The effect of doping in different layers on 2DEG for ultrathin-barrier AlN/GaN heterostructures

J. M. Al ABBAS*, P. NARIN, G. ATMACA, E. KUTLU, B. SARIKAVAK-LISESIVDIN, S. B. LISESIVDIN
Gazi University, Faculty of Science, Department of Physics, 06500 Teknikokullar, Ankara, Turkey

In this study, we have numerically investigated the two-dimensional electron gas (2DEG) carrier densities and electron probability densities of pseudomorphically grown ultrathin-barrier AlN/GaN heterostructures using self-consistent solutions of one-dimensional, non-linear Schrödinger–Poisson equations. In these calculations, we have focused on three different AlN/GaN heterostructures included fully undoped, the only Si-doped cap layer and the only Si-doped barrier layer. As a result of the calculations, it was found that doping of AlN barrier layer more effective than other cases on the 2DEG carrier density and the doping of GaN cap layer has not a significant effect on the 2DEG probability densities.

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1. Introduction

AlN material has been established as a main focal point for the development of deep ultraviolet optoelectronic devices as well as high-power and high-frequency electronic devices owing to outstanding properties such as wide and direct bandgap and high thermal conductivity. AlN/GaN High Electron Mobility Transistors (HEMTs) have been the subject of research to approach the theoretically predicted device performance [1]. In AlN/GaN heterostructures, extremely high two-dimensional electron gas (2DEG) density of up to 5.0×10^{13} cm^{-2} can be induced at the interface under an ultrathin AlN barrier due to the large difference in spontaneous and piezoelectric polarization between AlN and GaN [2-4]. Various barriers alternatives have been used in nitride-based HEMTs to improve the performance of devices [4-6]. Additionally, the electron mobility is expected to be high due to the absence of alloy disorder scattering in AlN barrier.

In this study, we have focused on ultrathin-barrier GaN/AlN/GaN heterostructures that are suitable for HEMT applications where high frequency and high current are required. 2DEG carrier density of these heterostructures is decisive on output characteristics, cut-off frequency, output conductance and drain current density for a device. One way to increase 2DEG carrier density is doped with Si of heterostructures. However, Si doping in different layers can be a different influence on some 2DEG properties included the conduction band energy, the sheet carrier density and the probability density. So, it is necessary to define how the Si doping in different layers influences 2DEG properties. For this purpose, we have investigated the influence of doping of the GaN cap and AlN barrier layers on 2DEG properties in ultrathin-barrier GaN/AlN/GaN heterostructures using the numerical calculations. The numerical investigations of 2DEG properties in GaN-based heterostructures will help to contribute to the development of transistors with higher carrier density and higher mobility [7-11].

2. Numerical model details

The numerical investigation of the ultrathin-barrier GaN/AlN/GaN heterostructures has been performed with the solutions of one-dimensional (1D) self-consistent Schrödinger-Poisson equations using TiberCAD software [11-12]. These solutions are included strain, polarization induced charges and band structures of wurtzite semiconductors [12]. Material parameters used in the calculations taken from Ref. [13] and listed in Table 1. Donor activation energy of Si doping is accepted as 25 meV in the calculations [14]. Fig. 1 shows the layer sequence of the simulated a) undoped GaN/AlN/GaN, b) n-GaN/AlN/GaN and c) GaN/n-AlN/GaN heterostructures. In this calculations, it is assumed that all layers of these heterostructures are pseudomorphically grown on a GaN substrate. Si doping density is 1×10^{18} cm^{-3}.

In the calculations, Schrödinger and Poisson equations are solved with a self-consistent method to obtain the conduction band structures, the 2DEG carrier densities and wave functions. The 2DEG which is populated in pseudotriangular quantum well located at the interface between AlN/GaN layers is largely induced by polarization fields. Therefore, the numerical calculation procedure begins with a strain calculation with homogeneous strain dispersion over the heterostructure [15]. With calculated the strain in layers of a heterostructure, piezoelectric polarization (P^{PE}) at each interface is calculated by

$$P^{PE} = 2\varepsilon_1 \left\{ e_{31} - e_{33} \frac{C_{13}}{C_{33}} \right\} \text{ (C/m}^2\text{)}. \quad (1)$$

Here, e_{31} and e_{33} are piezoelectric constants and ε_1 is in-plane strain [16]. The parameters of GaN and AlN materials are given in Table 1 [13].

