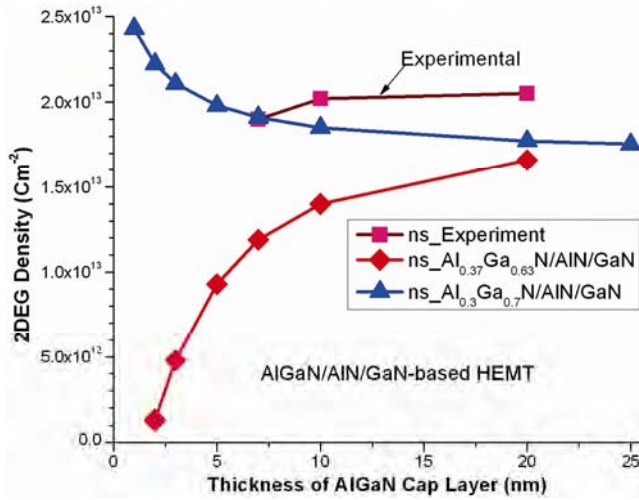


Fig. 4(a) — Simulated and experimental data of 2DEG densities of $Al_xGa_{1-x}N/AlN/GaN$ -HEMT as a function of AlGaN thickness

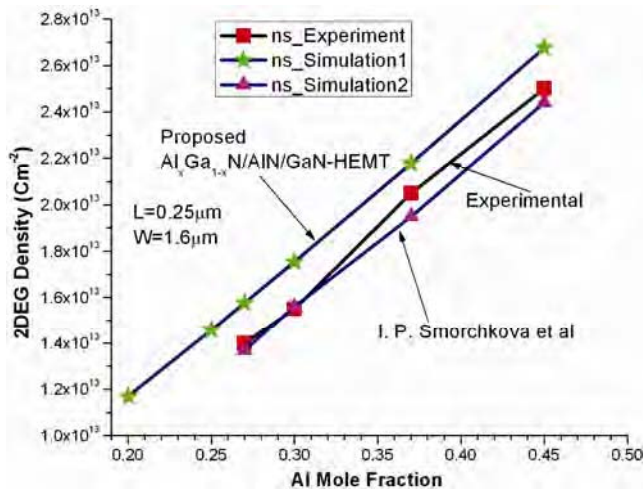


Fig. 4(b) — Simulated and experimental data of 2DEG densities of $Al_xGa_{1-x}N/AlN/GaN$ -HEMT as a function of Al mole fraction

from 0.5 to 5 nm are shown in Fig. 5. It is seen that the 2DEG density increases linearly and the charge density becomes saturated when the thickness of AlN increases from 0.5-1 nm, 1.5-2 nm, 2.5-3 nm and so on. Similarly, the sheet resistance decreases with certain slope and then getting saturated with respect to 2DEG density from 0.5-1 nm, 1.5-2 nm, 2.5-3 nm and so on.

$$R_{sheet} = \frac{1}{q \cdot n_s \cdot \mu_n} \quad \dots(11)$$

The 2DEG density is inversely proportional to the sheet resistance as per Eq. (11) and it is also verified from Fig. 5. As the 2DEG increases with the variation of AlN thickness in the same manner, the sheet

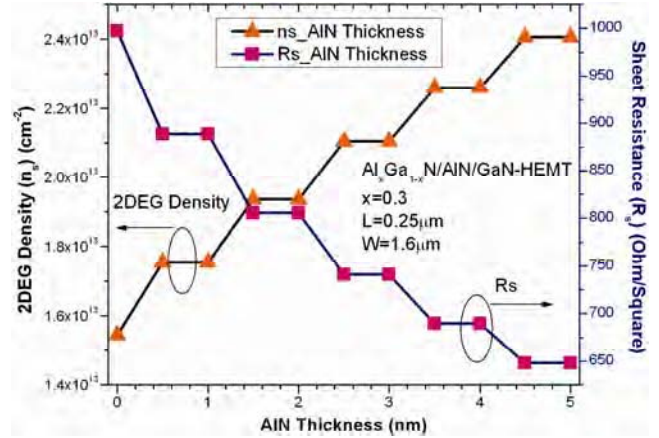


Fig. 5 — 2DEG Density (n_s) and sheet resistance (R_s) with the variation of AlN thickness

resistance also decreases. The mobility variation with the structural parameters is not discussed here.

