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.

![Graded barrier AlGaN/GaN HEMT structure](image)

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

The topmost Al$_{0.50}$Ga$_{0.50}$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 straightforward. 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

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

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where \(a_{\text{GaN}}\) and \(a_{\text{AlGaN}}\) 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:

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

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

\[
E_i = \gamma_i n_s^{2/3}
\]

for \(i = 0\) and \(1\)

Where \(\gamma_0 = 2.123 \times 10^{-12}\) and \(\gamma_1 = 3.734 \times 10^{-12}\) are obtained through experimental results [4].

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

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

Where \(d_{\text{AlGaN}}\) and \(d_{\text{GaN}}\) are AlGaN and GaN thicknesses, \(\varepsilon_{\text{AlGaN}}\) and \(\varepsilon_{\text{GaN}}\) are the dielectric constants of AlGaN and GaN, \(\phi_{\text{AlGaN}}\) is schottky barrier height of the gate contact, \(V_{GS}\) is the applied gate voltage, \(\Delta E\) 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

\[
\Delta(x) = E_0 + \frac{\pi h^2}{m_{\text{GaN}}} n_s(x)
\]

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 \(n_s\) over \(E_F\) is considered with an initial guess of \(n_s\) 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 1: Comparison between analytical calculation and experimental results

<table>
<thead>
<tr>
<th>Al molar fraction (%)</th>
<th>AlGaN Thickness (nm)</th>
<th>2DEG density from reference (cm-2)</th>
<th>By analytical calculation (cm-2)</th>
<th>(E_F) (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>35</td>
<td>20</td>
<td>1.30E+13</td>
<td>1.39E+13</td>
<td>1.292</td>
</tr>
<tr>
<td>25</td>
<td>28</td>
<td>9.00E+12</td>
<td>1.00E+13</td>
<td>0.88</td>
</tr>
<tr>
<td>24</td>
<td>20</td>
<td>6.00E+12</td>
<td>8.64E+12</td>
<td>0.7705</td>
</tr>
<tr>
<td>24</td>
<td>40</td>
<td>9.00E+12</td>
<td>1.02E+13</td>
<td>0.897</td>
</tr>
<tr>
<td>35</td>
<td>29</td>
<td>1.50E+13</td>
<td>1.50E+13</td>
<td>1.45</td>
</tr>
</tbody>
</table>

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 barrier 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 \( \sigma \) 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 \( \sigma \) value.

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 \( \sigma \) values for Structure 1 and Structure 2 are obtained as:

\[ P_{total} = [ -P_{SP1} + P_{SP2} + P_{PZ1} - P_{PZ2} + P_{PZ3} ] \]

and

\[ P_{total} = [ -P_{SP1} + P_{SP2} + P_{PZ1} - P_{PZ2} - P_{PZ3} ] \]

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:

\[ n_s (x) = \frac{\sigma_{Total}}{q} - C || E_F || \]

\[ -\frac{C}{q^2} [ q(\phi_{AlGaN(top)} - V_{GS}) + \Delta(x) - \Delta E_{AlGaN(bottom)} ] \]

where \( \sigma_{Total} \) is the total polarization generated charge, \( q\phi_{AlGaN(top)} \) is the Schottky barrier height of the gate contact and \( \Delta E_{AlGaN(bottom)} \) 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:

\[ C || = \frac{\varepsilon_1 \varepsilon_2 \varepsilon_3}{d_1 \varepsilon_1 + d_2 \varepsilon_3} \]

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>
<thead>
<tr>
<th>TABLE II</th>
<th>ANALYTICAL CALCULATION RESULTS FOR DIFFERENT DEVICE STRUCTURES</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Conventional HEMT (35% Al and 25 nm thick barrier)</td>
</tr>
<tr>
<td>2DEG carrier density (cm$^{-2}$)</td>
<td>1.46E13</td>
</tr>
<tr>
<td>Position of Fermi level $E_F$ (eV)</td>
<td>1.3859</td>
</tr>
<tr>
<td>Position of allowed ground energy level $E_0$ (eV)</td>
<td>0.5886</td>
</tr>
<tr>
<td>Position of allowed first energy level $E_1$ (eV)</td>
<td>1.0353</td>
</tr>
</tbody>
</table>

**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.

**CONCLUSIONS**

We have successfully analyzed and simulated the $\text{Al}_{0.50}\text{Ga}_{0.50}\text{N}/\text{Al}_{0.35}\text{Ga}_{0.65}\text{N}/\text{Al}_{0.20}\text{Ga}_{0.80}\text{N}/\text{GaN}$ 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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**REFERENCES**