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Effect of GaN buffer polarization on electron distribution of AlGaN/GaN heterostructure

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ABSTRACT

The formation of 2DEG in AlGaN/GaN heterostructure is discussed in detail. A misunderstanding about the 2DEG sheet density expression is clarified. It is predicted by theoretical analysis and validated by self-consistent Schrodinger–Poisson numerical simulation that under the force of GaN polarization, large amounts of electrons will accumulate at the GaN/substrate interface in AlGaN/GaN/substrate HEMT structure.

1. Introduction

High electron mobility transistors (HEMTs) based on AlGaN/GaN heterostructures have shown great potential in high-power and high-frequency applications [1]. Owing to improvements made during the last decades in both material quality and device processing, AlGaN/GaN HEMTs have been improved significantly in both DC and RF performance. An accurate expression of the 2DEG sheet carrier concentration n_s is of great importance to the further understanding of AlGaN/GaN HEMTs. There is an important and very much widely cited equation reported for calculating the 2DEG concentration n_s (see Eq. (1) in this article, which will be discussed later in detail). However, the meaning of "σ" in this formula is confusing and has some logical contradictions. In this work, we carefully analyze the process of the 2DEG formation and provide a clear physical image of the AlGaN/GaN heterostructure. The meaning of "σ" in the formula should be reinterpreted.

2. Aboudt the "σ"

The widely cited 2DEG sheet density expression is given as [2–4]:

$$n_s = \frac{\sigma}{q} - \frac{\varepsilon}{q^2 d}\left(q\varphi_b + E_f - \Delta E_c\right), \tag{1}$$

where ε is the dielectric constant of AlGaN, d is the AlGaN layer thickness, q is the electron charge, φ_b is the surface barrier height, E_f is the Fermi level, ΔE_c is the conduction band offset between GaN and AlGaN, as is shown in Fig. 1. By transposing, Eq. (1) can be changed into:

$$\frac{1}{q}\left(q\varphi_b + E_f - \Delta E_c\right) = d\left(\frac{\sigma}{\varepsilon} - \frac{qns}{\varepsilon}\right). \tag{2}$$

According to Fig. 1, the potential drop of AlGaN barrier layer can be expressed as:

$$q\Delta V_{AlGaN} = q\phi_b + E_f - \Delta E_C. \tag{3}$$

Putting Eq. (3) into Eq. (2), we can get:

$$\frac{\Delta V_{AlGaN}}{d} = \frac{\sigma}{\varepsilon} - \frac{qns}{\varepsilon}. \tag{4}$$

Eq. (4) indicates that the electric field in AlGaN barrier layer is determined by two parallel plate capacitors, of which sheet charge density is $\pm\sigma$ and $\pm qns$ respectively.

The structural profile and charge distribution of a AlGaN/GaN heterojunction is shown in Fig. 2. We can see that there are indeed two pairs of coupled sheet charges at the upper surface and the lower interface of AlGaN: ① σ_s and $-qn_s$, ② $\pm\sigma_{AlGaN}$. σ_s is the sheet charge density of ionized surface donors. It equals to the product of

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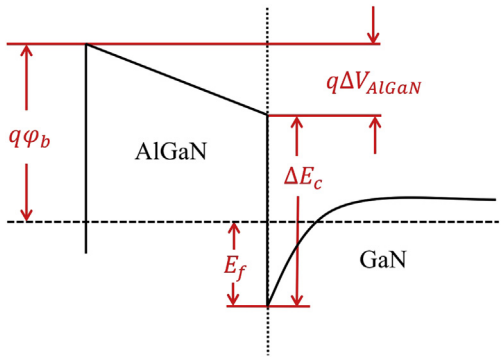

Fig. 1. Conduction band diagram of AlGaN/GaN heterostructure.

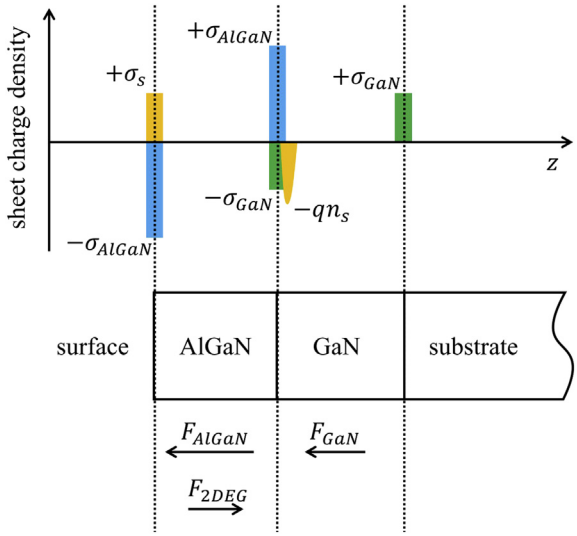

Fig. 2. Structure profile and charge distribution of AlGaN/GaN/substrate heterostructure.

electron charge and the 2DEG sheet density qn_s, because the electrons in 2DEG is considered coming from the surface states of AlGaN [5,6]. σ_{AlGaN} is the polarization charge sheet density of AlGaN. Therefore, according to the above mentioned discussion, the "σ" in Eq. (4) refers to the AlGaN polarization charge density, i.e., $\sigma = \sigma_{AlGaN}$.