4.2 C~V Characteristics

The capacitance voltage (C~V) characteristics with the variation of gate voltage from -4 to 4 V of the proposed device for different Al mole fractions and different AlN thickness are shown in Fig. 6(a and b), respectively. Similar to MOSFET, the C~V characteristics of HEMT also undergoes through accumulation, depletion and inversion process with the variation of gate voltage^{8,17} from -4 to 4 V.

From Fig. 6(a), it is seen that, as Al mole fraction increases from $x=0.2$ to $x=0.45$ of the $Al_xGa_{1-x}N$ barrier layer, then the capacitance decreases from 75 to 40 $\mu F/cm^2$ at a gate voltage of -4 V and then maintained almost constant with the variation of gate voltage up to 4V. It represents the high frequency characteristics of the device⁹⁻¹⁷. But as AlN thickness increases from 1 to 10 nm, then the capacitance is not being affected with the variation of gate voltage from -4 to 4V and is shown in Fig. 6(b).

$$C = \frac{\partial Q}{\partial V_{gs}} = \frac{\partial(en_s)}{\partial V_{gs}} \quad \dots(12)$$

As per Eq. (12), the differential change in the capacitor voltage in the ideal case causes a differential change in the 2DEG surface charge density at the hetero interface of AlGaN/GaN. The source of electrons produces a change in 2DEG charge density. The electron concentration in 2DEG cannot be changed instantaneously. If ac voltage across the gate electrode changes rapidly due to its alternating nature, the change in 2DEG density will not be able to

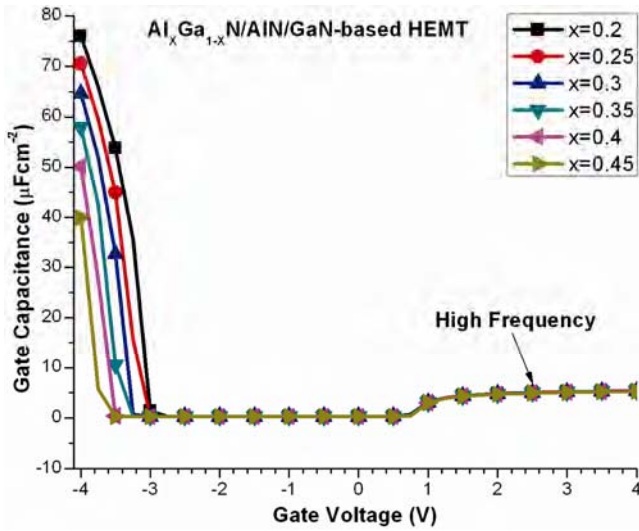


Fig. 6(a) — Gate capacitance with the variation of Al mole fraction

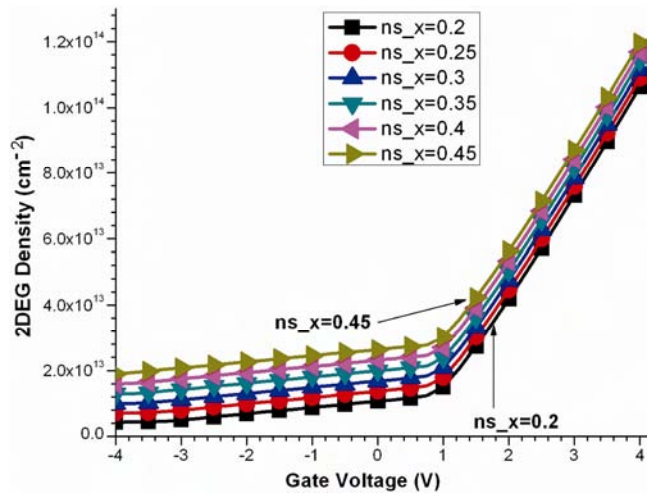


Fig. 7(a) — 2DEG density for different mole fractions in $\text{AlGa}_n/\text{AlN}/\text{GaN}$ -based HEMT

