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Theoretical Study of InAlN/GaN High Electron Mobility Transistor (HEMT) with a Polarization-Graded AlGaN Back-Barrier Layer

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Abstract: An inserted novel polarization-graded AlGaN back barrier structure is designed to enhance performances of In_{0.17}Al_{0.83}N/GaN high electron mobility transistor (HEMT), which is investigated by the two-dimensional drift-diffusion simulations. The results indicate that carrier confinement of the graded AlGaN back-barrier HEMT is significantly improved due to the conduction band discontinuity of about 0.46 eV at interface of GaN/AlGaN heterojunction. Meanwhile, the two-dimensional electron gas (2DEG) concentration of parasitic electron channel can be reduced by a gradient Al composition that leads to the complete lattice relaxation without piezoelectric polarization, which is compared with the conventional Al_{0.1}Ga_{0.9}N back-barrier HEMT. Furthermore, compared to the conventional back-barrier HEMT with a fixed Al-content, a higher transconductance, a higher current and a better radio-frequency performance can be created by a graded AlGaN back barrier.

Keywords: In_{0.17}Al_{0.83}N/GaN HEMT; graded-polarization; back barrier; parasitic electron channel; electron confinement

1. Introduction

Over the years, gallium nitride (GaN) which is a typical representative of third-generation wide bandgap semiconductor materials, has attracted enormous interest due to it having a high critical electric field, electron gas owing to polarization, higher electron mobility and saturation velocity [1–3]. Therefore, the GaN-based high electron mobility transistors (HEMTs) allows us to achieve higher breakdown voltage, lower on-resistance and high operation switching frequency [4–6]. Considering the reliability problems of AlGaN/GaN HEMTs, which are caused by lattice defects due to lattice mismatch and piezoelectric effect at the AlGaN/GaN heterojunctions [7–9], an AlInN barrier layer has attractively replaced a commonly applied AlGaN barrier layer to improve performances of GaN-based HEMTs. The In_xAl_{1-x}N is lattice matched to GaN when the Al composition of In_xAl_{1-x}N is 0.83 [10]. Thus, a significantly higher two-dimensional electron gas (2DEG) density can be induced by spontaneous polarization at In_{0.17}Al_{0.83}N/GaN interface and the HEMT's reliability can be enhanced [6,11–14]. An additional thin AlN interlayer is set between the AlInN barrier layer and the GaN channel layer to further improve performances of the In_{0.17}Al_{0.83}N/GaN HEMT. The AlN can increase discontinuity of the conduction band at heterojunction interface due to its larger forbidden band width, which plays a dominant factor for the significant increase of 2DEG concentration [15]. In addition, the AlN in In_{0.17}Al_{0.83}N/GaN heterojunction interface can reduce the alloy scattering which increases the mobility of the device [16]. Although the proposed InAlN/AlN/GaN structure has the stated advantages, part

of the 2DEG will spill from the channel into the buffer layer, resulting in the reduction of mobility and reliability. It can be explained that GaN is both a buffer layer and a channel layer in a single heterojunction structure [17]. The most direct way to enhance the confinement of heterojunction 2DEG and suppress the overflow of carriers into the buffer layer is to use a back barrier, which constitutes a double heterojunction structure. Recently, many researches have reported on effects of the AlGaIn back-barrier layers on the HEMTs with the double heterojunction structures [18–21]. To some extent, it can enhance carrier confinement but also produce an unwanted parasitic channel at the AlGaIn back-barrier/GaN buffer interface. According to our previous works [22,23], the graded AlGaIn back-barrier with Al content changing linearly from 0 to 0.1 can weaken the polarization between AlGaIn and GaN buffer layer, and reduce the adverse effect of parasitic channel.

