A new expression of $N_S$ versus $E_F$ to an accurate control charge model for AlGaAs/GaAs

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Abstract. Semi-conductor components become the privileged support of information and communication, particularly appreciation to the development of the internet. Today, MOS transistors on silicon dominate largely the semi-conductors market, however the diminution of transistors grid length is not enough to enhance the performances and respect Moore law. Particularly, for broadband telecommunications systems, where faster components are required. For this reason, alternative structures proposed like hetero structures IV-IV or III-V [1] have been. The most effective components in this area (High Electron Mobility Transistor: HEMT) on III-V substrat e. This work investigates an approach for contributing to the development of a numerical model based on physical and numerical modelling of the potential at heterostructure in AlGaAs/GaAs interface. We have developed calculation using projective methods allowed the Hamiltonian integration using Green functions in Schrödinger equation, for a rigorous resolution “self coherent” with Poisson equation. A simple analytical approach for charge-control in quantum well region of an AlGaAs/GaAs HEMT structure was presented. A charge-control equation, accounting for a variable average distance of the 2-DEG from the interface was introduced. Our approach which have aim to obtain $n_s$-$V_g$ characteristics is mainly based on: A new linear expression of Fermi-level variation with two-dimensional electron gas density in high electron mobility and also is mainly based on the notion of effective doping and a new expression of $\Delta E_c$

1. Introduction
The IV-IV or III-V hetero structures [1] use semi-conductors in which, the electrons effective mass is less than the massive Si mass, thus enhancing their mobility. In this domain The most efficient devices are HEMTS on III-V substrate.
The development of semi-conductor materials hetero structures gave clear illustrations on some quantum mechanics concepts as confinement or quantification of energy levels. A new electronic devices generation especially the HEMT have been developed benefitting from these quantum effects. The HEMT) or TEGFET (Two Dimensional Electron Gas FET) is essentially made of one hetero junction GaAsAl/GaAs, which is considered as abrupt of references because both materials have the same crystal structure and the physical parameters of these materials are very close (parameters of meshes very close to the two semiconductors) [2].
The study of this hetero junction (abrupt) inevitably passes by the resolution of the Schrödinger-Poisson equation system due to its quantum effects occurring at the interface level [3, 4].
Different models of TEGFET have been suggested, but in the literature the modeling of TEC is abundant, the amount of works about the modeling of TEGFET is limited.
However, two types of models have been suggested: analytic models and the two dimensional classical models or Monte-Carlo type [5]. The first models are based on controlling the accumulated charge suggested by Dr. Delagebeaudeuf [5]. The potential well combined with the hetero junction is supposed triangular, giving a simple analytic expression of the energies from different sub-bands. The second models based on the two-dimensional analysis of devices, in this case transport phenomenon is governed by standard electro kinetics equations or of Monte-Carlo type. Therefore, it seems interesting to us to precisely study this component from a theoretical point view in order to assess its performances.

This work is dedicated to nanometric modeling of HEMT in a rigorous and complete manner. That we started with a preliminary and precise study of the hetero junction, then, the exact numerical resolution of globally non linear system Schrödinger-Poisson, in an self coherent way, was carried out[6, 7]. Thus allowing to have the repartition the potential model of GaAsAl/GaAs hetero junction interface. This allowed to us to deduce the influence of the different physical and geometric parameters (as doping and the rate of aluminum) on characterizing parameters of quantum wells (such as the density of charge, ΔEc), which led us to a study of the accumulated charge and its command, to highlight its importance in the comprehension of the principle functioning of HEMTs.

2. Theory
Generally, high gap materials are preferred for manufacturing high power components; many of them have used these materials especially, the HEMT. The development of Semiconductors materials hetero structures led to clear illustrations of some quantum mechanics concepts as the confinement and/or energy levels quantification.

One of quantum hetero structures applications is the HEMT transistor. Which is made of e GaAs substrate, a low gap buffer layer, 2D GaAs will be formed in this material at the upper defining the canal which is the confinement zone of carriers; and then, the non doped AlGaAs layer it allows to reduce interactions between donor’s electrons and donor layer which provide electrons to the canal [3].

