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Exploring the impact of AlGa_N barrier thickness and temperature on normally-on Ga_N HEMT performance

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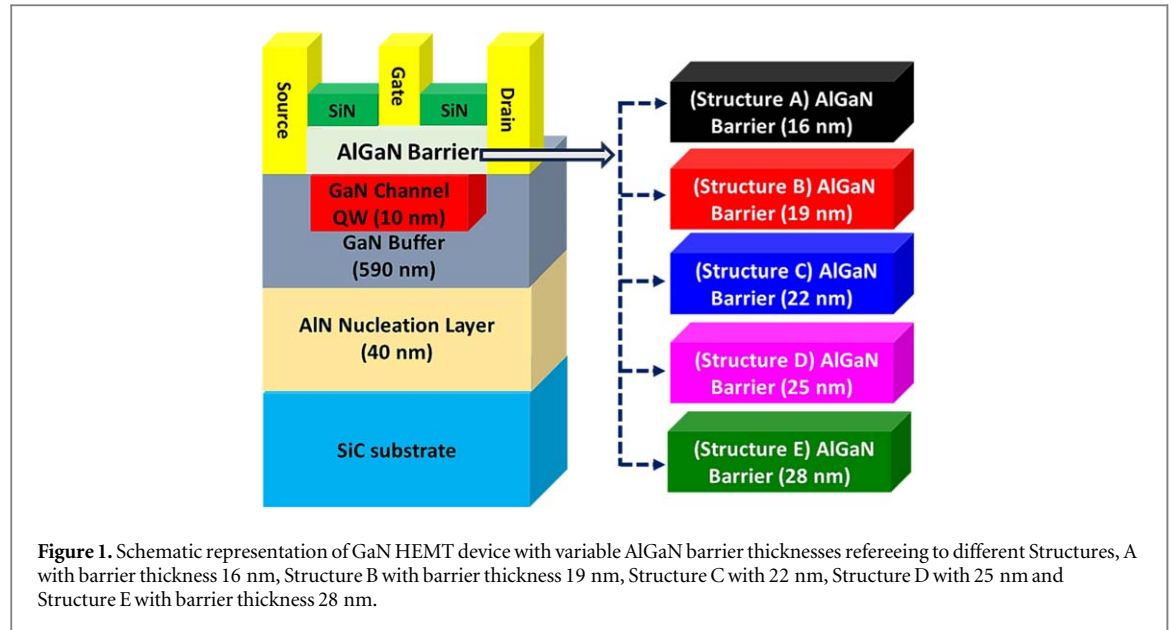
Abstract

We study varying barrier thicknesses in Ga_N/AlGa_N HEMTs as well as the effect of temperature fluctuation on device functionality theoretically. Structures A, B, C, D, and E are designed each with barrier thickness 16 nm, 19 nm, 22 nm, 25 nm, and 28 nm respectively. The impact of barrier thickness on the surface barrier height, strain relaxation and 2DEG concentration is explained including Ga_N HEMT's drain and transfer properties. At elevated temperatures, the polar-optical phonon dispersion is the predominant process. Yet, at lower temperatures, the interface-roughness (IFR) and alloy disorder dispersion both satisfactorily account for the calculated mobilities.

1. Introduction

The superior electrical features of WBG (wide bandgap) semiconducting materials such as Ga_N and SiC make them the preferred choice for power electronic appliances. They are reliable, and efficient, and exhibit reduced thermal restriction compared to silicon technology since their bandgap is up to four times higher than Si [1]. In contrast to SiC, which has greater thermal conductance than both Ga_N and Si, Ga_N systems have a higher saturation on-current as well as an accelerated recovery time [2]. AlGa_N/Ga_N high-electron-mobility transistors (HEMTs) are now at the forefront of investigation for developing the foreseeable future of power electronics. Owing to their exceptional ability to combine minimal channel resistance losses with quick switching, HEMTs have been shown to be a good option for systems requiring high-power switching. AlGa_N/Ga_N HEMTs operate in D-mode (depletion mode), which is a normally-on operation mode, as well as E-mode (enhancement mode), which is a normally-off operation mode. In recent years, numerous methods are being investigated, such as recessed gates [3], p-Ga_N gates [4, 5], fluorine implantation [6], and cascade design [7] to achieve normally-off operation of Ga_N HEMTs. Depending on the application, normally-on or normally-off Ga_N HEMTs are used. In high-frequency applications, normally-off devices are preferable because they offer better control, reduced power consumption, and higher efficiency [8, 9]. Nonetheless, it has been reported in some publications that normally-on Ga_N HEMTs have high-speed switching capabilities [10]. Presently, researchers are working to increase the AlGa_N/Ga_N HEMTs' reliability because of trapping issues that might occur during the operation and, thus, lead to performance losses such as frequency dispersion, gate delay and drain delay transients, as well as reduced microwave power generation [11].

