Numerical optimization of In-mole fractions and layer thicknesses in Al$_x$Ga$_{1-x}$N/AlN/GaN high electron mobility transistors with InGaN back barriers

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**Abstract**

The effects of the In-mole fraction ($x$) of an In$_x$Ga$_{1-x}$N back barrier layer and the thicknesses of different layers in pseudomorphic Al$_x$Ga$_{1-x}$N/AlN/In$_x$Ga$_{1-x}$N/GaN heterostructures on band structures and carrier densities were investigated with the help of one-dimensional self-consistent solutions of non-linear Schrödinger–Poisson equations. Strain relaxation limits were also calculated for the investigated Al$_x$Ga$_{1-x}$N barrier layer and In$_x$Ga$_{1-x}$N back barriers. From an experimental point of view, two different optimized structures are suggested, and the possible effects on carrier density and mobility are discussed.

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1. Introduction

The superior material properties of GaN/AlN/InN and the related quaternary and ternary alloys make them the ideal choice for high power and high frequency applications [1,2]. Important progress has been made with improvements in the material quality, device fabrication, and the epitaxial layer designs [3]. However, more advanced device structures are being investigated for further performance improvement. Recently, double-hetero-junction HEMTs were explored to improve carrier confinement, which may result in improved carrier mobility and better pinch-off characteristics for HEMT devices [4–7]. Micovic et al. [4] demonstrated an AlGaN/GaN/AlGaN double-heterojunction HEMT with improved buffer isolation by using an AlGaN buffer layer with an Al composition of 4%. Maeda et al. [5] presented AlGaN/InGaN/AlGaN double heterostructures to improve the confinement of two-dimensional electron gas (2DEG). In addition to all these efforts, thin InGaN layers have also been employed as back...
barriers (by increasing the conduction band offset of the GaN buffer with respect to the GaN channel) in order to increase the confinement of electrons in the channel [6,7].

GaN-based heterostructures are unique in that the 2DEG is accumulated not by intentional doping, but rather by the polarization charges formed at the interface between the bulk GaN region and the AlGaN barrier layer. These polarization charges are composed of two parts: spontaneous and piezoelectric [8,9]. This property is unlike many other semiconductors and, for this reason, as for the AlGaN/GaN system and other III–V nitrides, the effects of both spontaneous and piezoelectric polarization fields must be included in an electrical analysis. Further investigations and understanding of the energy band diagram and charge distribution, which can be obtained by self-consistent Schrödinger–Poisson calculations, are required for the design and analysis of GaN-based HEMT devices.

In this study, we theoretically investigate the effects of the In mole fraction (x) of an InGa1−xN back barrier layer and the thicknesses of different layers on the carrier densities and band structures in pseudomorphic Al0.2Ga0.8N/AlN/GaN/InGa1−xN/GaN heterostructures by solving one-dimensional non-linear Schrödinger–Poisson equations self-consistently including polarization induced carriers [10]. The strain relaxation limits were also calculated with a simple critical thickness calculation approach [11].

2. Device structures and simulation

The general layer sequence of the modeled HEMT structures is shown in Fig. 1. All of the layers are assumed to be grown on a GaN buffer pseudomorphically. The optimum values of the

Fig. 2. (a) Calculated conduction band energy diagram of an AlGaN/AlN/GaN/InGaN/GaN HEMT structure with different GaN channel thicknesses. Inset: a closer view of GaN/InGaN region. (b) Sheet carrier density of the designed HEMT structure versus GaN channel thickness.
In several references [15–18], the AlN, GaN, and InN used in the calculations are taken as wave functions and related eigenenergies. The material parameters are solved self-consistently in order to obtain the carrier distribution, this value and starts to decrease more rapidly with thicknesses up to 10 nm GaN channel thickness, and makes a peak at a thickness of 1 nm, and the In-mole fraction is kept at 0.1. The sheet carrier density increases in very small increments up to 10 nm GaN channel thickness, and makes a peak at this value and starts to decrease more rapidly with thicknesses greater than 12 nm. Although the change in the sheet carrier density is not very significant, the electron confinement effect of the InGaN back barrier layer is smaller for higher GaN channel thicknesses. Therefore, a 10 nm thickness value is chosen as the optimum value for GaN channel thickness.

