Analytical and Simulative Viewpoint of Graded Barrier AlGaN/GaN HEMT for High Input Impedance, Breakdown Voltage and Channel mobility

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Abstract

This paper presents a unique compositional grading of barrier layer of an AlGaN/GaN HEMT, thereby benefiting in different aspects. Extensive calculations are used to determine a simple model for determining 2DEG carrier density with respect to Al molar fraction and AlGaN barrier thickness. The analytical calculation and simulation results are depicted for the $Al_{0.50}Ga_{0.50}N/Al_{0.35}Ga_{0.65}N/Al_{0.20}Ga_{0.80}N/GaN$ HEMT structure. The physical interpretations show that improvement of input impedance, carrier confinement and 2DEG mobility can be achieved by the graded barrier HEMT structure.

INTRODUCTION

An intense outlook of Gallium Nitride (GaN) and its alloys always create attention towards their application in very high power, high temperature, high frequency devices as well as these devices are also better for high linearity demands. In AlGaN/GaN heterostructure, discontinuity of the spontaneous polarization vector at the AlGaN/GaN heterointerface and the piezoelectric charge due to lattice-mismatch of AlGaN on GaN induces high channel charge to the AlGaN/GaN HEMT. Higher channel charge increases the device's current handling capability. The increasing aluminum percentage in the barrier increases the polarization driven charges thus increases the effective 2DEG concentration in the channel [1]. However there is a limiting factor to the increment of Al molar fraction in AlGaN barrier. This is the critical thickness of AlGaN over GaN. Hence there is a solution of graded AlGaN barrier which introduces the effectively high Al concentration in the barrier such that the polarization driven charges get increased. Other advantage is that the lower Al mole fraction next to GaN channel gives improvement in the channel-barrier interface quality. Thirdly, the higher Al mole fraction below the gate contact decreases the gate leakage current.

DEVICE STRUCTURE

We approached in a different way such that the requirement of high Al in the channel is maintained for the higher 2DEG achievement as well as the gate leakage current can be minimized as much as possible. We present the device as shown in Fig. 1 which contains a graded barrier with highest Al content at the gate barrier interface.

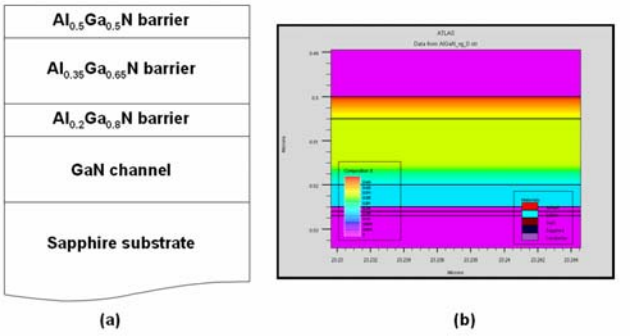

Fig. 1: Graded barrier AlGaN/GaN HEMT structure (a) Device structure (b) Simulated structure

The topmost $Al_{0.5}Ga_{0.5}N$ barrier layer is having the maximum energy bandgap; hence it must have the better resistivity to the gate current flowing from gate to channel through barrier. The AlGaN layer in the channel vicinity is having lowest lattice mismatch with the substrate. It interprets that the defect density at the channel adjacent region will be very less and thus it will improve the 2DEG mobility a lot.

CALCULATION OF 2DEG CARRIER CONCENTRATION:

The behavior of 2DEG concentration vs the AlGaN barrier of a HEMT is quite straight forward. 2DEG concentration increases with the increment of Al molar fraction and the AlGaN barrier thickness. The most important concern about the source of this accumulated charge is the polarization effect in III-nitride materials. The polarization generated charge can be calculated using the below mentioned formula:

$$\sigma = P_{sp(AlGaN)} + P_{pz(AlGaN)} - P_{sp(GaN)}$$

and $$P_{pz(AlGaN)} = \frac{2(a_{GaN} - a_{AlGaN})}{a_{AlGaN}} \times \left(e_{31} - \frac{e_{33} \bullet C_{13}}{C_{33}} \right)$$

where a_{GaN} and a_{AlGaN} are the lattice constants of GaN channel layer and AlGaN barrier layer, *e31, e33, C13* and *C33* are the materials' elastic and piezoelectric constants for strain calculations.