Over the past few years, Gallium Nitride (Ga_N) power transistors have accomplished enormous strides [12]. Due to sufficient polarization-driven surface charge at the heterojunction, undoped AlGa_N/Ga_N double-layers are favored. AlGa_N barrier in Ga_N HEMTs is employed to keep electrons contained in a two-dimensional electron gas (2DEG) layer at the AlGa_N barrier's junction with the Ga_N channel. The device's ability to effectively regulate electron mobility is made possible by this confinement. The selection of AlGa_N for the barrier is crucial because it possesses a wider energy band (6 eV) than Ga_N (3.4 eV) [13, 14]. This broader bandgap aids in sustaining the 2DEG's high electron mobility, which is necessary for HEMTs to function at elevated speeds and frequencies. The greater breakdown voltage of AlGa_N devices (up to 900 V), is a result of their wider bandgap which enables them to withstand larger voltages without breaking down or suffering



damage [15]. The thermal resilience of GaN HEMTs may additionally be increased by the AlGaIn barriers [16]. They aid in decreasing electron capturing and dispersing at elevated temperatures, thus, enabling the device to continue operating at extreme temperatures. With the benefits of the AlGaIn barrier in mind, we studied the thickness variation with its effect on the operation of the HEMTs. To comprehend device operation better, we also investigated temperature effects on the drain characteristics as well as mobility of carriers in GaN HEMTs.

2. Design parameters

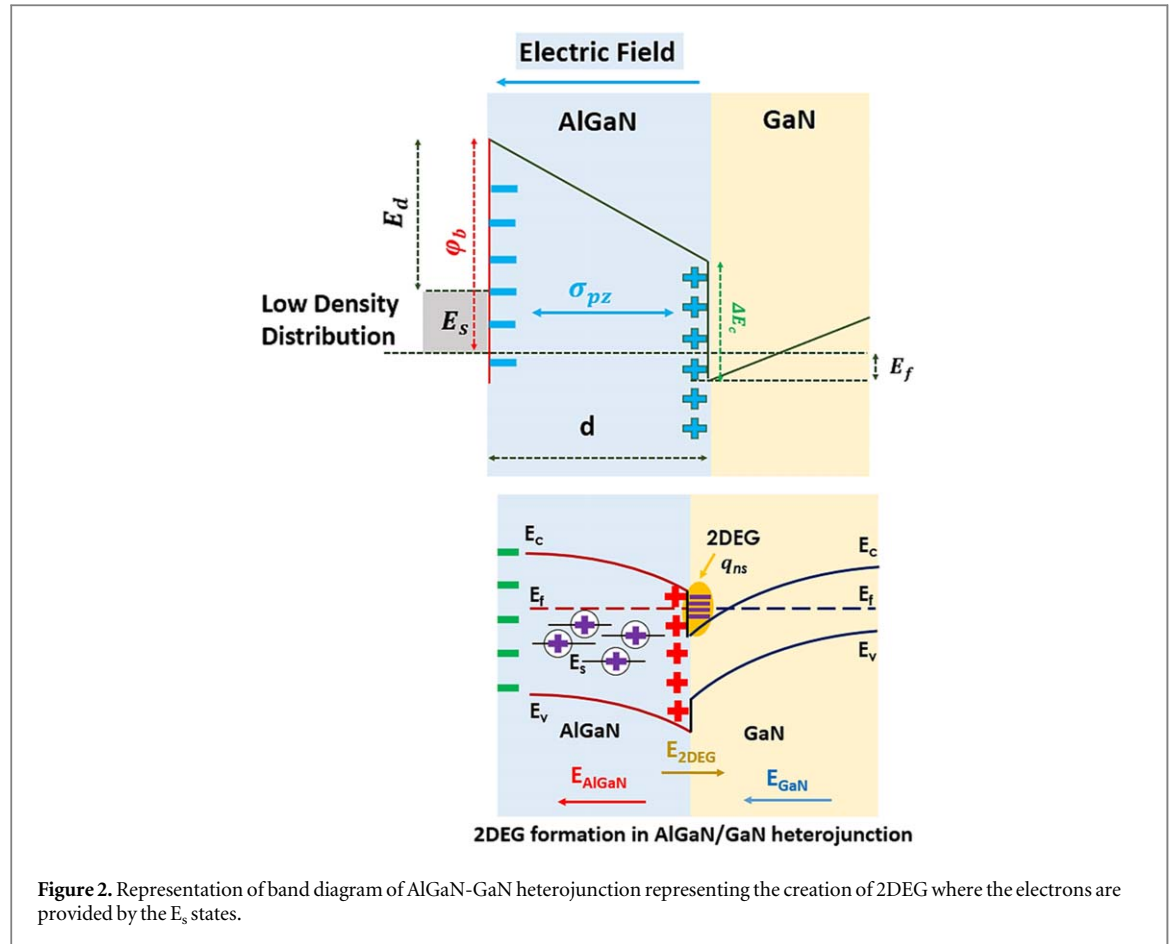
The device structure, as seen in figure 1, was inspired by [17–19] which served as an idea for the geometric dimensions and the epi-layer stack. It comprises of a 500 μm thick SiC substrate [20, 21], an AlN nucleation layer (40 nm thick), a GaN buffer layer (590 nm thick), a local GaN channel layer quantum well (QW) (10 nm thick), and an undoped AlGaIn barrier film with 30% aluminum content). We have five possible structures based on varied barrier thicknesses, namely Structures A, B, C, D and E designed with barrier thickness 16 nm, 19 nm, 22 nm, 25 nm, and 28 nm respectively, as illustrated in figure 1. By managing electron flow, the barrier reduces current leakage and improves performance. The device is protected from corrosion and environmental effects by a protective SiN covering. The source, drain and gate contacts are all ohmic. APSYS simulator is utilized to study the GaN HEMTs in this work. The output current characteristics in our work exhibit a pattern that is comparable to the findings of [22].