In this work, we propose a conventional $\text{In}_{0.17}\text{Al}_{0.83}\text{N}/\text{AlN}/\text{GaN}$ structure with a 25 nm-thick $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back-barrier layer that can improve confinement of the channel, but a parasitic channel would be generated at the $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ barrier/GaN buffer interface. Therefore, a polarization-graded AlGaIn back barrier replaces the $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back barrier to reduce the harm of parasitic channel. The Al composition of graded AlGaIn back-barrier layer near the side of GaN main channel is 0.1, and gradually reduces to 0 far away from the main channel. Numerical simulations can support the design of non-conventional devices in a short time, and a large amount of works on devices have been investigated by Atlas-Silvaco physical simulation [24–29]. The electron distributions and the conduction band profiles of HEMTs with an $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back-barrier and a graded back-barrier are calculated by Atlas-Silvaco physical simulator. The influences of two structures on performances of the HEMTs are compared theoretically. The results indicate that confinement of 2DEG can be effectively enhanced by a polarization-graded back barrier. In addition, the electron concentration in the parasitic channels can be weakened by the AlGaIn back barrier layer with a gradient of polarization. It is beneficial for the improvement of transconductance, drain current, current gain cut-off frequency and power gain cut-off frequency, compared with the conventional $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back-barrier HEMT.

2. Device Description and Physical Models

Figure 1a,b shows the schematic cross-sectional diagram of the designed conventional HEMTs with an $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back barrier and a polarization-graded AlGaIn back barrier. The epitaxial structure of an $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back-barrier HEMT was composed of a 2 μm unintentionally n-type doped GaN buffer layer, with a background carrier concentration of $1 \times 10^{16}\text{cm}^{-3}$ [30], a 1 nm AlN space layer, a 10 nm undoped $\text{In}_{0.17}\text{Al}_{0.83}\text{N}$ barrier layer, a 14-nm-thick GaN channel and a 25 nm undoped $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back-barrier layer. Compared with the conventional back-barrier structure, the optimized structure introduced a 25 nm graded AlGaIn back barrier with Al content linearly changing from 0% (bottom) to 10% (top) along the epitaxial growth. In both structures, Ohmic contacts were formed in the source and drain terminals. The distance of gate–source, gate–drain, and length of gate were 0.5 μm , 10 μm , and 2 μm , respectively. The device surface was passivated by using Si_3N_4 thin film to reduce the current collapse effect in the HEMT [31]. For all the simulations, donor trap was introduced at the $\text{In}_{0.17}\text{Al}_{0.83}\text{N}$ with a trap level of 0.42 eV and a density of $3.86 \times 10^{13}\text{cm}^{-3}$ [32], while acceptor trap was considered in the unintentional doped (UID) GaN buffer with a trap level of 0.4 eV below the conduction band and a trap density of $1 \times 10^{17}\text{cm}^{-3}$.

Figure 1. Schematic diagram of the designed lattice-matched $\text{In}_{0.17}\text{Al}_{0.83}\text{N}/\text{GaN}$ high electron mobility transistor (HEMT) structure (a) with an $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back barrier and (b) with a graded AlGaIn back barrier.

During the two-dimensional numerical calculation, the drift-diffusion transport model as well as several important physical models such as Fermi-Dirac, low field electron mobility, high field mobility, Shockley–Read–Hall (SRH) and polarization were used to simulate the device response. The physical parameters of GaN, AlN, $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ and $\text{In}_{0.17}\text{Al}_{0.83}\text{N}$ during the simulation are shown in Table 1 [33–36].

Table 1. Parameters of GaN, AlN, $\text{Al}_{0.83}\text{In}_{0.17}\text{N}$, $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ in the simulation.

