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# Dependence of Sheet Charge Density on Strain Relaxation and Material Composition for 2DEG

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## Abstract

Sheet charge density of $Al_xGa_{1-x}N/GaN$ 2DEG structure is analytically computed as a function of material composition. Strain relaxation factor, carrier concentration and quantized length of the well are also taken into account for computation purpose. Both spontaneous and piezoelectric polarizations are calculated as function of mole fraction and charge density is determined from the simulated findings. Results are important for calculating electrical characteristics of HEMT.

**Keywords:** Mole Fraction, Piezoelectric Polarization, Quantized Length, Sheet Charge Density, Sheet Resistance, Spontaneous Polarization; Strain Relaxation Factor

## 1. Introduction

High Electron Mobility Transistor (HEMT) is one of the preferred research area[1,2] now-a-days for the device engineers due to the possibility of microwave and millimeter wave application. Among the different materials, nitride based devices are used to form heterostructures owing to the higher bandgap, higher thermal conductivity, larger breakdown voltage, higher electric field[3]. More precisely, $Al_xGa_{1-x}N/GaN$ material composition is suitable of high frequency and high power operation[4]. By virtue of bandgap engineering, this composition is the choicest candidate for HEMT design owing to the formation of Two-Dimensional Electron Gas (2DEG)[5,6].

Among the III-V materials, nitride based materials have exhibit the polarization properties. Spontaneous polarization arises due to asymmetric bonding and piezoelectric polarization arises due to mechanical stress. Hence from design perspective of the heterostructure based devices, it is better to include the effect of polarization while computing electrical parameters[7–9]. Ambacher[10] and co-workers showed the effect of structural parameter and material composition for nitride based heterostructures on spontaneous and piezoelectric polarization

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induced by 2DEG. Works is also carried out to study the effect on sheet charge density and well thickness[11], where carrier–carrier and carrier–phonon scattering effects are considered. Polarization effects on effects on electronic and optical properties are also investigated[12].

Later, strain relaxation effect of AlGaN barrier layer on conduction band structure, electron concentration and 2DEG sheet charge density is calculated by self-consistent solution of Schrödinger and Poisson's equation[13]. It is also shown very recently that strain effect can be reduced by altering doping concentration in the heterostructure[14]. Current-voltage characteristics are developed considering these effects for HEMT and reported[15].

In the present paper, sheet charge density of $Al_xGa_{1-x}N$/GaN based structure is calculated after evaluating polarization effect and the effect of strain relaxation factor, carrier concentration and quantized length are taken into consideration. Result will play important role for HEMT design.

## 2. Mathematical Modeling

Strain (ε) generated due to band-bending at the hetero-interface of AlGaN and GaN is given by:

$$\varepsilon = (1-r)\frac{(a_{AlGaN}-a_{GaN})}{a_{AlGaN}} \tag{1}$$

where $a$ is the in-plane lattice constant and $r$ is the amount of strain relaxation. The piezo-polarization component of AlGaN is given by:

$$P_{pz}(AlGaN) = 2\varepsilon\left[e_{31} - e_{33}\left(\frac{c_{13}}{c_{33}}\right)\right] \tag{2}$$

Therefore, the total polarization vectors for GaN and AlGaN are given by:

$$P_{Tz}(GaN) = P_{sp}(GaN) \tag{3.1}$$

$$P_{Tz}(AlGaN) = P_{sp}(AlGaN) + P_{pz}(AlGaN) \tag{3.2}$$

The total hetero-interface charges (σ) can be computed for the AlGaN surface and the AlGaN/GaN interface given as:

$$\sigma_{surf} = -[P_{Tz}(AlGaN) - P_{Tz}(GaN)] \tag{4}$$

where the total piezoelectric polarization of AlGaN layer is given as:

$$P_{pz}(AlGaN) = 2\left(\frac{a(0)-a(x)}{a(x)}\right)\left(e_{31} - e_{33}\frac{c_{13}}{c_{33}}\right) \tag{5.1}$$

$$P_{sp}(AlGaN) = = -0.052x - 0.29 \tag{5.2}$$

$$P_{sp}(GaN) = = -0.029 \tag{5.3}$$

where a(0) and a(x) are the lattice constants, $c_{13}$ and $c_{33}$ are the elastic constants, $e_{31}$ and $e_{33}$ are piezoelectric constants. In the above expression, it has been assumed that GaN layer is fully relaxed.
The 2DEG density of the AlGaN/GaN HEMT can be written as:

$$n_s = \frac{\sigma_{AlGaN}t_{AlGaN} - \frac{\varepsilon\varepsilon_0}{q}\phi_B + \frac{\varepsilon\varepsilon_0}{q^2}\Delta E_c(AlGaN)}{t_{AlGaN} + d_0} \tag{6}$$

where the symbols have usual significances.
Sheet resistance of the 2DEG is given by:

$$R_{sheet} = \frac{1}{qn_s\mu_n} \tag{7}$$

## 3. Results and Discussions

Based on the mathematical formulation as mentioned in the previous section of this paper, spontaneous and piezoelectric polarizations are

first calculated as a function of material parameters. Figure 1 shows the variation of Al concentration with spontaneous polarization for the structure. The graph shows that spontaneous polarization varies inversely with the Al concentration. Figure 2 shows the variation of piezoelectric polarization where it is seen that the variation of Al concentration is directly proportional to the piezoelectric polarization. The plot is made for three different strain relaxation factors ('*r*'). With the increase in the value of *r*, it is observed that the slope of the line monotonically decreases.

The total polarization is a sum of the spontaneous and piezoelectric polarizations which provides Figure 3, which insinuates that the total polarization is inversely proportional to the Al concentration. This is due to the fact that GaN bulk is fully relaxed and, therefore, its polarization vector contains only the spontaneous component Psp (GaN). But for AlGaN layer, in addition to the spontaneous component Psp (AlGaN), the piezo-polarization component due to the presence of strain because of Al content in AlGaN must be considered. The piezo-polarization component of AlGaN is a function of strain and lattice constant.

Figure 4 shows the total polarization charge density as a function of mole fraction for different strain relaxation. The total hetero-interface charge (σ) is a function of total piezoelectric polarization, which, in turn, depends on lattice constants, elastic constants and piezoelectric constants of AlGaN layer.

As strain increases the amount of strain relaxation decreases. As strain is directly related to piezoelectric polarization, so with the decrease in the value of *r*, the total polarization charge density increases at a constant value of mole fraction *x*. Therefore, we observe an increase in the slope of the graph with the decrease in the value of r. This is plotted in Figure 5. This is due to that fact that increasing the carrier concentration enhances the probability of scattering and thus sheet charge density decreases.

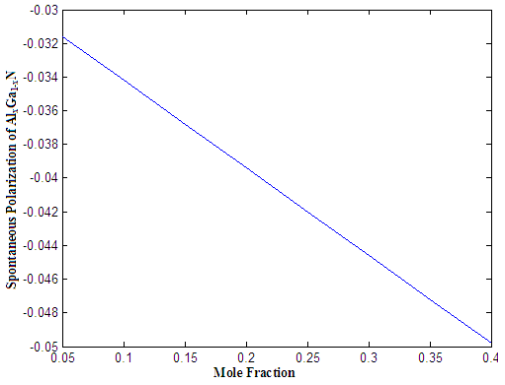


**Figure 1.** Spontaneous polarization variation with mole fraction of AlGaN.

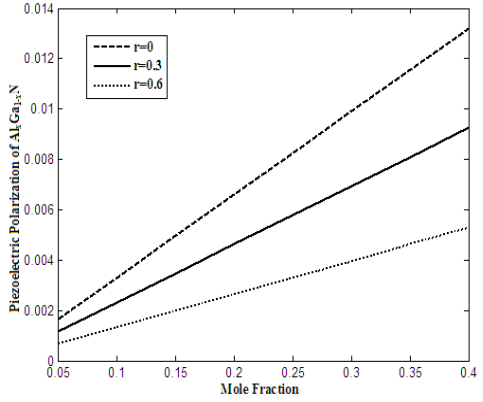


**Figure 2.** Piezoelectric polarization variation with mole fraction of AlxGa1-xN for different amount of strain relaxation.

Increasing the Al mole fraction of AlGaN barrier can increase 2DEG density. In an AlGaN/GaN HEMT, the 2DEG sheet charge density approaches the net polarization charge density at AlGaN/GaN interface with increasing AlGaN thickness. The polarization charge