3. Results and discussion

3.1. Effects of barrier thickness

In this work, GaN HEMT five structures have been designed and analyzed namely Structure A (with barrier thickness (d_1) 16 nm), Structure B (with barrier thickness (d_2) 19 nm), Structure C (with barrier thickness (d_3) 22 nm), Structure D (with barrier thickness (d_4) 25 nm), and Structure E (with barrier thickness (d_5) 28 nm). The variations in the surface barrier height (SBH), represented by φ_b , and the 2DEG are analyzed with thickness variation in HEMTs. In figure 2, we display the distribution of small-density surface-donor-states (E_s), across a range of energy values, under a specific donor energy level (E_d). The E_d level rises as barrier thickness (d) increases. As thickness of AlGaIn barrier increases, the E_s states get close to the Fermi level and begin transferring electrons to produce 2DEG in the AlGaIn/GaN junction. Owing to the lower surface-donor densities E_s , the SBH ' φ_b ' would be allowed to rise as ' d ' increases [23]. Experimental analysis and computer simulations have reported that the 2DEG concentrations ' q_{ns} ' and SBH ' φ_b ' initially climb directly and then reach saturation as ' d ' increases [24, 25].

The subsequent formula describing the SBH is derived from the Poisson equation with the appropriate boundary conditions while assuming charge neutrality through the barrier layer [23]:



$$\varphi_b = \frac{\left(n_o E_d + \frac{\sigma_{pz}}{q}\right)d + \varepsilon_{AlGaIn} \frac{\Delta E_c}{q^2}}{n_o \left(\frac{d + \varepsilon_{AlGaIn}}{q^2 n_o}\right)} \quad (1)$$

wherein n_o is the number of surface states per unit energy per unit area, E_d denotes the difference between the CBM and the Fermi level, σ_{pz} is the corresponding positive surface charge at the heterojunction, ε_{AlGaIn} is the AlGaIn barrier's permittivity, and ΔE_c represents the conduction band offset. By analyzing this statement, we observe that the barrier height saturates considering enough thick barriers, at the value given below [23]:

$$\varphi_b \approx E_d + \frac{\sigma_{pz}}{qn_o} \quad (2)$$

Poisson's expression for the density of a 2DEG layer may additionally be solved, and the result is the connection shown below [23]:

$$n_s = \frac{\frac{\sigma_{pz}}{q}}{1 + \frac{\varepsilon_{AlGaIn}}{dq^2 n_o}} \left(1 - \frac{d}{d_{cr}}\right) \quad (3)$$

here $d_{cr} = \varepsilon_{AlGaIn}(E_d - \Delta E_c)/\sigma_{pz}q$ is the thickness at which appreciable charge at the junction first appears. Above a particular threshold thickness value, relaxation of strain occurs in the barrier sheet [25]. 2DEG concentration at various thicknesses of the barrier layer have also been reported [26]. This has a substantial impact on reducing the effective polarization. Parallel to this, the piezoelectric polarization steadily decreases. To determine the critical thickness of the AlGaIn barrier layer, we employed the empirical relationship given in [23].

$$d_{crr} = x^k d_o \quad (4)$$

where k is a constant which has a value approximately -1.04 and d_o is approximately equal to 4.17 nm. Since we have employed $Al_{0.3}Ga_{0.7}N$ barrier in our device with $x = 0.3$, this implies that for our device $d_{crr} \approx 15$ nm. This is in consistent with the extracted result of $d_{crr} = 15.5$ nm at aluminum mole fraction $x = 0.29$ [23, 25]. It is generally accepted that piezoelectric and spontaneous polarizations combine to form the overall polarization charge in the AlGaIn/GaN heterostructure. Additionally, because AlGaIn's piezoelectric polarization is specifically linked to lattice strain, varying barrier thickness and ultimately strain relaxation has a significant