However, according to previous works [2–4,7–10] which have mentioned the 2DEG sheet density expression (Eq. (1)), the term "σ" refers to the difference value of AlGaN polarization charge and GaN polarization charge, i.e., $\sigma = \sigma_{AlGaN} - \sigma_{GaN}$. This argument makes the formula conforms to the result of experiment well, but has some logical contradictions. Admittedly, the net polarization charge sheet density at the AlGaN/GaN interface is $\sigma_{net} = \sigma_{AlGaN} - \sigma_{GaN}$. However, if $\sigma = \sigma_{AlGaN} - \sigma_{GaN}$, according to Eq. (4), the absolute value of net polarization charge density at the AlGaN upper surface should be equal to $\sigma_{AlGaN} - \sigma_{GaN}$, too. But this is obviously contradictory to the fact that the only polarization charge at the AlGaN surface is $-\sigma_{AlGaN}$. There is not a "$+\sigma_{GaN}$" at the AlGaN surface. Moreover, it should be noticed that there is a positive polarization charge $+\sigma_{GaN}$ at the GaN/substrate interface, as is shown in Fig. 2. $\pm\sigma_{GaN}$ at the upper and lower interface of GaN layer form a parallel plate capacitor, which will only have nonzero electric field outside the GaN buffer layer. This means that polarization charge of GaN buffer will have no affect on the potential drop of AlGaN barrier layer.

Actually, in previous works, polarization effect of GaN buffer is neglected when calculating the band diagram. Polarization sheet charge density of AlGaN is considered as the relative value comparing with GaN's: $\sigma_{AlGaN} - \sigma_{GaN}$, and polarization charge of GaN is regarded as zero. But why?

3. New calculation

Taking polarization effect of GaN buffer into consideration, there will be a polarization field F_{GaN} in GaN layer pointing from bottom to the top. Adding the potential drop caused by this electric field, the conduction band diagram should be like the one shown in Fig. 3, but not the one in Fig. 1. Moreover, we should notice that all the above-mentioned discussion is based on an *a priori* assumption that the 2DEG locates at the AlGaN/GaN interface. In fact, charge distribution shown in Fig. 2 is not stable, because that electrons will move towards the GaN/substrate interface under the force of F_{GaN}, rather than fix at the AlGaN/GaN interface.

The conduction band diagram and the corresponding electron distribution of a 20 nm $Al_{0.25}GaN_{0.75}$/20 nm GaN/substrate HEMT structure is calculated by self-consistent Schrodinger–Poisson numerical simulation, as is shown in Fig. 4a. The lattice parameter *a*, polarization intensity of *Psp*, *Ppz*, P_{total} of GaN and AlGaN that we used in the calculation are shown in Table 1. Here we only discuss under an assumption that the substrate material has a higher conduction band minimum than GaN's (e.g., sapphire). Since the specific band structure of substrate does not affect the electron distribution much, the conduction band edge of substrate is artificially set as 3 eV higher than GaN's. According to our calculation, electrons not only accumulate at the AlGaN/GaN interface, there is also another electron distribution peak at the GaN/buffer interface. It is found that the width of GaN buffer affect neither the shape of the two electron peaks nor the shape of conduction band near the two interfaces. As long as the polarization of GaN is taken into consideration, electrons will move toward the substrate, and as long as the substrate has a higher conduction band edge than GaN, electrons will accumulate at the GaN/substrate interface. The band diagram and electron distribution of a HEMT structure with 40 nm GaN buffer is shown in Fig. 4b as an example. Therefore, for definiteness and without loss of generality, we will only discuss the characteristics of the HEMT structure with 20 nm GaN buffer in the following discussion.

Comparing with conventional works, the only difference of our calculation is that polarization of AlGaN and GaN is set as the original value, i.e., σ_{AlGaN} and σ_{GaN} respectively. For comparison, band diagram and electron distribution of a 20 nm AlGaN/20 nm GaN/20 nm substrate HEMT structure is also calculated under conventional conditions, i.e., polarization sheet charge density of AlGaN and GaN is considered as $\sigma_{AlGaN} - \sigma_{GaN}$ and 0 respectively, as is shown in Fig. 4c. It can be found that Fig. 4a and c are almost the same at the region of 0–30 nm. They have very similar band diagram and electron distribution shape. The electron sheet density of 20 nm AlGaN/20 nm GaN/substrate structure from 0 to 30 nm, i.e. the integral intensity of the first electron distribution peak, is

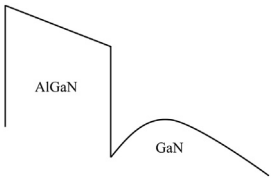

Fig. 3. Conduction band profile of AlGaN/GaN heterojunction when taking polarization effect of GaN buffer into consideration.