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Two-dimensional electron gas densities in AlGaN/AlN/GaN heterostructures

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ABSTRACT The dependence of two-dimensional electron gas (2DEG) density and distribution in an $Al_xGa_{1-x}N$/AlN/GaN heterostructure on the thicknesses of the $Al_xGa_{1-x}N$ barrier layer and the AlN interfacial layer are investigated theoretically. A competitive contribution of the AlGaN and AlN layers to the 2DEG density is revealed. For an AlN interfacial layer thinner than a critical value d_{cAlN}, the 2DEG density is dominated by the AlGaN barrier and the 2DEG density increases with the increase of the AlGaN barrier thickness, as in the case of a simple AlGaN/GaN heterostructure. While the AlN interfacial layer will take the dominant contribution to the 2DEG density as its thickness exceeds d_{cAlN}. In this case, the increase of AlGaN barrier layer thickness leads to the decrease of the 2DEG density. Detailed calculations show that the critical AlN thickness increases with the increase of Al content in the AlGaN barrier.

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1 Introduction

It has been well known that the electron mobility in AlGaN/GaN heterostructure can be remarkably improved by incorporating an thin AlN interfacial layer between the AlGaN and GaN layers [1–5]. Conventional AlGaN/GaN heterostructures usually have carrier mobility of 1000–1600 cm^2/Vs. By inserting an AlN interfacial layer, carrier mobility high up to 2100 cm^2/Vs can be achieved as a result of the reduced electron spillover into the barrier layer and less alloy disorder scattering [2]. With this advantage, the AlGaN/AlN/GaN heterostructure has been attracting much attention due to its promising use in high-electron-mobility transistors (HEMTs) applications [6–9]. In addition to carrier mobility, the two-dimensional electron gas (2DEG) density is also an important aspect which determines the channel current and the access resistance of the HEMTs. However, few attention was paid on the study of 2DEG density in the AlGaN/AlN/GaN heterostructure, in which the inserted AlN layer could play an important role [6].

In this letter, we present a theoretical investigation on the 2DEG density and distribution in $Al_xGa_{1-x}N$/AlN/GaN heterostructures. The results show that the AlN layer thickness is crucial for further improvement of the 2DEG density in AlGaN/AlN/GaN heterostructure, especially when the AlGaN barrier is thin. This brings great advantage for the development of short channel HFETs where a smaller gate to channel separation is desired. The 2DEG sheet density is found to increase linearly with the increase of the AlN thickness. With the AlN thickness smaller than certain critical value d_{cAlN}, the 2DEG density increases with the increase of AlGaN barrier thickness, this is similar to the case of a simple AlGaN/GaN heterostructure. However, when the AlN thickness is in excess of the d_{cAlN}, the 2DEG will decrease with the increase of the AlGaN barrier layer thickness. The critical AlN thickness d_{cAlN} increases with the increase of Al content x of the $Al_xGa_{1-x}N$ barrier layer. This may provide a guideline for the epilayer structure optimization of AlGaN/AlN/GaN HEMTs, especially short channel devices for mm wave applications.

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2 Model descriptions

Our calculation is based on a self-consistent solution of the coupled Schrödinger and Poisson equations [10]. The boundary conditions are specified as follows: the surface barrier energy of the heterostructure is set as 1.2 eV relative to the ground energy which is defined to be the energy close to the substrate. Polarization effect is incorporated into the calculation as the boundary condition at the heterointerface, i.e., the electric displacement must be continuous, yielding:

$$P_1 - \varepsilon_1\varepsilon_0\frac{\mathrm{d}V_1}{\mathrm{d}z} = P_2 - \varepsilon_2\varepsilon_0\frac{\mathrm{d}V_2}{dz}\,, \tag{1}$$

where P is the sum of the spontaneous polarization (P_{SP}) and piezoelectric polarization (P_{PE}), ε is the dielectric constant and V is the potential energy of the conduction band-edge. Due to the discontinuity of the total polarization at the heterostructure, polarization charges are induced and assumed to be fixed at the heterointerface with the sheet density given by:

$$\sigma = P(\text{lower}) - P(\text{upper}) = [P_{SP}(\text{lower}) + P_{PE}(\text{lower})] - \left[P_{SP}(\text{upper}) + P_{PE}(\text{upper})\right]\,. \tag{2}$$