Parameter	GaN	AlN	$\text{Al}_{0.83}\text{In}_{0.17}\text{N}$	$\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$
Band gap (eV)	3.42	6.15	4.62	3.58
Permittivity	10.28	10.31	11.04	10.28
Hole mobility (cm^2/Vs)	22	14	82	-
Saturated velocities (v_{sat}) for electrons (10^7 cm/s)	2.0	2.17	1.1	-
Spontaneous polarization, P_{sp} (C/m^2)	−0.034	−0.090	−0.072	−0.038

The two mobility models have been used to consider various types of scattering mechanisms [37]. The low field mobility model can be given by [34]:

$$\frac{1}{u(N,T)} = a \left(\frac{N}{1 \times 10^{17}} \right) \left(\frac{T}{300} \right)^{-\frac{3}{2}} \times \ln \left[1 + 3 \left(\frac{T}{300} \right)^2 \left(\frac{N}{1 \times 10^{17}} \right)^{-\frac{2}{3}} \right] + b \left(\frac{T}{300} \right)^{\frac{3}{2}} + \frac{c}{\exp\left(\frac{1065}{T}\right) - 1} \quad (1)$$

where $a = 2.61 \times 10^{-4} / \text{V} \cdot \text{s} \cdot \text{cm}^{-2}$, $b = 9.8 \times 10^{-4} / \text{V} \cdot \text{cm}^{-2}$ and $c = 1.7 \times 10^{-2} / \text{V} \cdot \text{s} \cdot \text{cm}^{-2}$. $u(N,T)$ is the mobility as a function of doping and ambient temperature, N is the total doping concentration, and T is the ambient temperature.

The high field mobility model can be specified as below [38]:

$$u(E) = \frac{u(N,T) + v_{sat} \frac{E^{(N_1-1)}}{E_c^{N_1}}}{1 + a_n \left(\frac{E}{E_c} \right)^{N_2} + \left(\frac{E}{E_c} \right)^{N_1}} \quad (2)$$

where $u(N,T)$ is the low field mobility, v_{sat} is saturation velocities, and E is the electric field. The values of E_c , a_n , N_1 , and N_2 can be referred to [38].

SRH and Fermi–Dirac statistics are also considered. SRH recombination occurs when an electron gets trapped, referring to a trap-assisted recombination process. In order to investigate the specific

physical mechanism of electron trapping, electron trapping process of each trap level should be calculated in the SRH recombination model. The rate of electron trapping [38–41] is given by

$$R_{net}^{SRH} = \frac{pn - n_{ie}^2}{\tau_p [n + n_{ie} \exp(\frac{E_{trap}}{kT})] + \tau_n [p + n_{ie} \exp(\frac{-E_{trap}}{kT})]}, \quad (3)$$

where E_{trap} is the difference between the trap energy level and intrinsic Fermi level, n_{ie} is intrinsic carrier concentration, and T is the lattice temperature. τ_n and τ_p are the lifetimes of electrons and holes, respectively, both of which are assumed to be 10^{-9} s.

Polarization modeling is critical for GaN based devices. Here, P_{PE} and P_{SP} represent the piezoelectric polarization and spontaneous polarization, respectively. The total polarization-induced polarization charge density is defined as [35]:

$$P_{total} = [P_{PE}(bottom) + P_{SP}(bottom)] - [P_{PE}(top) + P_{SP}(top)] \quad (4)$$

Since $\text{In}_{0.17}\text{Al}_{0.83}\text{N}/\text{GaN}$ is lattice-matched and the graded back barrier layer is assumed as complete lattice relaxation, the sum of polarization in the device is spontaneous polarization without any piezoelectric polarization. A space polarization-induced charge would be generated by a gradient of polarization of the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ back barrier which varies along the growth direction. The corresponding density is given by [42,43]:

$$\rho P = -\nabla \cdot P = -\frac{\partial P}{\partial Z}. \quad (5)$$

With

$$P = P_{sp}(\text{Al}_x\text{Ga}_{1-x}\text{N}) = xP_{sp}(\text{AlN}) + (1-x)P_{sp}(\text{GaN}). \quad (6)$$