The calculated piezoelectric polarization is used in Poisson equation. The numerical methods were based on the self-consistent solution of the reciprocally coupled equations of the Poisson model for carrier transport given by

$$-\nabla(\varepsilon\nabla\varphi - P) = -e(n - p - N_d^+ + N_a^-) \quad (2)$$

where ε, φ, n, p, N_d^+, N_a^- are the permittivity, the electric potential, the electron and the hole densities, densities of the ionized donors and acceptors, respectively. P is also the electric polarization included spontaneous and piezoelectric polarization. From the solution of the Schrödinger equation, eigenstates, carrier densities and probability densities of electrons in a quantum well are obtained. The carrier density can be included in the Poisson equation for self-consistent Schrödinger-Poisson calculations.

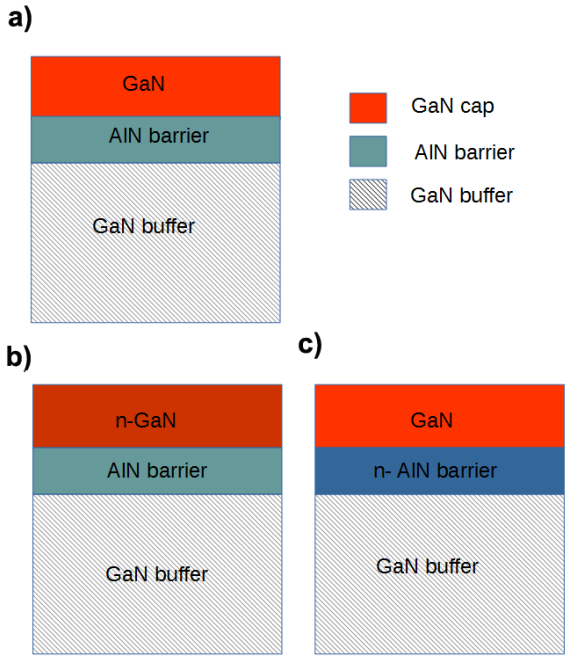

Fig. 1. Schematic cross section for a) GaN/AlN/GaN heterostructure, b) n-GaN/AlN/GaN heterostructures and c) GaN/n-AlN/GaN heterostructure

Table 1. Lattice parameters, spontaneous polarization, piezoelectric and elastic constant values of GaN and AlN materials [13]

	GaN	AlN
a (nm)	0.3189	0.3112
e_{31} (C/m^2)	-0.49	-0.60
e_{33} (C/m^2)	0.73	1.46
C_{13}(GPa)	106	108
C_{33}(GPa)	398	373
P^{SP}(C/m^2)	-0.029	-0.081

3. Results and discussions

Fig. 2 shows the conduction band structures of the investigated heterostructures are given in Fig. 1. The thicknesses of the GaN cap layer, the AlN barrier layer, and the GaN buffer layer are set 2 nm, 3 nm and 1 μm, respectively. It can be seen that the quantum well in a heterostructure with the only Si-doped barrier layer is deeper than other heterostructures. Because the carriers from Si-doped barrier layer create additional the electrical field and this electrical field bends conduction band in the interface.

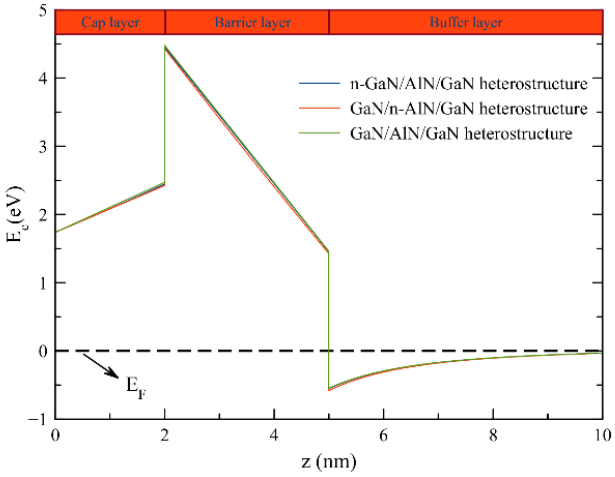

Fig. 2. Calculated conduction band structures of investigated heterostructures. The Fermi level E_F is indicated by the horizontal dash line

