Equations for the Electron Density of the Two-Dimensional Electron Gas in Realistic AlGa_N/Ga_N Heterostructures

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Abstract: This paper presents equations for the electron density of the two-dimensional electron gas (2DEG) in AlGa_N/Ga_N heterostructures in three realistic scenarios: (1) AlGa_N/Ga_N heterostructure with surface exposed to ambient with mobile ions, (2) metal gate deposited on the AlGa_N surface, and (3) a thick dielectric passivation layer on the AlGa_N surface. To derive the equations, we analyzed these scenarios by applying Gauss's law. In contrast to the idealistic models, our analysis shows that the 2DEG charge density is proportional to the difference between spontaneous polarization of AlGa_N and Ga_N, whereas surprisingly, it is independent of the piezoelectric polarization.

Keywords: AlGa_N/Ga_N heterojunctions; electron density; heterostructures; piezoelectric polarization; semiconductors; spontaneous polarization; two-dimensional electron gas

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1. Introduction

Aluminium Gallium Nitride/Gallium Nitride (AlGa_N/Ga_N) heterostructures are widely used in devices for high power and radio frequency applications because they enable higher current and faster switching speed [1–5]. Both capabilities are the results of high electron mobility and high electron density of the two-dimensional electron gas (2DEG), which is formed at the AlGa_N/Ga_N heterojunction even in the absence of intentional doping [6]. The formation of 2DEG is considered to be due to the spontaneous and piezoelectric polarizations in the AlGa_N/Ga_N heterostructure [7,8], however, the existing equations for the electron density in the 2DEG, N_{2DEG} , are inconsistent and confusing [6,9]. For example, the prevalent equations for N_{2DEG} do not include its dependence on the polarization charges [10,11]. This confusing result corresponds to the implicit assumption that the polarization charges at the AlGa_N/Ga_N heterojunction and AlGa_N surface balance each other [10,11]. It should be noted that there have been follow-up works to revise the original equations. In our approach presented herein, we analyze the charge balance for the following three realistic scenarios:

- (1) AlGa_N surface is unpassivated and accessible by free ions from the ambient;
- (2) Metal gate is deposited on the AlGa_N surface;
- (3) The AlGa_N surface is passivated by a thick dielectric layer.

The results of this analysis are realistic equations for N_{2DEG} .

2. Equations for 2DEG in AlGa_N/Ga_N Heterostructures

2.1. Unpassivated AlGa_N Surface Accessible to Free Ions from Air

GaN is a polar crystal because the formation of the interatomic bonds creates asymmetric electron clouds of Ga and N atoms [11], which is illustrated by the dipole symbols in Figure 1. This effect leads to the spontaneous polarization in GaN, which is quantified by the effective spontaneous polarization charge per unit area, N_{p-GaN} . In AlGa_N, the polarization effect is analogous, with the difference that the spontaneous polarization charge

per unit area ($N_{p\text{-AlGaN}}$) is larger [9,12,13]. The fact that $N_{p\text{-AlGaN}} > N_{p\text{-GaN}}$ is illustrated in Figure 1 by showing five columns of dipoles in AlGaN and three columns of dipoles in GaN. The arrows in Figure 1 show electric field lines.

Figure 1. Impact of spontaneous polarization (modelled using dipoles) on the electron density at the AlGaN/GaN heterojunction (N_{2DEG}) and on the density of mobile ions at the surface (N_{ions}). Cases A and B show dashed rectangles enclosing zero net charge. Case A corresponds to the ideal case of AlGaN surface in vacuum without mobile ions that could be attracted to the surface, whereas Case B shows electric fields attracting mobile positive ions to the AlGaN surface and electrons to the 2DEG at the heterojunction.

The statement by Ibbetson et al. that “polarization charge in AlGaN is balanced” [10] implies that there is no field outside the AlGaN layer and that there is no impact on N_{2DEG} from the spontaneous polarization charge. This result can be obtained by applying Gauss’s theorem in a way that is illustrated by the dashed rectangle labeled as Case A in Figure 1. However, this case excludes the possibility that the positive polarization charge at the heterojunction can attract mobile electrons to the 2DEG and that, likewise, the negative polarization charge at the AlGaN surface can attract positive mobile ions from the ambient. The dashed rectangle in case B shows the application of Gauss’s law that includes electrons next to the heterojunction and positive ions at the AlGaN surface. The total charge inside the Gauss’s rectangle is equal to zero in both cases, which means that the following Gauss’s equation applies to each of them:

$$\varepsilon_{\text{AlGaN}} E_s - \varepsilon_{\text{AlGaN}} E_h = 0 \quad (1)$$

In (1), E_s is the electric field at the AlGaN surface, E_h is the electric field at the AlGaN/GaN heterojunction, and $\varepsilon_{\text{AlGaN}}$ is the permittivity of AlGaN. Case A, which excludes both the electrons next to the heterojunction and the positive ions at the surface, corresponds to $E_s = 0$ and $E_h = 0$. In case B, the heterojunction and the surface fields are equal to each other, $E_s = E_h$, but they are not equal to zero. The field E_s attracts mobile positive ions from the ambient, whereas the field E_h attracts mobile electrons to the 2DEG. This means that the density of 2DEG electrons balances the difference between the spontaneous polarizations of AlGaN and GaN:

$$N_{2DEG} = N_{p\text{-AlGaN}} - N_{p\text{-GaN}} \quad (2)$$

It should be noted that the potential impact of the piezoelectric polarization charge, N_{pz} , is not included by the analysis based on Figure 1. However, the AlGaN bonds near the