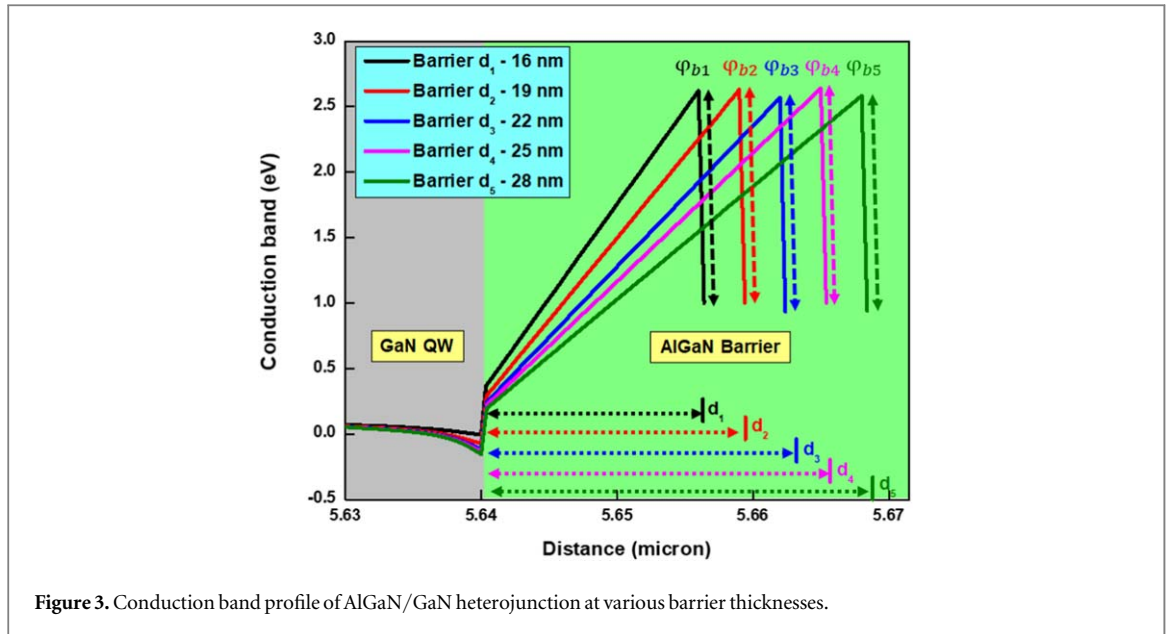


Figure 3. Conduction band profile of AlGaIn/GaN heterojunction at various barrier thicknesses.

impact on it. However, it has been established that spontaneous polarization does not depend on the AlGaIn barrier thickness meaning that strain relaxation has no impact on it. The piezoelectric polarization ' P_p ' might be represented as:

$$P_p = 2 \left(\frac{a_{AlGaIn}}{a_{GaN}} - 1 \right) \left(e_{31} - e_{33} \frac{C_{13}}{C_{33}} \right) \quad (5)$$

here C_{33} and C_{13} are elastic constants and e_{33} , e_{31} represents piezoelectric coefficients while a_{AlGaIn} and a_{GaN} defines the lattice constants of AlGaIn and GaN respectively. The spontaneous polarization is given by:

$$P_s = -0.052x - 0.029 \quad (6)$$

As the barrier thickness increases beyond the critical thickness, Bykhovski *et al* [27] demonstrated that overall strain-induced polarization decreases exponentially as the barrier thickness ' d ' increases. Thus, at $d > d_{crr}$ the remaining strain might be represented as:

$$S_r = S_{crr} \exp \left(1 - \frac{d}{d_{crr}} \right) \quad (7)$$

in which S_{crr} denotes the critical strain at relaxation's beginning. Moreover, when $d > d_{crr}$ the associated effective piezoelectric polarization changes to:

$$P_p = 2S_r \left(\frac{a_{AlGaIn}}{a_{GaN}} - 1 \right) \left(e_{31} - e_{33} \frac{C_{13}}{C_{33}} \right) \quad (8)$$

Conduction band for various AlGaIn thicknesses are visually depicted in figure 3 indicating that increasing AlGaIn barrier thickness tends to increase barrier height. Larger barrier height leads to a low gate leakage current and better confinement of charge carriers within the GaN channel. As discussed earlier, AlGaIn's piezoelectric polarization is specifically linked to lattice strain which greatly depends on barrier thickness. As the barrier thickness increases, the lattice strain decreases, thus, strain relaxes. Consequently, this results in less piezoelectric polarization at AlGaIn/GaN interface [27]. This information enables researchers to optimize GaN HEMT structures. Furthermore, increasing barrier thickness increases 2DEG concentration, which can result in higher output current as evident from figure 5 and, hence, can lead to faster switching of GaN HEMTs [28].

