Double subband occupation of the two-dimensional electron gas in $\text{In}_x\text{Al}_{1-x}\text{N}/\text{AlN}$/GaN heterostructures with a low indium content ($0.064 \leq x \leq 0.140$) barrier

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1. Introduction

GaN/AlN-based field effect transistors have been extensively studied due to the availability of high power and high frequency applications even at high temperatures [1]. Several improvements have been made in the growth and layer structures of the system, such as AlN buffer growth [2] and AlN interlayer insertion at the interface of 2DEG [3]. In addition to GaN/AlN-based heterostructures, InAlN/GaN and InAlN/InGaN/InGaN-based heterostructures were also proposed as a successor of GaN/AlN-based heterostructures because of their higher sheet carrier densities, which are provided by the spontaneous polarization of these systems [4,5]. With the higher carrier densities, the occupation of more than one subband may occur. Because of the highly polar structure of these materials, the electron interactions of each subband with interface related scattering mechanisms would be different [6]. Therefore, investigations of the transport properties of each subband have a great importance in producing better devices that have higher mobilities and higher carrier densities. Recently, Gonschorek et al. [7] reported two subband occupancy in $\text{In}_x\text{Al}_{1-x}\text{N}/\text{GaN}$-based structures with low indium ($0.03 \leq x \leq 0.23$) barriers.

Herein, we present a study on $\text{In}_x\text{Al}_{1-x}\text{N}/\text{GaN}$/AlN heterostructures ($0.064 \leq x \leq 0.140$) that were grown with metal organic chemical vapor deposition (MOCVD) with very high sheet carrier densities ($\approx 7.46 \times 10^{13}$ cm$^{-2}$ at 33 K). We studied temperature dependent Hall measurements, and we proved two subband occupancy in most of the samples via the quantitative mobility spectrum analysis (QMSA) method and one-dimensional (1D) self-consistent solution of non-linear Schrödinger–Poisson equations.

2. Experimental details

The $\text{In}_x\text{Al}_{1-x}\text{N}/\text{GaN}$/AlN heterostructures on c-plane (0001) Al$_2$O$_3$ substrates were grown in a low-pressure MOCVD reactor. Prior to the epitaxial growth, Al$_2$O$_3$ substrates were annealed at 1100 °C for 10 min in order to remove surface contamination. The growths were initiated with a 10-nm-thick low-temperature (840 °C) AlN nucleation layer. Then, 460-nm high-temperature AlN buffer layers were grown at a temperature of 1150 °C. A 500-nm-thick undoped GaN buffer layer was then grown at 1070 °C with a reactor pressure of 200 mbar. After the GaN buffer layers, a ~2-nm-thick AlN interlayer was grown at 1085 °C with a pressure of 50 mbar. Then, $\text{In}_x\text{Al}_{1-x}\text{N}$ layers with low indium content were grown under various temperatures (770–830 °C) for different samples at 50 mbar. Finally, ~3-nm-thick GaN cap layer growths were carried out at a temperature of 1085 °C at the same pressure. All of the layers are nominally undoped.

The thicknesses and indium contents of the barrier layers were determined by high-resolution X-ray diffraction (HRXRD) measurements. HRXRD measurements were taken with D8-Discover diffractometer equipped with a monochromator with four Ge (220) crystals for a CuK$_\alpha$ X-ray beam ($\lambda = 1.5406$ Å). The resolution of the $\psi-\theta$ measurements (where $\phi$ and $2\theta$ are the angles of the sample and detector relative to the incident X-ray beam) was $18^\circ$ ($\sim 0.005^\circ$).
The thicknesses of the barrier layers \(t\) were estimated by using \(t = \frac{\lambda}{2 \sin \theta_B} \cdot \frac{1}{2}\) [8]. Here, \(d\) and \(\theta_B\) are full width at half maximum (FWHM) and the angular position of the peak of the barrier layer, respectively.