The spontaneous polarization P_{SP} and piezoelectric polarization P_{PE} are determined by [11]:

$$P_{\mathrm{SP}}\left(\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{N}\right) = (-0.052x - 0.029)\ \mathrm{C/m^2} \quad (3)$$

$$P_{\mathrm{PE}} = 2\frac{a-a_0}{a_0}\left(e_{31} - e_{33}\frac{C_{13}}{C_{33}}\right) \quad (4)$$

where a and a_0 are the strain and equilibrium values of the lattice parameters, respectively, e_{33}, e_{31} are piezoelectric coefficients, and C_{13}, C_{33} are elastic constants. The conduction-band discontinuity ΔE_{c} is assumed to be given by [12]:

$$\Delta E_{\mathrm{c}} = 0.7\left[E_{\mathrm{g}}(x) - E_{\mathrm{g}}(0)\right] \quad (5)$$

Our calculated AlGaN/AlN/GaN model contains a 20–40 nm thick $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{N}$ top barrier layer with the Al content x ranging from 0.1 to 0.3, a 1–3.5 nm thick AlN interfacial layer and a 1 μm thick GaN buffer layer. The $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{N}$/AlN/GaN heterostructure is assumed to be unintentionally doped. Both the AlGaN barrier layer and the AlN interfacial layer were coherently on GaN layer. The calculation is done for 300 K temperature.

3 Results and discussion

Firstly, we perform calculation on a 20nm $\mathrm{Al_{0.3}Ga_{0.7}N}$/AlN/GaN heterostructure with an AlN thickness of 1 and 2.5 nm. The potential profiles and 2DEG distributions are shown in Fig. 1 in which z denotes the distance away from the surface to the inside of the heterostructure. With the increase of AlN thickness from 1nm to 2.5nm, the 2DEG peak concentration is considerably increased from $7.0\times10^{19}\ \mathrm{cm^{-3}}$ to $9.1\times10^{19}\ \mathrm{cm^{-3}}$, and the calculated 2DEG sheet density is increased from $1.53\times10^{13}\ \mathrm{cm^{-2}}$ to $1.87\times10^{13}\ \mathrm{cm^{-2}}$. The calculated 2DEG sheet density for the heterostructure with 1 nm-thick AlN interfacial layer shows a good agreement with the experiment data of $1.5\times10^{13}\ \mathrm{cm^{-2}}$ in [5]. While it is moderately larger than $1.22\times10^{13}\ \mathrm{cm^{-2}}$ reported in [1], mainly due to the weakened polarization effect by possible lattice defects and dislocations or higher surface barrier height. The increase of the 2DEG sheet density with increasing the AlN thickness can be explained as follows. The insertion of an AlN interfacial layer leads to a sharp increase of the positive polarization charges at the AlN/GaN interface (from $1.68\times10^{13}\ \mathrm{cm^{-2}}$ to $6.41\times10^{13}\ \mathrm{cm^{-2}}$ by calculation), which, however, does not contribute to the 2DEG density effectively for a thin AlN layer due to the tantamount of negative polarization charges at the AlGaN/AlN interface. By increasing the AlN thickness, charges at the AlN/GaN interface are less affected by the negative charges, thereby inducing more electrons in the quantum well. On the other hand, the presence of negative charges remarkably lifts the potential at the AlGaN/AlN interface upward; as a result, the direction of the electron field in the AlGaN barrier, which is shown by the slope of the potential profile, could turn from negative to positive under our boundary conditions. This is directly responsible for the unusual dependence of the 2DEG density on the thickness of the top AlGaN barrier, which will be discussed in detail with the subsequent calculations.

Figure 2 shows the potential profiles and 2DEG distributions of $\mathrm{Al_{0.3}Ga_{0.7}N}$/AlN/GaN heterostructures with the AlGaN barrier thickness of 20 or 30nm. The AlN interfacial layer thicknesses are a 1 nm or b 2.5 nm, respectively. For the AlGaN/AlN/GaN with a 1 nm-thick AlN interfacial layer, as shown in Fig. 2a, with the increase of AlGaN barrier thickness from 20 to 30 nm, the 2DEG concentration increases due to the enlarged potential drop over the AlGaN barrier (from 0.59 eV to 0.61 eV). Similar dependence of 2DEG on the AlGaN barrier thickness has been experimentally and theoretically demonstrated in a simple AlGaN/GaN heterostructure without employing an AlN interfacial layer [13, 14], therefore the insertion of a 1 nm-thick AlN interfacial layer does not substantially influence the 2DEG density, which is induced dominantly by the AlGaN barrier. Whereas for a 2.5 nm AlN interfacial layer, as shown in Fig. 2b, increasing the AlGaN