The field diagram is shown in figure 4. As a result of a decrease in effective polarization, we see that the effective field is lowered with increasing thickness. The 2DEG concentration (n_{2DEG}) grows when the barrier thickness rises as evident from the deeper quantum well as depicted in figure 4 [29]. In AlGaIn/GaN HEMTs, polarization Coulomb field (PCF) scattering is linked to n_{2DEG} [30]. The n_{2DEG} will change depending on the thickness of AlGaIn barrier, and this will influence the PCF scattering. Since Structure A's AlGaIn barrier layer is thin (16 nm), thus, at the same V_{GS} value, the electric field is more powerful (up to $14 \times 10^6 \text{ V m}^{-1}$) and the strain brought on by the inverse piezoelectric effect (IPE) is larger. As a result, there will be a more noticeable change in polarization charge, resulting in more polarized charges being produced underneath the gate. Structure E has a thick barrier (28 nm), thus, at the similar gate bias the electric field in the AlGaIn barrier is relatively weaker (up to $8 \times 10^6 \text{ V m}^{-1}$) due to weak IPE caused by larger strain relaxation. Hence, less

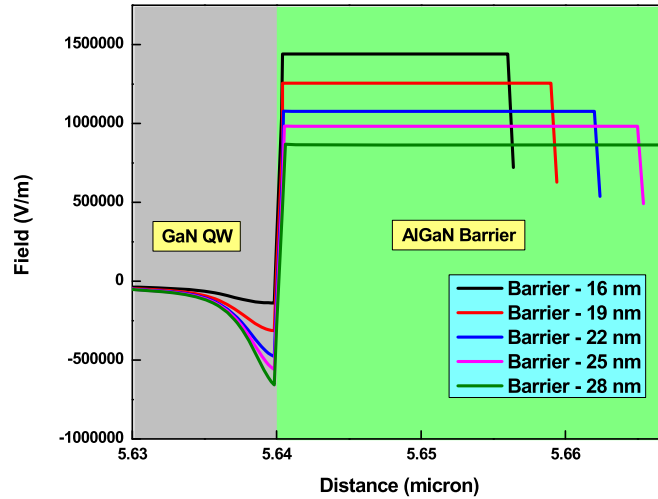


Figure 4. Field distribution at AlGaIn/GaN heterojunction at different barrier thicknesses.

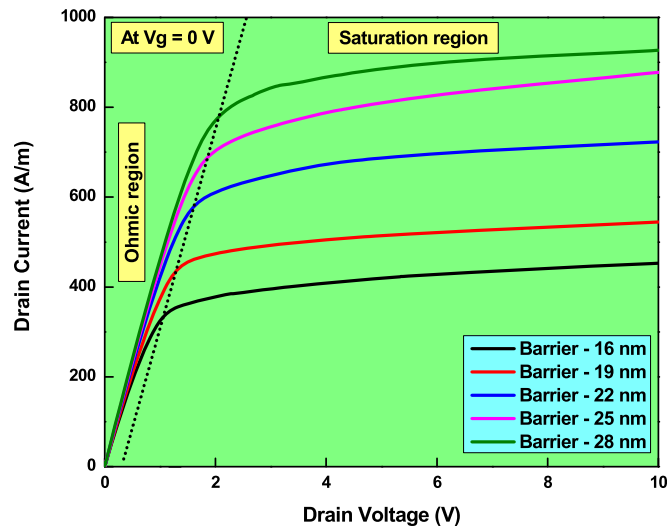


Figure 5. Drain characteristics of AlGaIn/GaN HEMT at various barrier thicknesses.

polarization charges will be induced underneath the gate. Consequently, when considering extra polarization-induced charges, thickening the AlGaIn barrier will reduce the PCF scattering. Ultimately, higher n_{2DEG} will lead to larger output currents, as shown in figure 5 and figure 6.

It is depicted in figure 5 that Structure A with thin barrier (16 nm) has relatively lower drain current ($I_d = 400 \text{ A m}^{-1}$) while structure E with thick barrier (28 nm) has relatively higher drain current ($I_d = 900 \text{ A m}^{-1}$) at the same gate bias ($V_g = 0 \text{ V}$). Because thick barriers have less PCF scattering and thin barriers have more PCF scattering, thick barriers have higher output currents as explained above. Because of a stronger electric field and more strain, Structure A's thin AlGaIn barrier layer generates more polarized charges leading to more PCF scattering, but Structure E's thicker barrier decreases PCF scattering due to comparatively lower electric field and less strain and ultimately, increases output currents. Figure 6 follows the same trend for similar reasons. The larger drain current indicates that the device has a high saturation velocity [31]. High saturation velocity in GaN HEMTs is a critical element that allows these devices to succeed in high-frequency and high-power applications.