3. Results and Discussion

The conduction band diagrams of two different structures with back barrier under zero bias voltage calculated by two-dimensional self-consistent simulations are shown in Figure 2. The conduction band diagram of a conventional HEMT was simulated to observe the conduction band discontinuity caused by a back-barrier layer. It is obvious that the back barrier can raise the conduction band edge of the side of the potential well and enhance confinement of the heterojunction 2DEG. Comparing with the HEMT with a single heterojunction structure, the conduction band edge of the potential well of the device with an $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back barrier is increased by 0.69 eV, while the structure with an Al-graded back barrier is increased by 0.46 eV. Furthermore, the depth of electron potential well of the parasitic electron channel at interface of AlGaIn/GaN in the polarization-graded AlGaIn back-barrier HEMT is shallower than that of the device with an $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back barrier. The results are attributed to a gradient of polarization of AlGaIn , which results in the complete lattice relaxation in the graded AlGaIn back barrier without any piezoelectric polarization.

Figure 3 shows the carrier distributions of the three different structures, it is evident that at the AlN/GaN interface generates the primary quantum well. The electron concentration of the conventional HEMT, graded back-barrier HEMT and back-barrier HEMT were about $11 \times 10^{19} \text{cm}^{-3}$, $8.81 \times 10^{19} \text{cm}^{-3}$, and $8.8 \times 10^{19} \text{cm}^{-3}$, respectively. Moreover, a shallower secondary quantum well was also produced at the interface between the AlGaIn layer and the GaN buffer layer, demonstrating the formation of a conductive parasitic channel. It is obvious from the inset of Figure 3 that the 2DEG concentration of secondary quantum well in the graded AlGaIn back-barrier HEMT was about $0.1 \times 10^{19} \text{cm}^{-3}$, lower than that of the secondary quantum well in the AlGaIn back-barrier HEMT with 2DEG concentration of $0.2 \times 10^{19} \text{cm}^{-3}$. Compared to the HEMT with a single heterojunction, the electron distribution of the main channel was narrowed due to a back-barrier layer, while the carrier distribution of the structure with a fixed Al-composition back barrier layer was narrower than that of the structure with a graded Al-composition back-barrier layer. In other words, the structure

with a graded Al-composition contributes to the improved confinement of 2DEG and the weakening of the generation of parasitic channels.

Figure 2. The conduction band diagrams of the $\text{In}_{0.17}\text{Al}_{0.83}\text{N}/\text{AlN}/\text{GaN}$ HEMT, HEMTs with graded back-barrier layer and $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back-barrier layer under zero applied voltage.

Figure 3. The electron concentration distributions of the $\text{In}_{0.17}\text{Al}_{0.83}\text{N}/\text{AlN}/\text{GaN}$ HEMT, the graded back-barrier HEMT and the $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back-barrier HEMT. The inset shows the electron concentration in the parasitic channel at $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interface.

Figure 4 specifically illustrates the two-dimensional contour map of the electron distribution inside the two HEMTs with different structure. Figure 4a,b corresponds to the polarization-graded AlGa_N back-barrier HEMT and the $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back-barrier HEMT, respectively. It can be seen that the electron concentration at the AlN/GaN interface was the highest, and formed a 2DEG potential well, which is consistent with the results shown in Figures 2 and 3. Figure 4a,b shows that the enhanced 2DEG confinement was obtained by introducing a back-barrier layer due to the creation of an obvious conduction band discontinuity. The electron concentration at 25 nm (GaN/AlGa_N) shown in Figure 4a is higher than that in Figure 4b, while that at the 50 nm (AlGa_N/GaN) is lower than Figure 4b. This is because the gradual change of the Al composition in AlGa_N back barrier weakened the polarization effect between AlGa_N back-barrier layer and GaN buffer layer.

Figure 4. Structure chromaticity plots of the electron concentration distributions inside the two different HEMT structures with (a) a graded AlGaIn back barrier and (b) an $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back barrier.