Fig. 3 shows the dependence of 2DEG carrier density on AlN barrier layer thickness in AlN/GaN heterostructures included fully undoped, the only Si-doped cap layer and the only Si-doped barrier layer. 2DEG carrier density is increased with increasing the AlN barrier layer thickness. This increment in AlN/GaN heterostructures with Si-doped AlN barrier layer is more than other two heterostructures according to Fig. 3. As a result of calculations, 2DEG carrier densities in GaN/AlN/GaN heterostructure, n-GaN/AlN/GaN

heterostructure and GaN/n-AlN/GaN heterostructure are 2.81×10^{20} cm^{-3}, 2.7×10^{20} cm^{-3} and 3.04×10^{20} cm^{-3} when thicknesses of GaN cap layer and AlN barrier layer are taken as 2 nm and 4 nm, respectively. Consequently, the doping of AlN barrier layer more effective than other cases on the 2DEG carrier density.

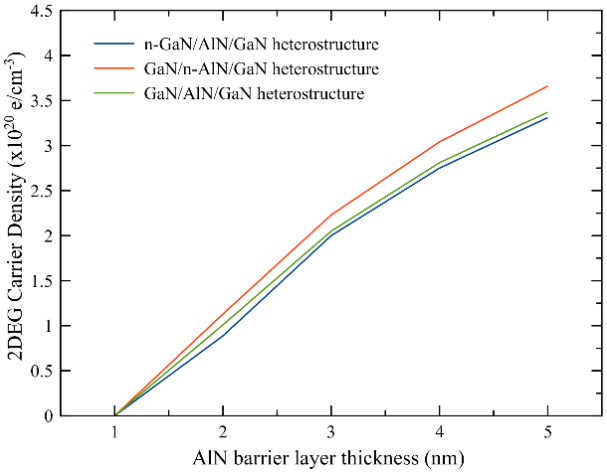

Fig. 3. 2DEG carrier density versus different AlN barrier layer thicknesses for investigated GaN/AlN/GaN heterostructures. Blue: heterostructure with Si-doped cap layer, Red: heterostructure with Si-doped barrier layer and Green: fully undoped heterostructure

Fig. 4 shows the probability densities of 2DEG carriers in the pseudotriangular quantum well for AlN/GaN heterostructures included fully undoped, the only Si-doped cap layer and the only Si-doped barrier layer. When electron probability density is close to the interface, the effects of mobility scattering mechanisms such as alloy disorder and interface roughness on 2DEG electrons may increase [17]. In this study, the alloy disorder scattering mechanism can be neglect due to AlN barrier layer [4]. On the other hand, when probability density of 2DEG electrons is far away from the interface, it could be more influenced by impurity-related scattering mechanisms [18]. Therefore, 2DEG electrons least affected these scattering mechanisms are located in the interface of AlN/GaN heterostructure with Si-doped AlN barrier layer according to Fig. 4. However, it was found that the doping of GaN cap layer has not a significant effect on the 2DEG probability densities.

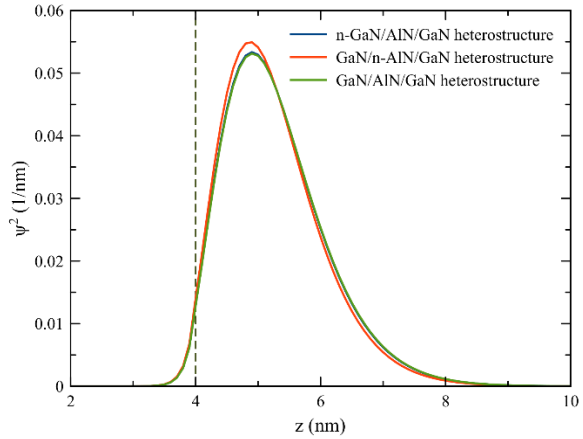

Fig. 4. 2DEG probability density for investigated GaN/AlN/GaN heterostructures. Blue: heterostructure with Si-doped cap layer, Red: heterostructures with Si-doped barrier layer and Green: fully undoped heterostructure

4. Conclusions

In this study, 2DEG properties in ultrathin-barrier AlN/GaN heterostructures included fully undoped, the only Si-doped cap layer and only Si-doped barrier layer were investigated. We have presented the influence of the AlN barrier layer thickness and doping in the GaN cap layer and AlN barrier layer on 2DEG properties in these heterostructures. As a result of the calculations, it was that the doping of AlN barrier layer more effective than other cases on the 2DEG carrier density and the doping of GaN cap layer has not a significant effect on the 2DEG probability densities.

Acknowledgements

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*Corresponding author: jangizafandy@gmail.com