In Fig. 3, the sheet carrier density of the designed HEMT structure is shown for different InGaN back barrier thicknesses. In these calculations, the InGaN back barrier layer thickness is swept from 1 to 6 nm, and the In-mole fraction is kept at \( x = 0.1 \). The critical thickness of \( \text{In}_x\text{Ga}_{1-x}\text{N} \) on GaN is calculated as 14.4 nm and, therefore, the InGaN layer used here is assumed to be strained. The GaN channel thickness is taken as 10 nm, which is found to be an optimal value in the previous step. There is no considerable change in sheet carrier density with respect to the InGaN back barrier thickness after 3 nm value. It is known that the potential barrier, formed by the InGaN layer, increases with the increase in the InGaN layer thickness [21]. However, as the InGaN layer thickness increases the conduction band offset at the interface between the InGaN-notch and GaN buffer loses its sharpness. As a result, the degree of electron confinement and, therefore, electron mobility is expected to decrease. For the next step of the simulations, the InGaN layer thickness is changed from 1 to 3 nm because more variations are observed and the maximum level is obtained in this interval.

3. Results and discussion

In order to observe the effects of optimizations, a standard AlGaN/AIn/GaN HEMT structure is first chosen as a template and used for comparison at the end of the optimizations. In this standard structure, \( t_{\text{AlGaN}} = 20 \) nm with an Al-mole fraction \( y = 0.3 \) and \( t_{\text{InN}} = 1 \) nm values were used. A higher Al-mole fraction at the barrier layer is required to increase 2DEG conductivity and the breakdown field [19]. However, the growth process of high quality AlGaN layers with high Al content on GaN is problematic due to large lattice mismatch, which can cause defects due to strain relaxation [20]. The critical thickness for \( \text{Al}_x\text{Ga}_{1-x}\text{N} \) is calculated as \( t_{\text{critical}} = 21.8 \) nm. First, the GaN channel thickness was changed and the effects of this change on the conduction band and sheet carrier density were analyzed to find an optimum structure. Second, the InGaN back barrier layer’s thickness was changed with a constant In-mole fraction. In the last step, the In-mole fraction of the InGaN back barrier layer was scanned with three different thicknesses in order to see the combined effects.

The calculated conduction band energy diagram of an AlGaN/AIn/GaN HEMT structure with different GaN channel thicknesses is shown in Fig. 2a. The sheet carrier density of the designed HEMT structure versus GaN channel thickness is shown in Fig. 2b. In these calculations, the InGaN back barrier layer’s thickness is taken as 1 nm, and the In-mole fraction is kept at \( x = 0.1 \). The sheet carrier density increases in very small increments up to 10 nm GaN channel thickness, and makes a peak at this value and starts to decrease more rapidly with thicknesses greater than 12 nm. Although the change in the sheet carrier density is not very significant, the electron confinement effect of the InGaN back barrier layer is smaller for higher GaN channel thicknesses. Therefore, a 10 nm thickness value is chosen as the optimum value for GaN channel thickness.

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Fig. 4 shows the sheet carrier density of the designed HEMT structure versus the In-mole fraction values of the InGaN back barrier layer with different thicknesses. In these calculations, the In-mole fraction is swept from 5% to 20%, and InGaN layer thickness is varied from 1 to 3 nm. As can be seen in the figure, the sheet carrier density is much more dependent on the In-mole fraction for 1 nm thickness when compared to 2 and 3 nm thicknesses. The maximum sheet carrier density is obtained for a 1 nm thick In$_{0.18}$Ga$_{0.82}$N layer. Another option for the back barrier would be a 3 nm thick In$_{0.09}$Ga$_{0.91}$N layer because the sheet carrier density obtained with this layer is very close to that of a 1 nm thick In$_{0.18}$Ga$_{0.82}$N layer. Therefore, one has to carry out further analysis for these two different configurations.