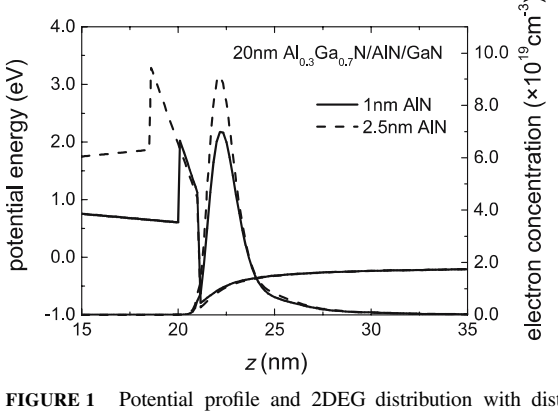

FIGURE 1 Potential profile and 2DEG distribution with distance z for a 20 nm $\mathrm{Al_{0.3}Ga_{0.7}N}$/AlN/GaN heterostructure with an AlN interfacial layer thickness of 1 and 2.5 nm

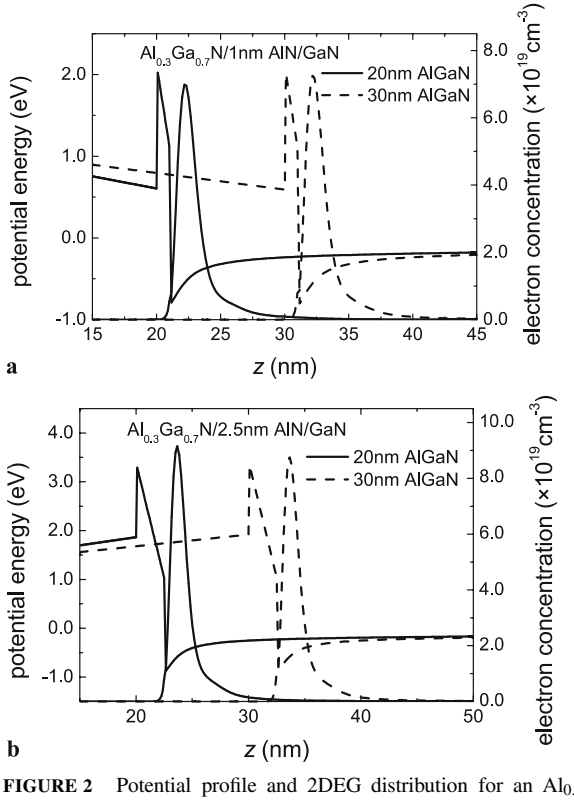

FIGURE 2 Potential profile and 2DEG distribution for an $\mathrm{Al_{0.3}Ga_{0.7}N}$/AlN/GaN heterostructure with an AlGaN barrier thickness of 20 nm and 30 nm and an AlN thickness of (**a**)1 nm and (**b**) 2.5 nm

thickness from 20 to 30 nm results in a slight decrease of the 2DEG concentration with the sheet density decreasing from $1.87 \times 10^{13}\,\mathrm{cm}^{-2}$ to $1.82 \times 10^{13}\,\mathrm{cm}^{-2}$, owing to the uplift of electron potential energy (from 3.29 eV to 3.34 eV) at the AlGaN/AlN interface. And this 2DEG dependence is similar to the case of an AlN/GaN heterostructure capped with a GaN layer [5], indicating that the AlN layer predominantly induce the 2DEG with a thickness of 2.5 nm in the AlGaN/AlN/GaN heterostructure. Comparing Fig. 2a and b, it is clear that the AlGaN barrier predominantly induce the 2DEG for a thinner AlN layer, while the AlN layer take the dominant contribution to the 2DEG formation when it is thick enough.

The 2DEG sheet density in dependence on the AlGaN barrier thickness of an $Al_{0.3}Ga_{0.7}$/AlN/GaN heterostructure is shown in Fig. 3a for different AlN thicknesses of 1–2.5 nm. The case of a simple $Al_{0.3}Ga_{0.7}N$/GaN heterostructure ($d_{\mathrm{AlN}} = 0$) is also shown for comparison. It is clear that insertion of an AlN interfacial layer tends to weaken the increasing dependence of the 2DEG sheet density on the AlGaN barrier thickness. This coincides with the experiment results in [5] which mentioned that the density of the 2DEG in an AlGaN/AlN/GaN structure ($d_{\mathrm{AlN}} = 1$ nm) does not vary with the width of the AlGaN cap layer as significantly as a common AlGaN/GaN structure. As discussed in Fig. 2, for a 1 nm-thick AlN interfacial layer, the 2DEG sheet density increases with the AlGaN thickness and tends to saturate, which is also found in the case of a 1.5 nm AlN layer. When further increasing the AlN thickness to 2 nm, the 2DEG sheet density begins to decrease with increasing the AlGaN thickness, and the decrease is heavier for a 2.5 nm AlN barrier. It can be learned from these results that an AlN/GaN structure should be an ideal structure in which the highest 2DEG density can be achieved. However, AlN/GaN heterostructure is not properly applied for devices for the very thin AlN barrier (only 3.5–5 nm) due to the large lattice mismatch between AlN and GaN. Besides, the increase in the AlN barrier thickness is accompanied by a significant reduction in the electron mobility [5]. As a result, there are very few reports in the literature on the devices based on AlN/GaN heterostructure. It is interesting to note from Fig. 3a that, there should be a "critical" AlN thickness at which the 2DEG does not change with the AlGaN thickness. This claim is confirmed by Fig. 3b which shows the 2DEG sheet density as a function of the AlN thickness for different AlGaN barrier thicknesses. All the curves intersect at one point where the thickness of the AlN layer is about 1.63 nm, indicating that the 2DEG sheet density is independent of the AlGaN thickness at $d_{\mathrm{AlN}} = 1.63$ nm. Also can be seen is that the 2DEG sheet density always linearly increases with the increase of the AlN thickness, which is stronger for thinner AlGaN barrier.