Figure 5 displays the transfer characteristics of the two different structures at $V_{ds} = 5$ V. It was found that the maximum saturation current and transconductance of the graded back-barrier HEMT can be increased compared with that of the $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back-barrier HEMT. Figure 5a shows the curves of V_g - I_d (the threshold voltages are about -4.5 V and -4 V) corresponding to the graded back-barrier HEMT and the $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back-barrier HEMT, respectively, which shifted negatively. The reason is that the back-barrier layer generates a negatively polarization field and then the 2DEG are confined in a narrower potential well. In addition, the threshold voltage negatively shifts about 0.5 V due to attenuation of the negatively polarization field in the polarization-graded AlGaIn back barrier and weaker confinement of carriers in the main channel, compared with that of the $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back-barrier HEMT. The variations in G_m with V_g for two devices are depicted in Figure 5b. The structure with a graded back barrier shows the G_m peak value of 304 mS/mm at $V_{gs} = -1.75$ V, which is higher than that of the structure with an $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back-barrier (295 mS/mm at $V_{gs} = -1.5$ V), indicating that an improved control of drain current by the gate voltage was obtained in the polarization-graded one. The increase in the peak transconductance results from the fact that the gradual Al composition can weaken the effect of the parasitic channel on the main channel and increase the mobility of the 2DEG.

Figure 5. Calculated (a) gate voltage–drain current (V_g - I_d) and (b) gate voltage–transconductance (V_g - G_m) transfer characteristics at drain voltage of 5 V for the HEMTs with a grade back barrier and an AlGaIn back barrier.

Figure 6 represents the current-voltage (I_d - V_d) output characteristics at V_g from 0 V to -5 V for the two devices. The density of the maximum drain saturation current of 1.25 mA/mm was obtained at $V_{gs} = 0$ V in a graded back-barrier HEMT, which was about 13.6% higher than that of the $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back-barrier HEMT (1.1 mA/mm at $V_{gs} = 0$ V). The larger drain current in a graded back-barrier HEMT

was mainly due to the lower threshold voltage shown in Figure 5a, while the concentrations of electron in the graded back-barrier HEMT and the conventional $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back-barrier HEMT were nearly the same.

Figure 6. The drain voltage–drain current (V_d – I_d) output characteristics at gate voltage from 0 V to –5 V for the two HEMT structures with (a) a graded AlGa_N back barrier and (b) an $\text{Al}_{0.1}\text{Ga}_{0.9}\text{N}$ back barrier.

Based on the small-signal AC simulation, the frequency characteristics of the devices are discussed. The variations in the f_{max} and f_T regarding to the change of gate voltage for the two HEMTs are shown in Figure 7. It can be seen that the RF performance was improved by a gradual Al-composition in the AlGa_N back barrier. The device with a graded back barrier achieved a peak value of current gain cutoff frequency of 5 GHz and a peak value of power gain cutoff frequency of 19 GHz, which were both higher than that of the conventional one. The reasons for this result are mainly due to the higher transconductance and the higher output resistance resulting from a graded polarization in the AlGa_N back barrier.

Figure 7. Simulated radio-frequency (RF) performance of the two devices at 8 V drain voltage.

4. Conclusions

In summary, a lattice-matched $\text{In}_{0.17}\text{Al}_{0.83}\text{N}/\text{AlN}/\text{GaN}$ HEMT with a polarization-graded AlGaIn back barrier is proposed by two-dimensional analysis of Atlas drift-diffusion simulations. The improved performance of the graded back-barrier HEMT is systematically demonstrated by comparing to the HEMT with an AlGaIn back barrier. The electron confinement in the channel is enhanced effectively by introducing a back barrier, resulting in the improved performance of the device. In addition, a gradient of polarization in the back barrier can reduce the 2DEG concentration in the parasitic channel and weaken adverse effect of the channel, which is beneficial to improve the electronic performance of the device. As a result, a polarization-graded AlGaIn back barrier can be an alternative to a fixed Al-content $\text{Al}_x\text{Ga}_{1-x}\text{N}$ back barrier design to obtain a high-performance InAlN/GaN HEMTs.

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