For the calculations of the indium content of InAlN barrier layers, Bragg’s law is used,

\[
d = \frac{\lambda}{2 \sin \theta_B} = n \lambda.
\]

Here, \(d\) is the spacing of the related reflection planes. For hexagonal crystals, \(d\) can be calculated for any \((hkl)\) plane with

\[
d = \frac{1}{\sqrt{\frac{4 a^2 + b^2 + c^2}{a^2} + \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}
\]

Here, \(a\) and \(c\) are the lattice parameters of the hexagonal crystal. For the measured \((0002)\) plane, Eq. (2) can be simplified to \(d = \frac{c}{2}\).

Therefore, the lattice parameter of the AlInN barrier layer can be calculated with Eqs. (1) and (2). With the help of Vegard’s law and the known lattice parameters of AlN and InN crystals, the indium content of the AlInN barrier layer was determined. The growth temperatures, thicknesses, and indium content of the barrier layers are shown in Table 1.

By means of Hall measurements with van der Pauw geometry, the temperature and magnetic field \((0–1.4 \, \text{T})\) dependent mobilities as well as sheet carrier densities were all taken. Contacts were prepared as four evaporated Ti/Al/Ni/Au contacts at the corners. Using gold wires and indium soldering, the electrical contacts were prepared and the ohmic behaviors were confirmed by the current voltage characteristics before the Hall measurements. Because of the single field Hall effect, the measurements only gave averaged mobility and carrier concentration information, and these measurements can only be used in those cases of single electron, hole conduction, or single subband conduction in the semiconductor. The case with more than one type of carrier in the investigated sample is called mixed conduction. The correct transport parameters of the individual carriers in mixed conduction can be determined with the magnetic field dependent resistivity and Hall effect measurements. Different magnetic field dependent methods such as the two-carrier fit, multi carrier fit, and mobility spectrum analysis methods have been introduced by several groups for mixed conductivity analyses [9–12].

In the present study, we used the QMSA method for the analyses of magnetic field dependent resistivity and Hall data [13]. The QMSA method is widely used in many studies to extract the mobilities and carrier densities of different carriers in semiconductor materials, including bulk samples, thin films, quantum wells, and multilayer device structures [14–17]. In addition, the mobilities and carrier densities of individual 2D and 3D electrons and holes in GaN-based heterostructures are reported with the implementation of the QMSA method [18,19].

### Table 1

<table>
<thead>
<tr>
<th>Sample</th>
<th>InAlN layer</th>
<th>Growth temperature (°C)</th>
<th>Thickness (nm)</th>
<th>Indium content (mol%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>800</td>
<td>9.3 ± 0.3</td>
<td>10.6 ± 0.2</td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>830</td>
<td>9.3 ± 0.3</td>
<td>9.2 ± 0.2</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>770</td>
<td>11.1 ± 0.4</td>
<td>14.0 ± 0.2</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>810</td>
<td>10.8 ± 0.4</td>
<td>6.4 ± 0.2</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 1 shows the temperature dependence of Hall mobilities \((\mu_H)\) and Hall sheet carrier densities \((n_H)\) of the investigated samples at 0.4 \, \text{T} in the temperature range of 33–300 \, \text{K}. The mobilities exhibited temperature independence under 100 \, \text{K}, in which the carrier densities were temperature independent within the studied temperature range. At high temperatures, the mobilities are highly limited by the polar optical phonon scattering mechanism [20]. It is clear that these mobility and carrier density behaviors are typical for those samples where two-dimensional conduction is dominant [21].

In order to extract individual carrier types in the samples, QMSA analysis was performed on magnetic field dependent Hall data at each temperature step for every sample. Fig. 2 shows the QMSA results for sample A. Two distinct electron carriers and a hole carrier were observed in the investigated temperature range.

The maximum magnetic field is better at a range of \(B_{\text{max}} \approx \mu_{\text{min}}\) for the extraction of carriers with the mobility spectrum analysis method. Here, \(\mu_{\text{min}}\) is the minimum mobility of a carrier that can be extracted. For the QMSA studies, the \(B_{\text{max}} \approx 0.5\mu_{\text{min}}\) condition can be accepted as a limit [22]. For the present study, this condition seems to be barely satisfied, in which the results scatter in the QMSA data.

