Relation between Microstructure and 2DEG Properties of AlGaN/GaN Structures

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(Received July 22, 2002; accepted October 1, 2002)
PACS: 68.37.Lp; 73.40.Kp

Several AlGaN layers are grown on top of a GaN buffer layer with the same Al concentration but different thickness. The electrical properties of these layers show a clear dependence on the AlGaN thickness. This electrical behaviour can be related to the microstructure, which is investigated by transmission electron microscopy. The formation of basal dislocations in the GaN and bending of the threading dislocations (in the samples with the thickest AlGaN/GaN cap layers) indicate a change of the stress in the GaN. This influences the piezo-electric field and increases the carrier density. The AlGaN cap layer is able to filter threading dislocations. The filtering mechanism is a strain-induced interaction with growth defects.

1. Introduction

Due to their remarkable physical properties, AlGaN/GaN structures are now attracting considerable attention for high temperature and high power microwave HEMT devices. The transistor performance, such as the cut-off frequency and the maximum output power, is directly related to the electrical properties of the conducting layer. The interest of AlGaN/GaN structures is that the two-dimensional electron gas (2DEG) forms spontaneously in the GaN near the AlGaN/GaN interface, due to polarisation effects [1]. Optimisation of the electrical characteristics thus requires a complete understanding of the strain state inside the layers. We have investigated the influence of the AlGaN layer thickness on the structural properties of the HEMT structures, in relation with their electrical properties.

2. Experimental

The AlGaN/GaN structures have been grown by low-pressure metal-organic vapor phase epitaxy (LP-MOVPE) on c-plane sapphire substrates [2], using ammonia, TMGa and TMAI as precursors. After deposition of a thin nucleation layer at low temperature, the wafer is brought to high temperature for recrystallisation. A 3 μm thick GaN layer is then grown at 1200 °C at a pressure of 100 Torr, using the so-called i.3 process [3]. The Al0.28Ga0.72N layer is then deposited at lower pressure, 50 Torr.

The investigated samples only differ by the thickness of the AlGaN cap layer (see Table 1). Van der Pauw Hall measurements have been performed at room tempera-

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ture, using In dot contacts to determine sheet carrier densities and mobility. With TEM, samples have been investigated in cross-section, samples A and D also in plan view.

3. Electrical Properties  The carrier density in the 2DEG and the mobility are given in Table 1 for the different samples. The resistivity of the thickest sample (sample E) is even too high to measure any 2DEG properties. This mobility drop for thicker AlGaN layers has already been reported on other samples by us [4] and by other groups [5].

4. Microstructure  AlGaN grows epitaxially on GaN. Strain, due to differences in lattice parameters, is easily visualised in plan view samples, thinned near the AlGaN/GaN interface. The stress at the interface spontaneously curls the film: GaN at the convex side.

At low magnification the interfaces look very sharp, but a probably not atomically flat interface makes it very hard to point out the interface with atomic precision.

Plan view investigations (samples A and D) reveal the presence of some very defected regions (Figs. 1a, b). They are 800 nm (sample A) to a few μm (sample D) wide and they spread out over at least several hundreds of μm along [1120] (no endpoints could be detected). Their density increases with increasing AlGaN thickness. In sample A, networks of 60° dislocations can be seen. All dislocations have the same Burgers vector (BV). They are found next to a deformation band, which shows some narrow

<table>
<thead>
<tr>
<th>AlGaN/GaN thickness (nm)</th>
<th>carrier density ($10^{13}$ cm$^{-2}$)</th>
<th>mobility (300 K) cm$^2$ (Vs)$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>sample A 14</td>
<td>1.03</td>
<td>1760</td>
</tr>
<tr>
<td>sample B 31</td>
<td>1.10</td>
<td>1313</td>
</tr>
<tr>
<td>sample C 46</td>
<td>1.20</td>
<td>1235</td>
</tr>
<tr>
<td>sample D 50</td>
<td>2.00</td>
<td>240</td>
</tr>
<tr>
<td>sample E 65</td>
<td>?</td>
<td>?</td>
</tr>
</tbody>
</table>

Fig. 1. Bright-field plan view images taken in (1120) two-beam diffraction conditions: they show the deformation regions in the AlGaN/GaN structures in a) sample A and b) sample D. c) A selected area diffraction pattern of the deformation band in sample A is shown; a rotation around the c-axis can be seen.
cracks perpendicular to the band. In this band a lot of glide has occurred. Here a lot of
dislocations are found with line direction along the c-axis and BV 1/3[11\(\overline{2}0\)] or equival-
ent. They can be distinguished from the threading edge dislocations by the fact that
neighbouring dislocations do not have the same BV, which should be the case for
threading dislocations (TD’s) (columnar growth). These deformation bands can produce
severe distortions to the structure. This is evidenced in the [0001]* diffraction pattern of
Fig. 1c which looks more like the pattern of a texture; rotations around the c-axis up to
10° are measured. In sample D, the cracks are more pronounced than the deformation
band. Basal dislocations, all with the same BV, are still found close to the band. In both
samples the BV of the dislocations is related to the direction of the cracks; the direction
of glide is the same for both defects. This means that the formation of the cracks is
related to or involves the presence of the dislocations.