![Figure 1. HEMT structure.](image)
The electrons provided by donor layer will pass from high gap material to low gap material. These electrons fill the lower states of GaAs side, as a result, energy bands bend, the curvature of $B_c$ conduction band become a potential well in which electrons are confined. Energies are always measured in electron volts and identified relative to the lower side of the conduction band of L valley) [2, 3, 7]. The high donor level $E_{dl}$, is linked to the low side of conduction band, therefore it is wise to suppose that all electrons belonging to this level participate in conduction (there is a total ionization of donor atoms). In the opposite, the deep level $E_{dx}$ is linked to the bottom of L valley, thus an electron trapped on this level must pass through a potential barrier of the order of 140 mev to reach the L.

Therefore we can suppose that the electrons of deep level $E_{dx}$ are trapped forever and can never participate in conduction.

With:

\[
\begin{align*}
E_{cg} &= 0 \\
E_{dl} &= 0.006 \\
E_{dx} &= 0.17 - 0.58x - 0.31x^2 \\
E_{cl} &= 0.31 - 0.58x - 0.31x^2
\end{align*}
\]

The values of the bottom of the $\Gamma$ and L conduction band, respectively denoted $E_{cg}$ and $E_{cl}$, where $x$ represents the rate of Aluminum GaAsAl.

These hypotheses will allow us to calculate the effective total concentration $N_{eff}$ in the GaAsAl according to the concentration of Si doping $N_D$ and the aluminum rate. Namely $N_D$ the doping in Si donor atoms, we call $N_{dl}$ and $N_{dx}$ the respective concentrations in light and deep donor atoms, in an evident manner, we have (figure 2):

\[
N_D = N_{dl} + N_{dx}
\]

According to the statistic of Fermi-Dirac, $N_{dx}$, $N_{dx}$ are given by the following formulas [8]:

Figure 2. Energy diagram.
Where $E_F$ is the level of Fermi and $N$ is a constant of the problem.

A simple calculation allows us to access the value $N_D$, that is, in our hypotheses simply effective doping $N_{\text{eff}} [8]$

$$N_{\text{eff}} = \frac{N_{d}}{1 + \left(1 + \frac{1}{2} e^{\frac{E_{\text{d}} - E_{F}}{kT}}\right) / (1 + \exp\left(\frac{E_{d} - E_{F}}{kT}\right))}$$

In our recent works [6, 7], we have determined the parameters characterizing the potential quantum well like as: potential energy, spatial dispersion, wave function and surfaced density, these parameters can be used to determine the behavior dynamics of the HEMT structure. In this work we have proposed a new expression for the offset $\Delta E$ and the second is for $N_S$ versus $E_F$ or while also studying the influence of physics parameterizes (Al rate) and the geometric parameters of this heterojunction.

In our model, this new linear expression of Fermi level varied with two-dimensional electron gas (2DEG) density in high electron mobility is proposed, we have obtained this expression by exploiting the numerical calculation of the reference [6,7] in the static case by numerical interpolation, it is given by the following formula:

$$n_s = a + B \times E_F$$

Where $a=2.43.10^{12}/m^2$, and $B=0.05$ev/m$^2$.

The surface density is given by [9]:

$$n_s = \frac{\varepsilon}{qd} (V_g - V_{\text{off}} - E_F)$$

$\varepsilon$: is the permittivity,

d: is the total thickness of the AlGaAs layer, $V_{\text{off}}$: is the threshold voltage of the HEMT, given by:
\[ V_{\text{off}} = \phi_B - \Delta E_C - \frac{q n_D d_d^2}{2\varepsilon} - \frac{d}{\varepsilon} \sigma ) \]  

(8)

\( \phi_B \): is the barrier of the Schottky gate,

\( \Delta E_C \): is the conduction band discontinuity at the hetero junction,

\( N_D \): is the doping concentration,

\( "dd" \): is the thickness of doped AlGaAs layer

\( \sigma \): is the polarization sheet charge density of the heterojunction AlGaAs/GaAs.