Taking $d_{\mathrm{AlN}} = 1.63$ nm into calculation, the corresponding results for an $Al_{0.3}Ga_{0.7}N$/AlN/GaN heterostructure with an AlGaN barrier thickness of 20 and 30nm are shown in Fig. 4. There is no observable difference between the potential profiles and 2DEG distributions for different AlGaN barrier thicknesses, and the 2DEG sheet density keeps about $1.68 \times 10^{13}\,\mathrm{cm}^{-2}$ when AlGaN thickness is increased from 20 to 30 nm. This is easy to understand when we notice that the potential energy in the AlGaN top barrier does not vary with the distance, therefore keeping the potential energy at the

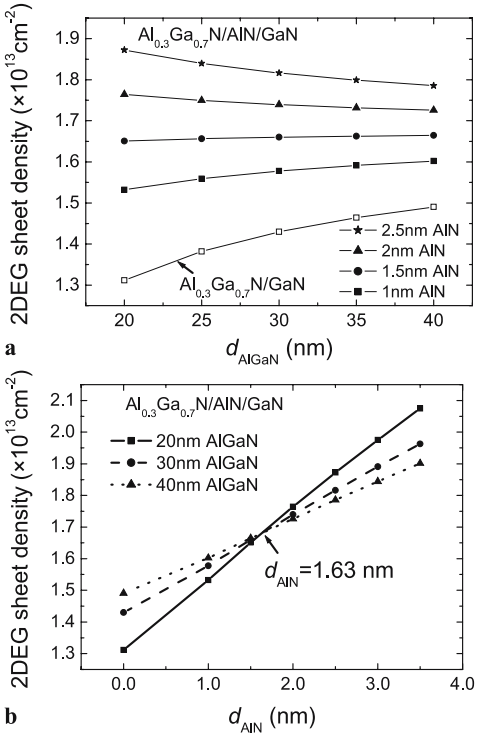

FIGURE 3 (**a**) 2DEG sheet density in dependence on the AlGaN barrier thickness for an $Al_{0.3}Ga_{0.7}N$/AlN/GaN heterostructure with different AlN thicknesses of 0–2.5 nm. (**b**) 2DEG sheet density in dependence on the AlN interfacial layer thickness with different AlGaN thicknesses of 20–40 nm

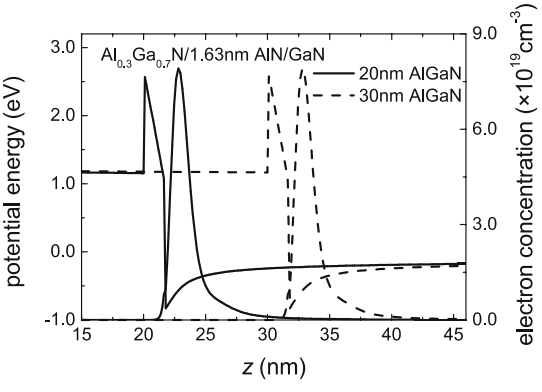

FIGURE 4 Potential profile and 2DEG distribution for an $Al_{0.3}Ga_{0.7}N$/1.63 nm AlN/GaN heterostructure with an AlGaN thickness of 20 and 30 nm

AlGaN/AlN interface unchanged and consequently resulting in a constant 2DEG density.