The values of polarization generated charges are the main factor for determining carrier concentration at the interface. Also it is necessary to calculate the position of the Fermi energy level (E_F) at AlGaN/GaN interface to determine whether 2DEG forms or not. E_F is related with the carrier concentration at the AlGaN/GaN interface by the following equation, which is obtained [2] by the self consistent solution of Schrodinger and Poisson's equations:

$$n_s = Dk_BT \ln\left(\left(1+\exp\left(\frac{E_F - E_0}{k_BT}\right)\right)\times\left(1+\exp\left(\frac{E_F - E_1}{k_BT}\right)\right)\right)$$

Here, E_0 and E_1 are the allowed energy levels and can be obtained by the following equations [3]:

$$E_i = \gamma_i n_s^{2/3} \quad \text{for i = 0 and 1}$$

Where $\gamma_0 = 2.123\times10^{-12}$ and $\gamma_1 = 3.734\times10^{-12}$ are obtained through experimental results [4].

Now, the carrier density under the gate contact is calculated as the following equation [5]:

$$n_s(x) = \frac{\sigma_{AlGaN/GaN(x)}}{q} - \frac{\varepsilon_0 E_F}{q^2}\left[\frac{\varepsilon_{AlGaN(x)}}{d_{AlGaN}} + \frac{\varepsilon_{GaN}}{d_{AlGaN}}\right] - \frac{\varepsilon_0\varepsilon_{AlGaN(x)}}{q^2 d_{AlGaN}}\left[q(\phi_{AlGaN(x)} - V_{GS}) + \Delta(x) - \Delta E^C_{AlGaN(x)}\right]$$

Where d_{AlGaN} and d_{GaN} are AlGaN and GaN thicknesses, ε_{AlGaN} and ε_{GaN} are the dielectric constants of AlGaN and GaN, $q_{\Phi AlGaN}$ is schottky barrier height of the gate contact, VGS is the applied gate voltage, ΔE^c is conduction band discontinuity between AlGaN and GaN, E_F is the position of the Fermi level with respect to the GaN conduction-band-edge close to the GaN/substrate interface and $\Delta(x)$ is approximated as

$$\Delta(x) = E_0 + \frac{\pi\hbar^2}{m^*_{GaN}} n_s(x)$$

We have used these equations for determining the 2DEG carrier density for AlGaN/GaN HEMTs with different Al molar fractions and AlGaN thicknesses. The dependency of ns over E_F is considered with an initial guess of ns and the obtained value of E_F is used for determining a new value of n_s. This procedure is continued till both the values of E_F and n_s satisfy all the relationships. This complete procedure is done with a set of experimental results and the calculated values are in good agreement as shown in Table 1.

TABLE I
COMPARISON BETWEEN ANALYTICAL CALCULATION AND EXPERIMENTAL RESULTS

Al molar fraction (%)	**AlGaN Thickness (nm)**	**2DEG density from reference (cm-2)**	**By analytical calculation**		**Reference**
			2DEG density (cm-2)	Ef (eV)	
35	20	1.30E+13	1.39E+13	1.292	[6]
25	28	9.00E+12	1.00E+13	0.88	[7]
24	20	6.00E+12	8.64E+12	0.7705	[8]
24	40	9.00E+12	1.02E+13	0.897	[8]
35	29	1.50E+13	1.50E+13	1.45	[9]

We fitted the calculated values of E_F and n_s with respect to the independent variables: Al molar fraction and AlGaN barrier thickness and plotted the dependency curve as shown in the below figure:

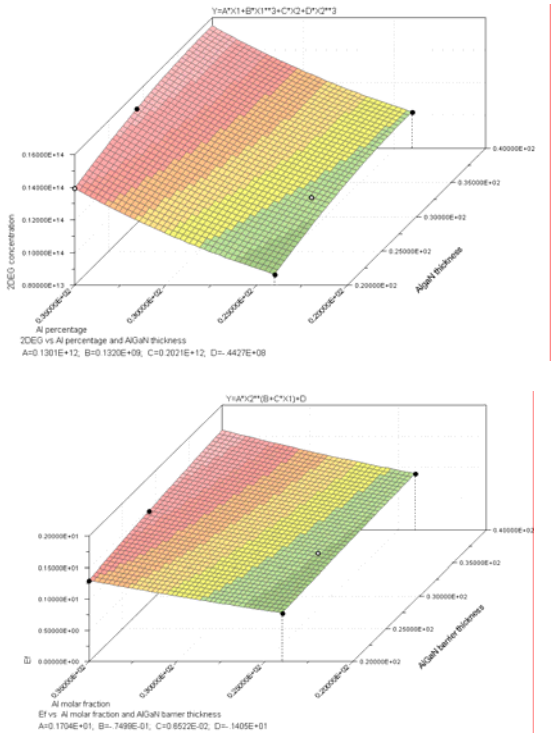

Fig. 2: Dependency of (up) 2DEG carrier density (down) E_F on Al molar fraction and AlGaN thickness in AlGaN/GaN HEMT

