Influence of AlN/GaN interfacial non-idealities on the properties of two-dimensional electron gas in AlGaN/AlN/GaN heterostructures

D S Arteev¹, A V Sakharov¹, W V Lundin¹, E E Zavarin¹ and A F Tsatsulnikov²

¹ Ioffe Institute, 26 Politekhnicheskaya, 194021 St. Petersburg, Russia
² Submicron Heterostructures for Microelectronics, Research & Engineering Center, RAS, 26 Politekhnicheskaya, 194021 St. Petersburg, Russia

e-mail: ArteevDS@mail.ioffe.ru

Abstract. The influence of two types of AlN/GaN interfacial non-idealities, namely unintentional Ga incorporation into AlN spacer and blurring of the spacer due to Al and/or Ga atomic diffusion on the mobility and density of two-dimensional electron gas in AlGaN/AlN/GaN heterostructure was studied theoretically. It was found that moderate amount of GaN in the nominal AlN spacer does not affect much the mobility and density of 2DEG as long as the interface is abrupt. In contrast, the blurring of AlN/GaN interface was found to have a significant impact on the mobility and sheet resistance of the structure since the GaN channel actually becomes AlGaN and alloy-disorder scattering takes place.

1. Introduction

III-nitride-based heterostructures are very promising for high-power and high-temperature electronics due to their unique properties, namely wide range of bandgap energies from 0.7 to 6.2 eV, high electron saturation velocity and high breakdown voltages. The polar nature of these materials and large conduction band offset allows achieving high-electron mobility transistors (HEMTs) with two-dimensional electron gas (2DEG) density of 1-3×10¹³ cm⁻² and mobility up to 2200 cm²V⁻¹s⁻¹ even without intentional doping [1]. However, doping of the buffer layers with different deep acceptor impurities (e.g. carbon, iron and other less common dopants like Mn, Cr, Be, etc. [2]) are usually used to compensate unintentional donor and ensure insulating character of the layers.

The mobility of 2DEG is one of the main parameters of the HEMT. The most common HEMT design includes GaN-channel and AlGaN barrier layer. Since AlGaN is a ternary alloy, the so-called alloy-disorder scattering takes place, resulting in degradation of the mobility of the 2DEG. To reduce the influence of alloy scattering, a thin AlN spacer may be introduced between GaN and AlGaN as theoretically proposed by [3].

Despite the fact that both metalorganic vapor phase epitaxy (MOVPE) and molecular beam epitaxy (MBE) techniques are used for a long time, the growth of high quality III-N layers with abrupt interfaces is still challenging. An unintentional gallium incorporation into subsequent layers are often observed for MOVPE-grown [4, 5, 6, 7] and MBE-grown [7] heterostructures. Moreover, composition profiles measured by atom probe tomography or secondary-ion mass spectrometry rarely show abrupt interfaces between the layers. However, it is questionable if they reflect “true” atomic distribution or it is just a measurement artifact due to poor spatial resolution or surface roughness [8, 9].
Since GaN-based HEMTs is one of the main candidates for high-temperature operation [10], one need to know how their properties may change in time during high-temperature operation. For example, it was both theoretically and experimentally shown that interdiffusion of Al and Ga occurs with high-temperature annealing [11, 12]. This could potentially lead to the blurring of the AlN spacer and increasing of alloy-disorder scattering rate since nominally AlN/GaN interface become gradient AlGaN/AlGaN one. This could be one of the reasons for the experimentally observe reduction of 2DEG mobility after the high-temperature annealing [13, 14].

In this paper, the influence of unintentional Ga incorporation into AlN spacer and blurring of the spacer due to Al and/or Ga atomic diffusion on the properties of 2DEG in AlGaN/AlN/GaN heterostructure was studied theoretically.

2. Model description

A HEMT structure with 25 nm Al$_{0.25}$Ga$_{0.75}$N, 1 nm AlN interlayer and thick GaN channel was used as a model. In order to obtain wave functions corresponding to 2DEG, the 1-D Schrödinger-Poisson equation system was solved self-consistently using Python programming language. The Schrödinger equation is given by:

$$
\left[ -\frac{h^2}{2} \frac{d}{dz} \left( \frac{1}{m^*(z)} \frac{d}{dz} \right) - q\phi(z) + \Delta E_c(z) \right] \psi_i(z) = E_i \psi_i(z)
$$

(1)

where $E_i$ and $\psi_i(z)$ are the energy level and wave function of the $i$th subband, $m^*(z)$ is electron effective mass, $\phi(z)$ is the electrostatic potential and $\Delta E_c(z)$ is a conduction band discontinuity. An improved shooting approach [15] was used to solve the equation.