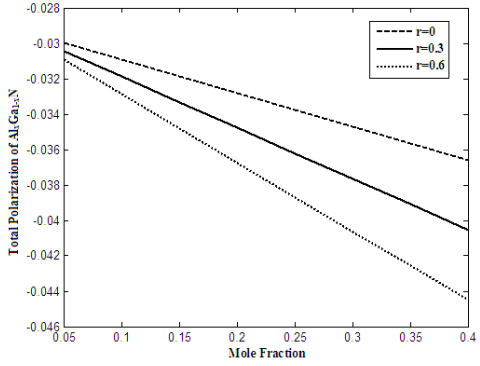


**Figure 3.** Total polarization variation with mole fraction of AlGaN for different amount of strain relaxation.

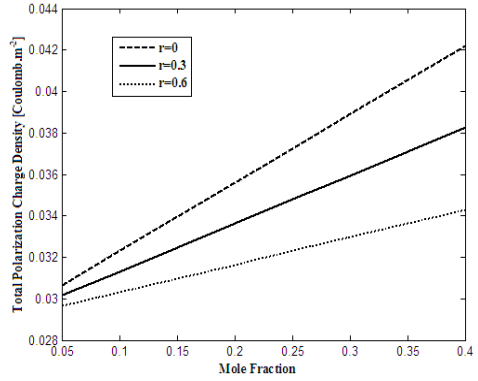


**Figure 4.** Total polarizaction charge density variation with mole fraction of AlGaN for different amount of strain relaxation.

density increases in turn with Al mole traction of the AlGaN barrier. This is plotted in Figure 6.

Figure 7 shows the sheet resistance profile with barrier layer thickness. It is seen from the plot that with increasing barrier dimension, sheet resistance increases as it increases more quantum confinement, thereby increasing the potential barrier. It is observed that the sheet resistance of AlGaN/GaN HEMT is increasing from 3.17 per square

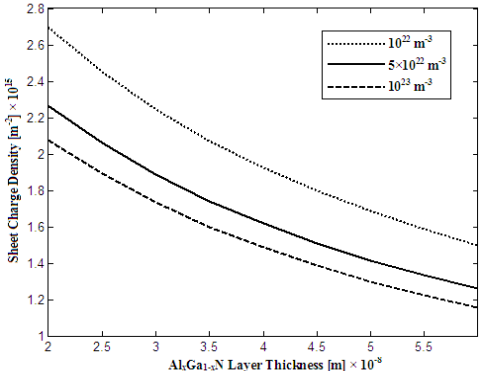


**Figure 5.** Sheet charge density with AlGaN layer thickness for different carrier concentrations.

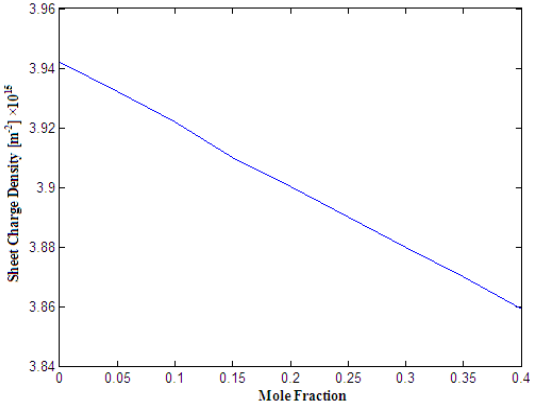


**Figure.6.** Sheet charge density of AlGaN/GaN based HEMT for different mole fractions.

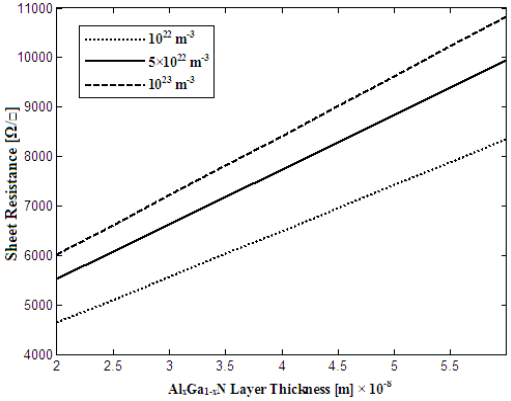


**Figure 7.** Sheet resistance with AlGaN layer thickness for different carrier concentrations.

at $x$ = 0 to 3.24 per square at $x$ = 0.4. Again, by reducing carrier concentration, sheet resistance increases as it lowers the conductivity.

## 4. Conclusion

Increase in Al mole fraction enhances the amount of spontaneous polarization but piezoelectric polarization varies inversely. The spontaneous polarization, has a negative value and is greater in magnitude as opposed to piezoelectric polarization. Change of Al mole fraction enhances the 2DEG density greatly for an AlGaN/GaN-based HEMT because of reducing the electron wave function penetration into the AlGaN barrier layer and the larger effective $\Delta E_c$ also increased the 2DEG density. The total polarization charge density increases with the increase in mole fraction. However, it decreases with the increase in the strain coefficient. The 2DEG sheet concentration at the $Al_xGa_{1-x}N$/GaN heterojunction is sensitively dependent on the Al mole fraction, which leads the GaN-based HEMT towards microwave and millimeter wave applications.

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