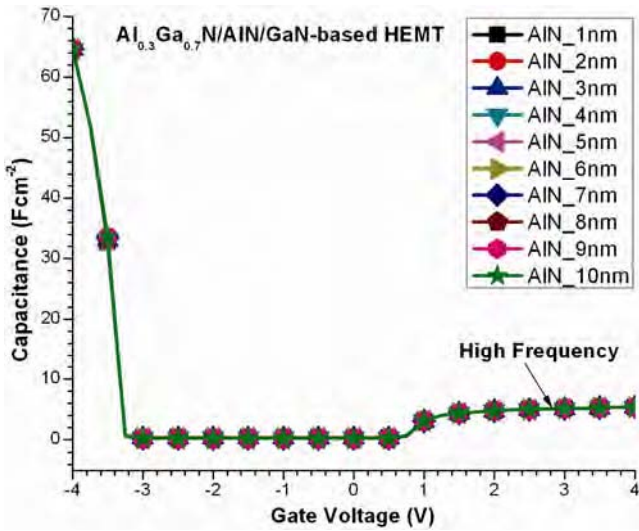


Fig. 6(b) — Gate Capacitance with the variation of AlN thickness

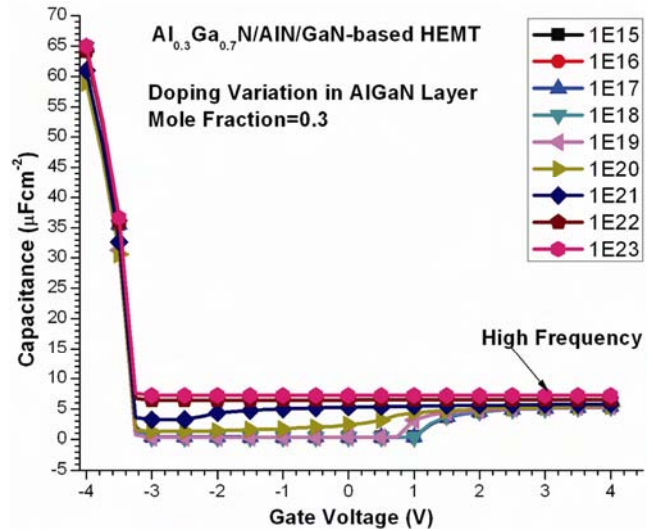


Fig. 7(b) — Capacitance for different doping concentrations in $\text{AlGa}_n/\text{AlN}/\text{GaN}$ -based HEMT

respond so quickly. Therefore, the $C\sim V$ characteristics is a function of frequency of the AC signal used to measure the capacitance^{8,17}. Therefore, for very high frequency of operation, the 2DEG density will not respond to the differential change in capacitor voltage, so that the capacitance is maintained constant, showing the high frequency nature^{8,17}. To maintain constant capacitance with the increase in the gate voltage, this results into a linear increase in the 2DEG density (n_s) for different mole fractions as shown in Fig. 7(a). As the gate voltage increases from -4 to 1 V, there is a minute increase in the 2DEG concentration and at the onset of 1 V, the 2DEG density suddenly rises to its peak value [Fig. 7(a)].

The capacitance is measured for different doping concentrations in the $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}$ cap layer. The doping concentrations (N_d) vary from $1\text{E}15$ to $1\text{E}23$. With the variation of gate voltage from -4 to 4 V, it is seen from Fig. 7(b), that the capacitance decreases from $65 \mu\text{F}/\text{cm}^2$ to a lower value and then maintained constant. It reveals the high frequency characteristics of the device. Higher the doping concentration, more is the tendency towards high frequency characteristics. From -3 to 1 V, the improvement in capacitance can be realized for lower doping concentrations. It also very peculiar to mark that from Fig. 7 that there is a significant increase of capacitance value at a gate voltage of 1 V, because the

pinch off voltage is measured to be 1 V of this device.

5 Conclusions

Introduction of thin AlN binary epitaxial layer promotes a tremendous improvement of 2DEG transport properties in the proposed HEMT structure. The conduction band offset also increases at the hetero interface. There is a significant improvement in 2DEG density with the variation of structural parameters such as thickness of AlGa_N cap layer, thickness of AlN layer and Al mole fraction and also in good agreement with the experimental results available from the literature. With the increase of Al mole fraction from 0.2 to 0.45, the 2DEG concentration increases. At a gate voltage of -4 to -3 V, there is a significant decrease of the capacitance for mole fractions from $x=0.25$ to $x=0.45$ and then maintained constant and represents the high frequency characteristics. With the variation of AlN thickness, there is no significant change in the capacitance of the device. But as the AlGa_N doping concentrations increase keeping the mole fraction into $x=0.3$, it is reported that there is a significant change in the capacitance from gate voltage from -3 to 1 V and then maintained constant and shows the high frequency characteristics.

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