Conduction band diagrams for the structures with 1 and 3 nm thick InGaN layers with varying In-mole fractions are shown in Figs. 5a and b, respectively. In Fig. 5c, the carrier density distributions for 1 nm and 3 thick InGaN back barriers are compared. The InGaN channel is more populated for the structure with 1 nm thick In$_{0.18}$Ga$_{0.82}$N when compared to 3 nm thick In$_{0.09}$Ga$_{0.91}$N. This can be seen as a disadvantage but from the figure it is possible to conclude that these electrons are well confined and spillover to the major channel will not occur. It is also clearly seen that electrons are more likely to spread into the GaN buffer layer for the structure with 3 nm thick InGaN back barrier. Therefore, we proposed an optimum Al$_{0.3}$Ga$_{0.7}$/ALN/IN$_{0.18}$Ga$_{0.82}$/In$_{0.18}$Ga$_{0.82}$/GaN HEMT structure for high 2DEG concentration and mobility with thicknesses of 20, 1, 10, and 1 nm for the layers Al$_{0.3}$Ga$_{0.7}$N, AlN, GaN, and In$_{0.18}$Ga$_{0.82}$N, respectively. However, it should be noted that sheet carrier density dependency to the In-mole fraction for this structure is an important issue from an experimental point of view because it is difficult to precisely control the In-mole fraction of the InGaN layer in growth processes [22].

The calculated conduction band energy diagrams of standard AlGaN/AlN/GaN structure and an optimized structure with an InGaN back barrier are shown in Fig. 6a. In Fig. 6b, carrier density distributions for standard AlGaN/AlN/GaN structure and an optimized structure with an InGaN back barrier are compared. According to the calculation results, a 16.6% increase in the sheet carrier density can be expected by using an InGaN back barrier and by optimizing the layers properly.

### 4. Conclusions

We have modeled Al$_x$Ga$_{1-x}$/N/AlN/In$_x$Ga$_{1-x}$/N/GaN HEMT structures by solving one-dimensional non-linear Schrödinger–Poisson equations self-consistently. Conduction band diagrams
and sheet carrier densities are calculated for different GaN channel and In$_x$Ga$_{1-x}$N back barrier layer thicknesses and for different In-mole fractions, including piezoelectric and spontaneous polarization fields. The effects of the GaN channel thickness, InGaN back barrier thickness, and In-mole fraction were investigated in order to increase carrier density and mobility. The pseudomorphic conditions were also satisfied for all the simulations, in which the optimizations were limited within the strain relaxation limits. According to the optimization results, Al$_{0.3}$Ga$_{0.7}$N/AlN/GaN/In$_{0.18}$Ga$_{0.82}$N/GaN structure with a thickness sequence of 20/1/10/1 nm is proposed for the high-performance devices with a high mobility and high carrier density. From an experimental point of view, Al$_{0.3}$Ga$_{0.7}$N/AlN/GaN/In$_{0.09}$Ga$_{0.91}$N/GaN structure with a thickness sequence of 20/1/10/3 nm should also be taken into account. According to the calculations, a 16.6% increase in sheet carrier density is predicted for an optimized AlGaN/AlN/InGaN/GaN structure compared to conventional AlGaN/AlN/GaN HEMT structures.

These simulation results show that, if optimized properly, AlGaN/AlN/GaN/InGaN/GaN heterostructures have the potential to be a promising structure for making high-performance GaN-based HEMTs due to their superior channel confinement and 2DEG density.

Fig. 6. (a) Calculated conduction band energy diagrams of a standard AlGaN/AlN/GaN structure and optimized structure with an InGaN back barrier (b) Comparison of the carrier density distributions for a standard AlGaN/AlN/GaN structure and optimized structure with an InGaN back barrier.
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