3.2. Effects of Temperature on device performance

GaN HEMTs' properties are influenced by the temperature, especially in GaN channel, where the temperature dependence of mobility plays a significant role. The mean velocity of carriers travelling under the effect of an electric field, as measured via the dispersion process, is referred to as electron mobility (μ). The time of relaxation τ , can be used to get the value of ' μ ' [32].

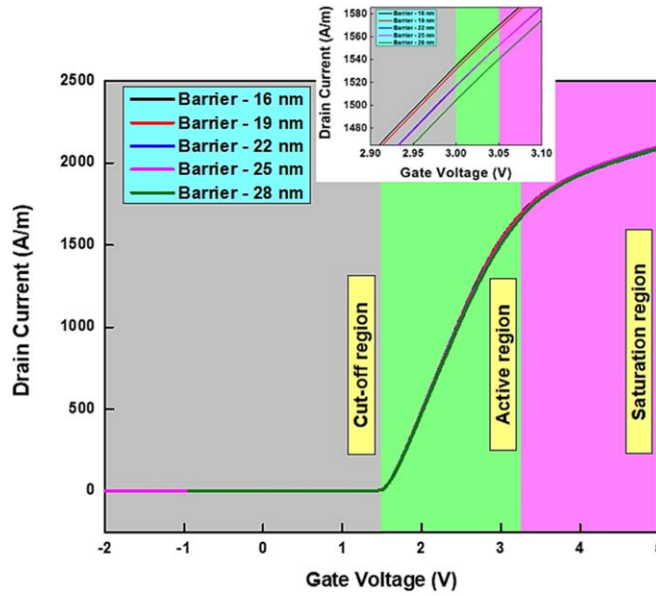


Figure 6. Transfer characteristics of AlGaIn/GaN HEMT at different barrier thicknesses.

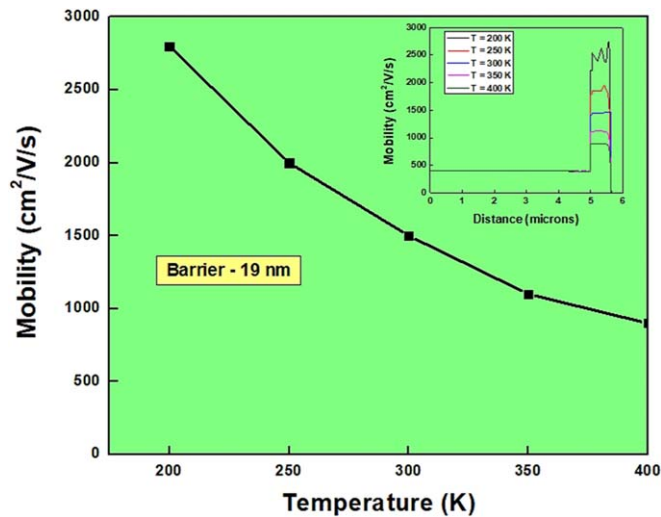


Figure 7. Temperature dependence of mobility for GaN HEMT.

$$\mu = q \frac{\langle \tau \rangle}{m^*} \quad (9)$$

m^* represents the effective mass of the charge carrier. Mobility in the GaN channel is primarily characterized by three scattering processes: interface roughness, alloy disorder, and polar optical phonon dispersion [33]. Figure 7 illustrates how the device's mobility steadily decreases as temperature rises. Alloy irregularity and interface roughness dispersion processes are the main factors limiting low-temperature mobilities [34–36]. It is widely acknowledged that a 2DEG develops in the GaN channel next to the AlGaIn barrier. The phrase 'alloy disorder scattering' refers to the dispersion of such electrons via the conduction band imbalance. In AlGaIn-GaN HEMTs, alloy disorder dispersion is primarily caused by two factors: First, the barrier layer is made of AlGaIn, a ternary alloy with a particular alloy misfit. The second explanation is that, as a result of a quantum effect, the 2DEG wavefunction passes through the AlGaIn barrier. Apparently, an alternative binary substance must be utilized for the barrier, or the penetration has to be impeded in order to lessen or eliminate this effect. The mobility representation of alloy disorder dispersion with no screening influences was described by Kearley and Horrell in [37]

$$\mu_{\text{alloy}} = \frac{16}{3b} \frac{e \left(\frac{h}{2\pi} \right)^3}{x(1-x)m^{*2}\Omega_o U_{AL}^2} \quad (10)$$