Cross-section samples provide information on the position of the defects with respect
to the AlGaN/GaN interface. All effects, described above, are also observed here
(Figs. 2a, b). As expected the cracks are running from the film surface to the AlGaN/ GaN interface. Surprisingly the basal dislocations are situated in the GaN, below the
AlGaN. Electron diffraction of defect free regions over the interface shows reflections
split along the \(c^*\) direction. This means perfect epitaxy in the (\(a\)–\(b\)) plane and only a
slight c-parameter difference (pseudomorphic growth). However, diffraction patterns
from a region with a dislocation array show also a small splitting perpendicular to \(c^*\)
(Fig. 2c). This indicates that the basal dislocations behave like misfit dislocations and
act as stress-releasers. It is clear that these defects are formed at the same time, they all
are a result of a large deformation. The fact that the basal dislocations are located in-
side the GaN shows that they were formed after growth. If not, misfit dislocations
would be created before a stress (the AlGaN layer) was applied. Probably cooling
down to room temperature alters the stress distribution.

It has also been observed that the AlGaN cap layer is able to filter all types of TD’s
(Fig. 3). Plan view investigation shows that this filtering is very efficient. These TD’s are
not bend into the AlGaN/GaN interface. Dislocations parallel to the interface have
only been found close to the so called “deformation bands”. The filtering mechanism is
some strain induced interaction with growth defects (type I\(I\) stacking faults, inversion
domains and insertion or extraction of c-halfplanes) that are present in high density in

![Fig. 2. Bright-field cross-section images taken in (1120) two-beam diffraction conditions showing
different deformations: a) basal dislocations in the GaN (sample D) and b) cracks in the AlGaN
(sample E). c) A selected area diffraction pattern taken over the AlGaN/GaN interface is shown.
The insets are enlargements of the (1124) reflection at a non-deformed (left) and a deformed
region (right)
and just below the AlGaN cap layer. Strain is an important parameter because interaction between the defects does not occur inside the GaN. These growth defects have unintentionally been introduced.

In samples D and E mixed type TD’s often bend between 80 and 130 nm below the AlGaN/GaN interface (Fig. 3). The angle of bending can be up to 45°; i.e. more than 15.6°, which is the lowest-energy inclination of mixed type TD’s [6]. As this bending is not observed in the other samples, the effect is probably related to the thickness of the AlGaN cap layer. The components perpendicular to the c-axis of those bent TD’s probably have the same function as misfit dislocations.

5. Relation between Microstructure and 2DEG Properties

The AlGaN layer is able to transfer strain into the GaN buffer; the stress in the GaN increases with increasing AlGaN thickness. This can be proven by the formation of the basal dislocations and by the bending TD’s in the samples with the thicker AlGaN layers. This way the increase in carrier density can be explained: the strain adds a piezo-electric field in the GaN, opposite to the spontaneous polarisation of GaN and AlGaN and opposite to the piezo-electric field in the AlGaN. This modification increases the positive space charge in the AlGaN and consequently increases the electron density in the 2DEG.

It is well known that TD’s in GaN are electron traps [7]. This is most likely the same for the basal dislocations. Besides breaking of the lattice periodicity, the dislocations act like charged lines for the electrons in the 2DEG. The basal dislocations certainly increase the sheet resistance dramatically: they are located at the same place as the 2DEG. A comparison between the two samples investigated in plan view, shows that the density of these defects in the 2DEG increases with increasing AlGaN thickness. On top, in the samples with the thickest AlGaN cap layers, the bending of the mixed TD’s increases their length in the 2DEG. This way the amount of scattering due to the TD’s will be larger. Thus, the accumulation of extra scattering centres in the 2DEG with increasing AlGaN thickness decreases the electron mobility. This explains the very high sheet resistivity of samples D and E.

6. Conclusions

By growing AlGaN on GaN, a certain amount of stress is transferred into the GaN. It increases the carrier density due to modification of the piezo-electric fields. The increase in crack and basal dislocation formation together with the bending of TD’s (samples with thickest AlGaN layer) decreases the electron mobility.

The AlGaN cap layer is able to filter the TD’s. The filtering mechanism is a strain-induced interaction with growth defects.
Acknowledgements This work has been performed within the framework of IUAP V-1 and with the support of the European Space Agency (ATHENA project, ESTEC contract No. 14205/00/NL/PA). B. Van Daele is grateful to the Fund for Scientific Research – Flanders (FWO – Vlaanderen), Belgium.

References