heterojunction are strained, which distorts the electron-cloud asymmetry of the nonstrained AlGaIn bonds and changes the spontaneous polarization charge, $N_{p-\text{AlGaIn}}$, by the value of N_{pz} . Therefore, the piezoelectric polarization charge can be modelled by additional dipoles next to the heterojunction, as illustrated in Figure 2. Case A shows that a mobile electron cannot be attracted to the heterojunction, and likewise, a mobile positive charge cannot be attracted to AlGaIn surface due to the piezoelectric dipole. The charge enclosed by the dashed rectangle in this case is zero, which means $E_s = E_h$. If we assume that $E_s = E_h$ is not equal to zero, we violate Kirchhoff's voltage law because $E_s d_1 > E_h d_2$. This is not possible as the potential difference between the AlGaIn surface and AlGaIn/GaN heterojunction has to be equal to zero because there is no electric field above the AlGaIn surface and no electric field below the AlGaIn/GaN heterojunction. Case B shows a dashed rectangle around a piezoelectric dipole with no mobile charges attracted towards it. This case satisfies both the Gauss's law and Kirchhoff's voltage law and shows that piezoelectric polarization near the heterojunction does not impact $N_{2\text{DEG}}$. Thus, as presented in (2), spontaneous polarization is the only reason for $N_{2\text{DEG}}$ at the AlGaIn/GaN heterojunction when the surface is exposed to ambient ions.

Figure 2. Illustration of the lack of impact of piezoelectric polarization (modelled using dipoles at AlGaIn/GaN heterojunction) on the electron density in 2DEG. Cases A and B show dashed rectangles with zero enclosed charge. The possibility of Case A is crossed out as it violates Kirchhoff's voltage law. Case B shows no mobile charges attracted from surroundings due to piezoelectric polarization.

2.2. Metal Gate Deposited on AlGaIn Surface

The electron density at the AlGaIn/GaN heterojunction with a metal gate deposited on the AlGaIn surface, $N_{2\text{DEG-M}}$ can also be stated in terms of spontaneous polarization in AlGaIn and GaN, with the difference that this parameter also depends on the metal–semiconductor work function difference, $q\phi_{ms}$, between the metal and the GaN acting as the semiconductor. This structure is analogous to metal–oxide–semiconductor (MOS) structures, the only difference being that the dielectric role of the oxide between the metal and the semiconductor is played by the AlGaIn layer. Adopting the dependence of electron density on the work–function difference from MOS theory [14,15], we obtain the following equation for $N_{2\text{DEG-M}}$:

$$N_{2\text{DEG-M}} = N_{p-\text{AlGaIn}} - N_{p-\text{GaN}} + C_{\text{AlGaIn}}\phi_{ms} \quad (3)$$

In (3), C_{AlGaIn} is the AlGaIn capacitance per unit area.

2.3. Thick Passivating Dielectric on AlGaN Surface

In the case of thick passivating dielectric, there are ions at the AlGaN surface, but they are fixed. This means that the electron density in the passivated case, $N_{2\text{DEG-P}}$, can be given in terms of the charge density at the passivation interface, N_{pass} , and the spontaneous polarizations in AlGaN and GaN layers by the following equation:

$$N_{2\text{DEG-P}} = N_{\text{p-AlGaN}} - N_{\text{p-GaN}} + N_{\text{pass}} \quad (4)$$

3. Comparison with Other Models

For the first scenario elucidated in Section 2.1, our model using Gauss's law indicates that 2DEG electron density is proportional to the difference between spontaneous polarization of AlGaN and GaN, whereas it is independent of the piezoelectric polarization. The simplified model by Ibbetson et al. [10] does not consider these factors. The other well-known model is developed by Ambacher et al. [12]. Their model states the dependence of 2DEG on both polarization and piezoelectric charges. Later on, several groups came up with more accurate models [9,16–18].

For the second scenario, as explained in Section 2.2, our model using MOS theory shows that 2DEG electron density is dependent on the difference between spontaneous polarization of AlGaN and GaN, as well as the work-function difference due to the metal-semiconductor junction. We have not seen other published model for the same scenario e.g. Morkoc [11] that employ the same approach.

For the third scenario, as documented in Section 2.3, our model indicates that 2DEG electron density is dependent on the difference between spontaneous polarization of AlGaN and GaN, as well as the charge density due to fixed ions at the insulator/AlGaN interface. There are several groups that have investigated this scenario, for example Shealy et al. [19] and Maeda et al. [20]. Both groups conducted experiments with variety of passivation dielectrics before deriving their equations. Despite differing complexities, all models agree that charge density of the passivation interface majorly influences the electron density of 2DEG.

4. Conclusions

We show that $N_{2\text{DEG}}$ depends on the difference between spontaneous polarizations of AlGaN and GaN, but surprisingly, it is independent of the piezoelectric polarization in all realistic scenarios: AlGaN surface exposed to free air with mobile ions, metal gate deposited on the AlGaN surface, and the AlGaN surface passivated by a thick dielectric layer. When a metal gate is deposited on the AlGaN surface, the work-function difference ($q\phi_{ms}$) impacts $N_{2\text{DEG}}$ in analogous way to the well-established dependence of the semiconductor-charge density on the work-function difference in MOS capacitors. Finally, the fixed charge at the interface between AlGaN and a thick passivating layer, which is usually positive, attracts equivalent density of electrons to the 2DEG. The resulting equations from this new analysis provide the ability to distinguish between these differences and realistic scenarios, which is a specific addition to the existing body of literature.

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