wherein Ω_o represents the space filled by one atom, x represents the alloy mole percent, and U_{AL} represents the alloy potential. Another important problem that significantly affects semiconductor heterojunctions is junction roughness. It can come through well-width variations or alloy variations, both of which can cause the electron's confining energy to change. The impact is more pronounced in narrower wells wherein changes in the well width of certain monolayers cause significant changes in the quantized energy. The wavefunction along with the energy levels are altered by spatial differences in junction roughness. The local potential for dispersion of electrons is produced by these potential fluctuations, which implies that electron dispersion is greatest for those that are nearest to the junction. The formula for the mobility of contact roughness dispersion is [35]

$$\mu_{IFR} = \left(\frac{2\varepsilon_o\varepsilon_s}{n_{2D}\Delta} \right)^2 \frac{\left(\frac{h}{2\pi} \right)^3}{e^3 m^{*2} J_{IFR}(k)} \quad (11)$$

where Δ is the distance between fluctuations' correlations and Δ is the roughness' lateral dimension. The definition of the integral J_{IFR} mentioned in the above equation is given as:

$$J_{IFR} = \int_0^{2k} \frac{e^{-\frac{q^2}{4}}}{2k^3(q+q_s)^2 \sqrt{1 + \left(\frac{q}{2k} \right)^2}} q^4 dq \quad (12)$$

where q_s represents screening constant. At lower temperature, the impacts of alloy disorder and interface scattering are lower because the temperature is reduced hence there are less atomic vibrations at the junction resulting in less dispersion. Furthermore, in our device, the barrier layer and channel layer only have one interface; as a result, alloy disorder and interface roughness dispersion will be reduced. As is evident from figure 7, this prompts electron mobility to rise at lower temperatures. These scattering mechanisms often have a greater influence on GaN HEMTs with two barriers [33]. It is evident from figure 7 that at 200 K the electron mobility has a value approximately equal to $2,810 \text{ cm}^2(\text{Vs})^{-1}$ and at 250 K it is near to $2,000 \text{ cm}^2(\text{Vs})^{-1}$.

The impacts of interface roughness as well as alloy disorder dispersion processes have just a small bearing on mobility at elevated temperatures, when the polar-optical phonon dispersion is the dominating mechanism [34, 36]. The mobility of 2D transport at elevated temperatures is primarily constrained by polar-optical phonon dispersion, which is one of the key elements influencing electron transport properties in polar semiconductor devices. Ridley provides the following expression for mobility that is constrained by polar-optical phonon dispersion [38]:

$$\mu_{po} = \frac{4\pi\varepsilon_o\varepsilon_p}{e\omega m^{*2}Z_o} \left(\frac{h}{2\pi} \right)^2 [e^{\frac{\hbar\omega}{kT}} - 1] \quad (13)$$

wherein

$$\frac{1}{\varepsilon_p} = \frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s} \quad (14)$$

In this case, ε_s and ε_∞ represents the low and high-frequency dielectric constants respectively while $\hbar\omega$ shows the polar-optical phonon energy. Additionally, the hall mobility is the combined result of bulk electrons as well as 2D electrons. With the use of Hall effect approach the possible way to represent the measured carrier mobility & density is [39]:

$$\mu_M n_M = \mu_{2DEG} n_{2DEG} + \mu_{buf} n_{buf} \quad (15)$$

here μ_M and n_M are the measured 2DEG sheet mobility and density, μ_{2DEG} and n_{2DEG} represents the actual 2DEG sheet mobility and density while μ_{buf} and n_{buf} values represent the carrier mobility and concentration of bulk electrons dispersed throughout the GaN buffer layer. The mobilities of bulk electrons traveling in three dimensions are less than that of 2D electrons. In GaN HEMT, shallow donor defects within the GaN buffer layer become ionized at elevated temperatures, which consequently increases background carrier concentration. In the meantime, when the temperature rises, certain channel electrons with enough energy can escape the potential well and transform into 3D electrons having lower mobility, and this has a significant impact upon the hall mobility of the entire material structure. These results can be clearly seen in figure 7. At $T = 300 \text{ K}$, the mobility is near to $1,500 \text{ cm}^2(\text{Vs})^{-1}$ and as the temperature increases to 350 K , the mobility value further reduces to approximately $1,100 \text{ cm}^2(\text{Vs})^{-1}$ while at $T = 400 \text{ K}$, the mobility is almost $800 \text{ cm}^2(\text{Vs})^{-1}$.