The obtained numerical relations between E_F, n_s, Al molar fraction and AlGaN thickness are determined as the following simple model:

$$n_s = A_1 x + B_1 x^3 + C_1 d + D_1 d^3$$

where A_1 = 0.1301E12, B_1 = 0.1320E9, C_1 = 0.2021E12, D_1 = –0.4427E8

$$E_F = A_2 d^{B_2 + C_2 x} + D_2$$

where A_2 = 1.704, B_2 = –0.07499, C_2 = 0.006522, D_2 = –1.405

We have verified the above equations with some other experimental results and those are also in good agreements.

Now we have considered the same approach for our proposed graded barrier structure. The main factor considered in this case is the value of σ is dependent on all of the AlGaN graded barrier layers. In a single barrier HEMT, the piezoelectric polarization field is caused only due to the single AlGaN strained layer. In graded barrier case, the strain is generated in the AlGaN layer (just above GaN channel) is also contributed by other AlGaN layers at top. So, we supposed the following polarization field schemes for calculating the total σ value.

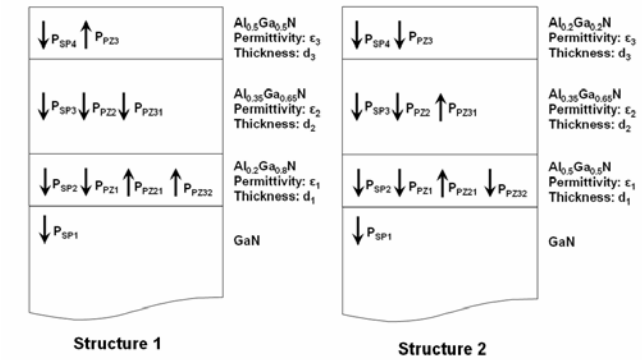

Fig. 3: Proposed polarization schemes for (left) high Al content AlGaN at top and (right) low Al content AlGaN at top. P_{PZ21} is the contribution from P_{PZ2} from the middle layer, P_{PZ31} is the contribution from P_{PZ3} from the top layer to middle layer and P_{PZ32} is the contribution from P_{PZ31} from the middle layer to the channel adjacent AlGaN layer. Here d_1 = 5 nm, d_2 = 15 nm and d_3 = 5 nm are the thicknesses of AlGaN layers

We considered that GaN channel layer is sufficiently thick, so that the AlGaN layer just above the channel will have the same lattice constant in perpendicular to growth direction. The upper AlGaN layers will change its lattice constant (in perpendicular to growth direction) after growth, because it is growing on an already strained layer. The dependence on this new lattice constant should maintain the following relation:

$$a_{new} = \frac{a_{old} d_{film} + a_{sub} d_{sub}}{d_{film} + d_{sub}}$$

where a_{old} is the original lattice constant, a_{new} is the lattice constant after pseudomorphic growth, a_{sub} is the substrate lattice constant, d_{film} is the epilayer thickness and d_{sub} is the substrate thickness

All of our polarization calculations for those graded barrier structures are done in accordance to the newly obtained lattice constants. Thus the total polarization charge for obtaining total σ values for Structure 1 and Structure 2 are obtained as:

$$P_{total} = \left| -P_{SP1} + P_{SP2} + P_{PZ1} - P_{PZ21} + P_{PZ32} \right|$$

and

$$P_{total} = \left| -P_{SP1} + P_{SP2} + P_{PZ1} - P_{PZ21} - P_{PZ32} \right|$$

respectively.