In our structures, we use a Ni-Schottky barrier contact at the surface; \( \phi_B \) and \( \Delta E_C \) are considered as the function of \( N_D \), \( N_{\text{eff}} \) and Al rate and we use the following formulations for the physical properties of AlGaAs in our calculations, Ni Schottky barrier [9]:

\[ \phi_B = 1.38x + 0.84 \]  

(9)

We also suggested a new formula at \( V_{\text{off}} \) level where we have introduced a new expression (our formula) of \( \Delta E_C \) given by the following expression [10]:

\[ \Delta E_C = 0.023 N_D^4 - 0.18 N_D^3 + 0.53 N_D^2 - 0.66 N_D + 0.34 \]  

(10)

With [9]:

\[ \sigma(x) = \left| \frac{2a(0) - a(x)}{a(x)} \left[ e_{31}(x) - e_{33}(x) \frac{C_{31}(x)}{C_{33}(x)} \right] \times P_{SP}(x) - P_{SP}(x) \right| \]  

(11)

Where the lattice constant: \( a = 5.6533 + 0.0078x \) Å°

The elastic constants: \( C_{31} = 5.x + 103; C_{33} = -32x + 405 \) C/m²

The piezoelectric constants: \( e_{31} = -0.11x - 0.49; e_{33} = 0.73x + 0.73 \) C/m²;

The spontaneous polarization: \( p_{sp} = (-0.034 - 0.124x) \times 10^{10} \) C/m²;

3. Results and Discussion

3.1. Variation of sheet carrier concentration (n_s) with applied gate voltage (v_{gs}-v_{off})
3.2. Sheet carrier density versus the gate bias

Figure 3 shows the surface density variation versus to the grid tension ($V_{gs}-V_{off}$). This increases followed by nearly a saturation of $n_s$ when $V_{gs}-V_{off}$ increases, however this limit value differs from the reference [9] because our result is simulated for AlGaAs, one band state, a fixed $x$ (25%) and $N_D=10^{24}/m^3$ additionally we used a linear formula for $E_f=f(n_s)$ and a polynomial formula of order 4 for $\Delta E_C$ but the result of the reference [9] was simulated for NGaAs, two band states, with a non linear formula of $\Delta E_C$.

Figure 4 shows the surface density variation versus to the grid tension ($V_{gs}-V_{off}$). This is perfectly agreed with the results obtained in the literature [9] (figure 4). This figure shows an increase followed by nearly a saturation of $n_s$. We can see that our result is different than the reference [9] because literature value of $V_{off}$ is fixed (it is a constant) while we have calculated $V_{off}$ which is a function of Al rate “$x$”, therefore the AlGaAs stays the basic material for manufacturing HEMT transistor.
3.3. Influence of Aluminum rate

The figure 6 shows that the decrease of x causes an increase of ns. This result is reasonable because the decrease of x causes an increase of effective N\textsubscript{d} which causes an increase of ns.

Figure 5. In-sheet carrier density versus the gate bias with regard to Results reported by the literature (reference [9]).

Figure 6. Influence of Aluminum rate on the sheet carrier density versus the gate bias.

Figure 7. The effect of d on the sheet carrier density versus with applied gate voltage.

Figure 8. Influence of thickness doped layer dd on the sheet carrier density versus with applied gate voltage.
The increase of the positive values of \((V_{gs} - V_{off})\) where \(d = 35\) the curve tends to a higher value where \(d = 100\) nm.

For negative value of \((V_{gs} - V_{off})\) where \(d = 35\) nm: the curve where \(d = 100\) nm shifts to the right which shows the directly influence of the thickness on the interval of \((V_{gs} - V_{off})\).

On the other side the increase of the “dd” (figure8) causes a shifted of curve to the right (for an increase of positive tension \(V_{gs} - V_{off}\)) with more elevated ns.

4. Conclusion

This work is based on an approach for contributing to the development of a numerical model based on physical and numerical modelling potential at the interface of a hetero structure in GaAsAl / GaAs .

We have elaborate a computation, using projective methods permit the Hamiltonian integration using Green functions in the equation of Schrödinger, for a rigorous resolution auto coherent with the equations of Poisson.

A serious approximation for Fermi level with sheet carrier density was made and some expressions were proposed. These expressions were important in an analytic model development for the HEMT, and it participates to of charge control model research.

A simple analytical approach for charge-control in quantum well region of a AlGaAs/GaAs HEMT structure was presented. A charge-control equation, accounting for a variable average distance of the 2-DEG from the top interface was introduced. Our approach to obtain ns-Vg characteristics is mainly based on: A new linear expression of Fermi-level variation with two-dimensional electron gas density in a high electron mobility and also is mainly based on the notion of effective doping and a new expression of \(\Delta E_c\).

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