The Poisson equation is given by

$$
\frac{d}{dz} \left( P_{tot}(z) - \varepsilon_0 \varepsilon(z) \frac{d\phi}{dz} \right) = q(N_D(z) - N_A(z) + p(z) - n(z))
$$

(2)

where total polarization $P_{tot}(z)$ is the sum of spontaneous $P_{sp}(z)$ and piezoelectric $P_{pz}(z)$ polarizations. In the present study, the structure is assumed to be undoped, so $N_D(z)$, $N_A(z)$ and $p(z)$ are equal to zero. Following an approach similar to that of [16], the electron density $n(z)$ was split into 2D and 3D components by introducing separation energy $E_{sep}$ to reduce a computation time without loss of accuracy. The 3D electron density $n_{3D}(z)$ of electrons with energy higher than $E_{sep}$ is expressed as

$$
n_{3D}(z) = N_c(z) F_{1/2}(\eta, b)
$$

(3)

where $N_c(z)$ is the effective density of states and $F_{1/2}(\eta, b)$ is the incomplete Fermi integral of the order of 1/2:

$$
F_{1/2}(\eta, b) = \frac{2}{\sqrt{\pi}} \int_b^\infty \frac{y^{1/2}}{1 + \exp(y - \eta)} dy
$$

(4)

where

$$
\eta(z) = \frac{E_F + q\phi(z) - \Delta E_c(z)}{kT} \quad \text{and} \quad b = \max \left[ 0, \frac{E_{sep} + q\phi(z) - \Delta E_c(z)}{kT} \right]
$$

(5)

For faster evaluation, the approximation from [17] was used for $b = 0$.

The 2D electron density $n_{2D}(z)$ is calculated as
The choice of $E_{\text{sep}}$ is somewhat arbitrary. We assumed that electrons become 3D when the separation between two adjacent energy levels becomes smaller than $kT$ (i.e. $E_{\text{sep}} = E_i$ when $E_{i+1} - E_i < kT$).

A predictor-corrector approach [18] was implemented for faster convergence.

The alloy disorder scattering rate for degenerate 2DEG can be expressed as [19, 20, 21]:

$$\frac{1}{\tau_{\text{AD}}} = \frac{\Delta V^2}{h^5} \int m^*(z)\Omega(z)x(z)[1-x(z)]\psi^4(z)dz$$

(7)

where $\Delta V$ is the alloy scattering potential, $\Omega(z) = (\sqrt{3}/2)a^2(z)c(z)$ is the volume of wurtzite unit cell with in-plane $a(z)$ and out-of-plane $c(z)$ lattice constants. It is easy to see that the expression reduces to the conventional one (e.g. [22]) when the alloy composition is constant through the region of interest. The structure is considered to be pseudomorphically-grown on a relaxed GaN buffer layer, therefore $a(z) = a_{\text{GaN}}$, and $c(z)$ is found as

$$c(z) = c_0(z)\left[1 - 2\frac{C_{13}(z)}{C_{33}(z)}\varepsilon_{xx}(z)\right]$$

(8)

where $c_0(z)$ is unstrained lattice constant, $\varepsilon_{xx}(z)$ is in-plane strain, $C_{13}(z)$ and $C_{33}(z)$ are elastic stiffness constants. Although the authors of [21] took screening into account, alloy disorder as a short-range potential is often considered unscreened. In the present work, the screening was neglected, and only the ground state wavefunction was taken into account. The total mobility was calculated by the Matthiessen rule as:

$$\frac{1}{\mu_{\text{total}}} = \frac{1}{\mu_0} + \frac{1}{\mu_{\text{AD}}}$$

(9)

where $\mu_0$ is the mobility, limited by the other scattering mechanisms. We assumed $\mu_0^{\text{RT}}=2100 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ and $\mu_0^{77K}=30000 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ as phonon- and dislocation-scattering limited mobility at room-temperature and 77 K, respectively [23]. Random-dipole scattering originated from a polarization charge fluctuations due to random distribution of dipoles in AlGaN is expected to be an order of magnitude weaker than alloy-disorder scattering [21, 24], therefore it was neglected in the present calculations. Most of the material parameters needed were taken from [25].

3. Results

Let us first consider unintentional gallium incorporation into the AlN spacer, but with an abrupt Al(Ga)N/GaN interface. In that case alloy disorder scattering takes place not only in AlGaN barrier, but in the spacer layer, which is AlGaN now as well (figure 1), leading to reducing the mobility (figure 2). Moreover, the higher Ga content in the spacer, the lower the 2DEG density. However, only relatively small part of the wavefunction penetrates the AlGaN layers, as one can see from figure 1, so the alloy-disorder scattering is weak, and, for the experimentally observed Ga mole fractions $\leq 0.4-0.5$, the reduction of 2DEG mobility and density is insignificant, leading to $\sim 10-15\%$ increase in sheet resistance in the worst case in comparison to ideal AlN/GaN interface. Therefore, an unintentional Ga incorporation into the AlN space does not influence much on the properties of the 2DEG at neither room nor liquid nitrogen temperature.
Figure 1. Conduction band energy (black lines) and electron ground level wavefunctions (color dashed lines) for the structures with AlN, Al\textsubscript{0.5}Ga\textsubscript{0.5}N and Al\textsubscript{0.25}Ga\textsubscript{0.75}N spacer. Grey gradient indicates normalized scattering rate; thick color lines show the part of the wavefunction that is scattered by alloy disorder.