As we can observe in previous n_s equation, that there are some capacitive terms. In the graded barrier case, we can observe that polarization dependent sheet charges are formed in each of the junctions (AlGaN/AlGaN and AlGaN/GaN), so we considered the series capacitance effect of all the AlGaN layers with different dielectric constants and layer widths. Hence, we considered the following modified version of Equation 1 to calculate the total 2DEG carrier density:

$$n_s(x) = \frac{\sigma_{Total}}{q} - \frac{C \| E_F}{q^2} - \frac{C \|}{q^2}\left[q(\phi_{AlGaN(top)} - V_{GS}) + \Delta(x) - \Delta E^C_{AlGaN(bottom)} \right]$$

where σ_{Total} is the total polarization generated charge, $q\Phi_{AlGaN(top)}$ is the schottky barrier height of the gate contact and $\Delta E^C_{AlGaN(bottom)}$ is the conduction band discontinuity between the channel adjacent AlGaN layer and GaN channel and $C \|$ is the effective capacitance per unit area and is given as follows:

$$C \| = \frac{\varepsilon_1 \varepsilon_2 \varepsilon_3}{d_1 \varepsilon_2 \varepsilon_3 + d_2 \varepsilon_1 \varepsilon_3 + d_3 \varepsilon_1 \varepsilon_2}$$

The previous method of calculating E_F and n_s (two mutually dependent terms) are applied with a number of iterations and finally we achieved the results shown in Table 2. The 2DEG result for graded barrier Structure 2 is approximately in good agreement with the experimental value [10]. We analyze from Table 2 that the difference between E_F and the first allowed energy state for Structure 2

is less than that of regular HEMT structure. So, it can be concluded that the carrier confinement must be better in graded barrier structure than the regular HEMT. The low temperature 2DEG density study for this structure showed the same agreement. Now, in our proposed structure (Structure 1) it is seen that E_F is below the first allowed energy level. Hence in this case, the 2DEG confinement should be better than Structure 2 also.

TABLE II
ANALYTICAL CALCULATION RESULTS FOR DIFFERENT DEVICE STRUCTURES

	Conventional HEMT (35% Al and 25 nm thick barrier)	**Graded barrier HEMT with high Al content at the upmost position (Structure 1)**	**Graded barrier HEMT with high Al content at the bottom most position (Structure 2)**
2DEG carrier density (cm-2)	1.46E13	5.07E12	1.08E13
Position of Fermi level E_F (eV)	1.3859	0.5089	0.9470
Position of allowed ground energy level E_0 (eV)	0.5886	0.2908	0.4815
Position of allowed first energy level E_1 (eV)	1.0353	0.5115	0.8468

DRAIN CURRENT SIMULATION

There are a lot of process techniques to minimize the gate leakage current in AlGaN/GaN HEMTs. Mainly the recessed gate technique [11], adjustment of the V-III ratio during AlGaN growth [12], oxygen plasma treatment of fabricated HEMT [13], and oxide filled MESA isolation [14] etc. have contributed towards achieving less gate current in AlGaN/GaN HEMT.

Our proposed structure, as mentioned earlier, has the inherent property of reducing the gate leakage current. The device structure has been simulated with the field dependent mobility model, lattice heating model etc. [15] for the best predictions. The 2DEG carrier density has been chosen from our proposed model of graded barrier HEMT.

The simulation of output current results in a maximum drain current of 350 mA/mm in case of the conventional HEMT structure. The incorporation of graded barrier lowers the maximum drain current to around 120 mA/mm. This is because of the decreased 2DEG carrier concentration in the AlGaN/GaN interface.

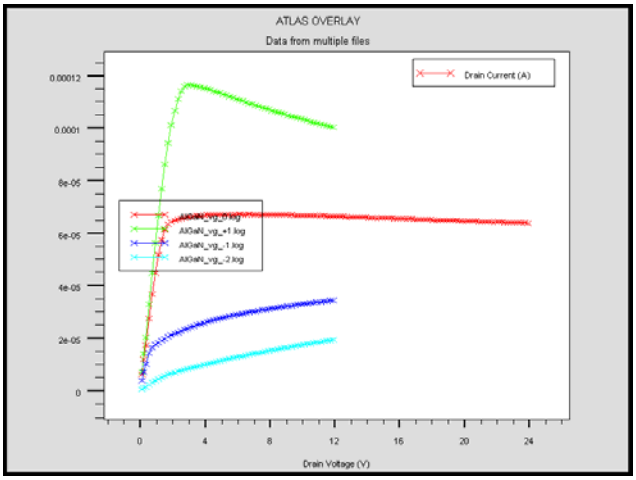

Fig. 4: Drain current vs drain voltage of proposed structure (Structure 1) at gate voltages of +1, 0, -1, and -2 V

CONCLUSIONS

We have successfully analyzed and simulated the $Al_{0.50}Ga_{0.50}N/Al_{0.35}Ga_{0.65}N/Al_{0.20}Ga_{0.80}N/GaN$ HEMT structure by theoretical calculations and ATLAS device simulator. We also proposed a simple model for extracting 2DEG charge carrier density of regular AlGaN/GaN HEMT.

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