So far in the calculation, the Al content of the top AlGaN barrier was fixed at 0.3, and we obtained a critical thickness of $d_{\mathrm{cAlN}} = 1.63$ nm. However, since the Al content strongly modulates the spontaneous and piezoelectric polarizations of the AlGaN barrier which contribute to the 2DEG density, the critical AlN thickness d_{cAlN} should largely depend on the Al content. Figure 5a shows the critical AlN thickness as a function of the Al content x in the $Al_xGa_{1-x}N$ barrier layer. The critical AlN thickness increases with increasing Al content x. This curve divides the coordinate plane into two parts; the upper half-plane represents the dominant contribution of AlN layer to the 2DEG density. That is, for an $Al_xGa_{1-x}N$/AlN/GaN heterostructure with parameters of Al content x and d_{AlN}

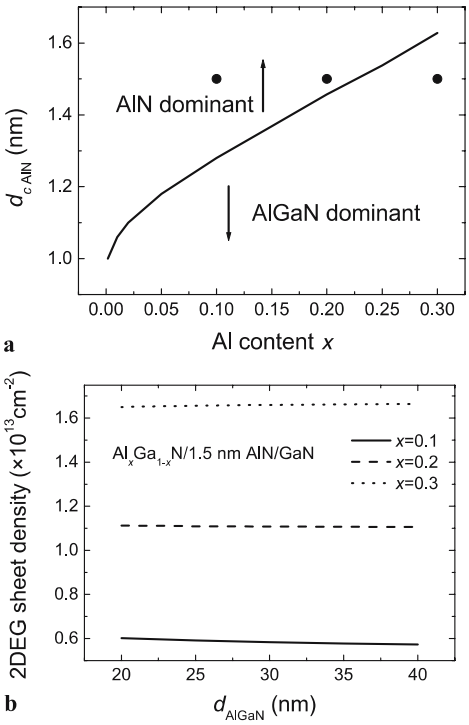

FIGURE 5 (**a**) The critical AlN layer thickness d_{cAlN} as a function of the Al content x of the AlGaN barrier. (**b**) 2DEG sheet density in dependence on the AlGaN barrier thickness for an $Al_xGa_{1-x}N$/1.5 nm AlN/GaN heterostructure with an Al content x of 0.1, 0.2 and 0.3

falling into the upper half-plane, increasing the AlGaN thickness leads to a decrease of the 2DEG density. While the 2DEG density increases with the AlGaN barrier thickness when the heterostructure parameters of x and d_{AlN} fall into the lower half-plane where the contribution of the AlGaN barrier to the 2DEG density is dominant.

For instance, we choose three points in Fig. 5a, the parameters are $d_{AlN} = 1.5$ nm and Al content $x = 0.1$, 0.2 and 0.3, respectively. The corresponding 2DEG sheet densities as a function of the AlN thickness are shown in Fig. 5b. For Al content $x = 0.1$, 0.2, the 2DEG decreases with increasing the AlGaN thickness, which is more slight for the case of $x = 0.2$. This agrees with the analysis before, since the points of $d_{AlN} = 1.5$ nm and $x = 0.1$, 0.2 fall in the upper half-plane of the Fig. 5a, and the point of $x = 0.2$ is closer to the critical curve. Further increasing the Al content to $x = 0.3$, as shown by the dotted line, the 2DEG sheet density turns to increase with increasing the AlGaN thickness due to the dominant contribution of the AlGaN layer, see from Fig. 5a, the parameter point falls into the lower half-plane.

4 Summary

In summary, 2DEG density and distribution in $Al_xGa_{1-x}N$/AlN/GaN heterostructure are theoretically investigated for different thicknesses of the AlGaN barrier layer and the AlN interfacial layer. Increasing the AlN interfacial layer thickness results in significant increment of the 2DEG sheet density, which is stronger for thinner AlGaN barrier layer. We found a critical AlN layer thickness d_{cAlN} below which the 2DEG sheet density increases with the increase of AlGaN thickness, indicating a dominant contribution of the AlGaN layer to the 2DEG density since the dependence is typical for a simple AlGaN/GaN heterostructure. Whereas the AlN layer exhibits a dominant contribution to the 2DEG density with thickness exceeding the critical value. In this case increasing the AlGaN thickness leads to a decrease of the 2DEG sheet density, similar to what happened in an AlGaN/GaN heterostructure capped with a GaN layer. Further investigation demonstrated the dependence of d_{cAlN} on the Al content x in the AlGaN barrier. It is suggested by our calculation that increasing the AlN interfacial layer thickness larger than commonly used 1nm, especially for an Al-rich AlGaN top barrier, will largely benefit the 2DEG in AlGaN/AlN/GaN heterostructure. While it should be carefully operated in experiment to avoid the possible large degradation of the crystal quality and hence the carrier mobility.

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