Figure 2. (a) Calculated mobility and density of 2DEG and sheet resistance at room temperature versus unintentional Ga mole fraction in the spacer. (b) Calculated alloy-disorder-limited mobility and total mobility at room and liquid nitrogen temperature in log scale.

Now consider blurring of the AlN spacer (e.g. due to Al-Ga interdiffusion). For simplicity, let’s assume concentration independent interdiffusion coefficient \( D \). Then, Al content \( x(z) \) can be expressed as

\[
x(z, t) = x_{\text{AlGaN}} + \frac{1 - x_{\text{AlGaN}}}{2} \left[ 1 + \text{erf} \left( \frac{z + d_{\text{Al}}}{2L} \right) \right] - \frac{1}{2} \left[ 1 + \text{erf} \left( \frac{z - d_{\text{Al}}}{2L} \right) \right]
\]

where \( x_{\text{AlGaN}} \) is Al content in AlGaN barrier layer, \( d_{\text{Al}} \) is the thickness of the AlN spacer, \( L = \sqrt{D \tau} \) is diffusion length (note that \( z = 0 \) corresponds the middle of the spacer). In that case, the channel region is not binary GaN, but ternary AlGaN, so alloy disorder scattering takes place. Figure 3 shows the calculated conduction band energies and wave functions for \( L = 0.25 \), 0.50 and 1.00 nm; the inset show concentration profiles. As one can see, a rather significant part of the 2DEG may undergo alloy disorder scattering, and the mobility may be reduced significantly (figure 4). The 2DEG density is slightly lower for more blurred interface. For instance, the diffusion length of one monolayer (~0.25 nm) resulted in ~30% increase of sheet resistance in comparison with the ideal structure. In the case of very blurred AlN the sheet resistance may increase fourfold. The obtained results are similar to that of [19], calculated for GaAs/AlGaAs with diffused interface.
**Figure 3.** Conduction band energy (black lines) and electron ground level wavefunctions (color dashed lines) for the structures with blurred AlN spacer for L=0.25, 0.50 and 1.00 nm. Grey gradient indicates scattering rate; thick color lines show the part of the wavefunction that is scattered by alloy disorder (for x>0.001). The inset shows corresponding concentration profiles.

**Figure 4.** (a) Calculated mobility and density of 2DEG and sheet resistance at room temperature versus diffusion length. (b) Calculated alloy-disorder-limited mobility and total mobility at room and liquid nitrogen temperature in log scale.

For comparison, we borrowed the data from [13]. It is difficult to compare the directly, since the authors studied the dependencies on annealing temperature. However, the diffusivity usually depends on temperature as \( D(T) = D_0 \exp(-E_a/kT) \), so \( L = \sqrt{D_0 \exp(-E_a/kT) \cdot t} \). Using the values \( E_a = 1.02 \) eV and \( D_0 t = 6 \times 10^{-11} \) cm² and the given as-grown mobility at 77 K of 13360 cm²/V·s as \( \mu_0 \), a good agreement is achieved (figure 5). The experimental values of the 2DEG density also agrees well (within 10%). Therefore, alloy disorder scattering due to blurring of the AlN spacer may considered as one of the possible mechanisms of degradation of GaN-based HEMTs.

**Figure 5.** Comparison of the mobility and density of 2DEG with experimental data from [13]. See text for details.
4. Conclusion
The influence of unintentional Ga incorporation into AlN spacer and blurring of the spacer due to Al and/or Ga atomic diffusion during the growth process or Al-Ga interdiffusion due to thermal annealing on the properties of 2DEG in AlGaN/AlN/GaN heterostructure was studied theoretically. It was found that moderate amount of GaN in the nominal AlN spacer does not affect much the mobility and density of 2DEG as long as the interface is abrupt. In contrast, the blurring of AlN/GaN interface was found to have a significant impact on the mobility and sheet resistance of the structure since the GaN channel actually becomes AlGaN and alloy-disorder scattering takes place. The interface blurring can be resulted either from atomic diffusion during the growth or from prolonged exposure to high temperatures.

It should be noted that there could be other processes caused by exposure to high temperatures, leading to the degradation of the structure, such as strain relaxation or surface oxidation. There is another scattering mechanism that usually considered to significantly reduce the 2DEG mobility, namely interface roughness scattering. And could the impact of alloy-disorder scattering due to the blurred interface be distinguished from interface roughness scattering – that is an open question, and further theoretical and experimental investigations are needed.

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