In a previous study, we presented extracted two-dimensional electron gas (2DEG) and two-dimensional hole gas (2DHG) carriers with low mobilities in an AlGaN/GaN/AlN heterostructure grown on sapphire [23]. In the present study, two distinct electron carriers and a hole carrier show 2D behavior with respect to the previous study. Temperature independent carrier densities for the low mobility 2DEG, high mobility 2DEG, and 2DHG carriers were found as \(3.05 \times 10^{13}\), \(4.95 \times 10^{12}\), and \(2.53 \times 10^{11} \, \text{cm}^{-2}\), respectively. These two 2DEG
carriers can be considered as the carriers populated at the first two subbands of a 2DEG system, which are located at the InAlN/AlN/GaN interface. 2DHG is populated at the GaN buffer/AlN buffer [23]. Because of an increase in the 2DHG mobility at low carrier densities via acoustic and interface roughness scatterings [20], and the absence of alloy scattering at the GaN/AlN interface, the mobility of the hole carrier is slightly higher than the mobility of electron carriers.

For GaAs-based multisubband occupied 2DEG systems, the lower subband is expected to have higher carrier density and also higher mobility [24], except for the case of high impurity diffusing into a two-dimensional channel [25]. In this study, the carrier with higher carrier mobility is defined near the interface than the second subband. Therefore, the first subband will be more scattered by non-uniform polarization field scattering as well as interface roughness scattering. Therefore, the mobility of the second subband will be higher than the first subband.

In order to see the change in the carrier densities of these subbands, all of the analysis was extended to all the samples that we measured. The results are shown in Fig. 4. With increasing $n_H$, a second subband was populated after $n_H > 1.93 \times 10^{13}\, \text{cm}^{-2}$. The carrier densities of the subbands increase with increasing $n_H$. The carrier densities of the 2DHG well at $\sim 2\,\mu\text{m}$ deep below the surface are more independent of $n_H$ because of the unchanged conditions for the 2DHG related layers for all the samples.

### Calculated in-plane strains ($\epsilon_{xx}$), critical thicknesses and strain relaxation expectations for the investigated samples

<table>
<thead>
<tr>
<th>Sample</th>
<th>Growth temperature (°C)</th>
<th>Calculated $\epsilon_{xx}$ at AlN/ GaN interface ($\times 10^{-3}$)</th>
<th>Critical thickness ($t_{cr}$) (nm)</th>
<th>Expectations</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>800</td>
<td>1.47 ± 0.2</td>
<td>10.8 ± 0.2</td>
<td>Highly strained</td>
</tr>
<tr>
<td>B</td>
<td>830</td>
<td>1.59 ± 0.2</td>
<td>10.0 ± 0.2</td>
<td>Strain relaxation may occur</td>
</tr>
<tr>
<td>C</td>
<td>770</td>
<td>9.0 ± 0.1</td>
<td>17.6 ± 0.1</td>
<td>Strained</td>
</tr>
<tr>
<td>D</td>
<td>810</td>
<td>19.7 ± 0.2</td>
<td>8.1 ± 0.2</td>
<td>Above strain relaxation limit</td>
</tr>
</tbody>
</table>
4. Conclusion

As a conclusion, the transport properties of the subbands of InAlN-based systems can be analyzed via the implementation of the QMSA method, even by using low magnetic fields at high lattice temperatures. It was found that a second subband begins to populate above $n_H > 1.93 \times 10^{13} \text{ cm}^{-2}$ for the investigated samples. For the GaN-based heterostructures, it is shown that the electrons in the lowest subband interact with the interface related scattering mechanisms more than the second subband’s electrons. Therefore, for those GaN-based devices with a higher mobility-carrier density product, investigating multisubband heterostructures, i.e., InAlN/GaN heterostructures with low indium content barriers, shows great importance.

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References