Figure 8 represents the drain characteristics of our device. It can be seen that the drain current decreases with increasing temperature. The drain current is $\sim 820 \text{ A m}^{-1}$ at $T = 200 \text{ K}$ and $\sim 640 \text{ A m}^{-1}$ at $T = 250 \text{ K}$. The drain current drops to about $\sim 430 \text{ A m}^{-1}$ when the temperature rises to 300 K . Like this, it is $\sim 400 \text{ A/m}$ at $T = 350 \text{ K}$

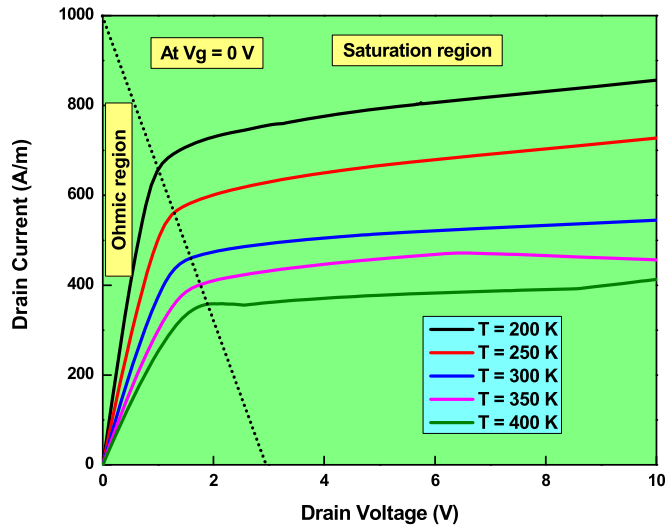


Figure 8. Drain characteristics of GaN HEMT at different temperatures.

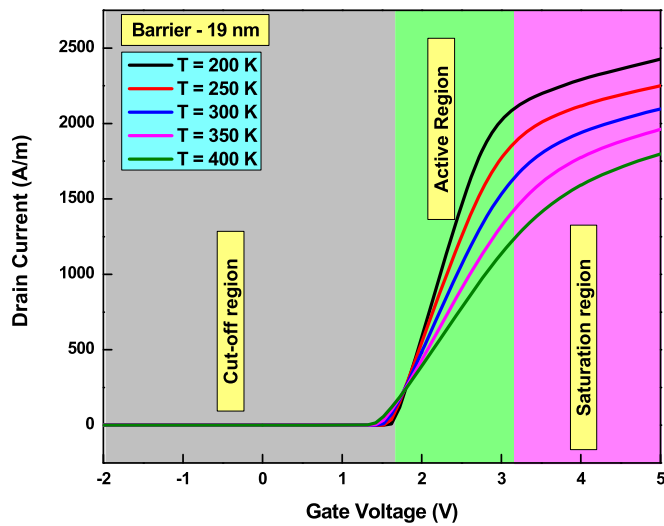


Figure 9. Transfer characteristics of GaN HEMT at various temperatures.

and over 380 A m^{-1} at $T = 400 \text{ K}$. Low drain currents with respect to drain voltage (figure 8) and gate voltage (figure 9) at higher temperatures result from lower mobilities due to optical phonon scattering phenomena [34, 36, 38]. Three-dimensional bulk electron mobility is smaller than that of two-dimensional electron mobility [33]. At high temperatures, the concentration of background carriers increases due to ionization of shallow donor defects in the GaN buffer layer. Thus, increase in temperature affects the mobility of the material structure because channel electrons with sufficient energy can escape the potential well and change into 3D electrons with less mobility [33]. Further rise in temperature leads to a further decrease in mobility. The drain current is greatly dependent on mobility of carriers as can be seen from the equation below:

$$I_{DS} = d\mu q n_{2DEG}(x) \frac{dV(x)}{dx} \quad (7a)$$

where ' d ' represents channel thickness, and ' μ ' is the carrier mobility. The drain current is higher at lower temperatures due to greater mobility, while the drain current is lower at higher temperatures due to decreased mobility in figures 8 and 9. In conclusion, the aforementioned events cause the carrier mobility to diminish at high temperatures and decreased output currents.

4. Conclusion

We discussed how surface barrier height, polarization charge, strain relaxation, and 2DEG concentration are impacted by barrier thickness. Increase in barrier thickness has been observed to result in higher surface barriers. Also, once a critical thickness is reached, strain relaxation occurs. With an Al mole fraction of 0.3 in the AlGa_N barrier, we were able to determine the critical thickness value for our device, which is roughly 15 nm. Further, temperature effects on the functionality of the device are presented in terms of polar-optical phonons, alloy disorder, and interface-roughness dispersion. The polar-optical phonon dispersion is the main mechanism at elevated temperatures. However, at lower temperatures, the measured mobilities can be effectively explained by both the IFR and alloy disorder dispersion.

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Data availability statement

The data cannot be made publicly available upon publication due to legal restrictions preventing unrestricted public distribution. The data that support the findings of this study are available upon reasonable request from the authors.

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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