Degradation mechanism of two-dimensional electron gas density in high Al-content AlGaN/GaN heterostructures

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This paper finds that the two-dimensional electron gas density in high Al-content AlGaN/GaN heterostructures exhibits an obvious time-dependent degradation after the epitaxial growth. The degradation mechanism was investigated in depth using Hall effect measurements, high resolution x-ray diffraction, scanning electron microscopy, x-ray photoelectron spectroscopy and energy dispersive x-ray spectroscopy. The results reveal that the formation of surface oxide is the main reason for the degradation, and the surface oxidation always occurs within the surface hexagonal defects for high Al-content AlGaN/GaN heterostructures.

Keywords: degradation mechanism, two-dimensional electron gas, AlGaN/GaN heterostructures, surface oxidation

PACC: 7280E, 7360L

1. Introduction

Aluminium gallium nitride/gallium nitride (AlGaN/GaN) heterostructures have many advantages, such as wide band-gap, high saturation electron velocity, high breakdown electric field strength, and can form a two-dimensional electron gas (2DEG) with high sheet density ($>1 \times 10^{13} \text{ cm}^{-2}$) and high mobility ($>2000 \text{ cm}^{2} \cdot \text{V}^{-1} \cdot \text{s}^{-1}$). AlGaN/GaN heterostructures are suitable to fabricate microwave power devices and high temperature devices.\[1]\] In order to improve 2DEG density, researchers often increase Al-content of AlGaN barrier layer or insert a thin AlN barrier layer.\[2,3]\] However, Gotthold et al.\[4]\] found that the high Al-content AlGaN/GaN heterostructures exhibited a time-dependent degradation of the 2DEG mobility that varied from days to weeks, because gradual relaxation of high strains in the high Al-content AlGaN barrier layer caused the degradation.

However, a time-dependent degradation of the 2DEG density in high Al-content AlGaN/GaN heterostructures was observed and studied in depth in this paper. The degradation reveals the reduction of the 2DEG density within several days after the epitaxial growth, but the 2DEG mobility always keeps constant. The degradation mechanism was investigated in depth using Hall effect measurements, high resolution x-ray diffraction (HRXRD), scanning electron microscopy (SEM), x-ray photoelectron spectroscopy (XPS) and energy dispersive x-ray spectroscopy (EDX). The analytical results discovered that the formation of surface oxide is the main reason of the degradation, and the surface oxidation always occurs within the surface hexagonal defects caused by high strains in high Al-content AlGaN/GaN heterostructures.

2. Experiment

The low Al-content Al$_{0.25}$Ga$_{0.75}$N/GaN (Sample A) and high Al-content Al$_{0.4}$Ga$_{0.6}$N/GaN (Sample B) heterostructures were grown on a $c$-plane sapphire substrate by low-pressure metal-organic chemical vapour deposition (MOCVD). Hydrogen was used as the carrier gas and triethylgallium (TEGa), trimethylaluminium (TMAI) and ammonia (NH$_3$) were used as source compounds. Prior to the epitaxial growth, sapphire substrates were annealed at 1050 °C.
for 10 min in order to remove surface contamination. A 20 nm-thick low-temperature AlN nucleation layer was deposited at 600 °C. Then, the growth temperature was ramped to 1020 °C and a 2 µm-thick GaN buffer layer was grown, followed by 24 nm-thick AlGaN barrier layer. The reactor pressure kept at 4.332 × 10^3 Pa during the growth.

After unloading the samples from the reactor, the two samples were immediately characterized by HRXRD (Bruker D8) and SEM (JEOL JM-6360LV) within a half hour. Then the electron density and mobility of the two samples were measured at different time intervals within 200 hours by room-temperature Hall effect system. After 200 hours, the XPS (AXIS ULTRA) and EDX (SystemSix) were used to analyze the surface element composition of the degraded sample.

3. Results and discussion

3.1. Time-dependent degradation of 2DEG density

After the epitaxial growth, the two samples were measured at different time intervals by room-temperature Hall effect measurements, shown in Fig. 1.

As can be seen in Fig. 1, within 200 hours after the growth, only the 2DEG density of the sample B with high Al-content has an obvious degradation, which first decreases quickly within the initial period of about 100 hours and finally saturated. However, the electron mobility of the sample B remains almost constant all the time. Because the 2DEG mobility is mainly affected by the interface quality of the AlGaN/GaN heterostructure, we thought that the stress relaxation in AlGaN barrier layer should not be the main reason for the degradation. The 2DEG sheet density is mainly affected by the surface variation, so the degradation may be directly related to the surface variation.

3.2. Relation between time-dependent degradation and crystal quality, surface morphology

The XRD 2θ − ω scans of the samples A and B within a half hour after the growth were shown in Fig. 2. The full width at half maximum (FWHM) values of the symmetric plane (002) of AlGaN (GaN) layers in the two samples were obtained as 211(582)° for sample A and 214(703)° for sample B, respectively. The Al-content of the AlGaN barrier layer in samples A and B were determined as 25.48% and 39.6%, which were in good agreement with the designed Al-content. As the FWHM values of AlGaN and GaN layers in samples A and B are compared, it is clearly seen that sample A with low Al-content AlGaN layer has better crystal quality than sample B with high Al-content AlGaN layer. The 2µm-thick GaN buffer layer in the two samples has almost the same good crystal quality.

Figure 3 shows the SEM images of the two samples. The surface of sample A is very smooth and has little hexagonal defects, while on the surface of the sample B, many hexagonal defects can be clearly seen. The results reveal that sample A has better surface morphology and crystal quality than those of sample B, which are in good agreement with XRD results.
Based on the above analysis, it is concluded that sample B with high Al-content has a AlGaN barrier layer with poorer crystal quality and the high strain of high Al-content AlGaN barrier layer had relaxed during the growth by forming hexagonal defects. After unloading the samples from the reactor, the strain relaxation of the AlGaN barrier layer can be neglected because the mobility of the samples always remains constant. So the surface variation may be the main reason for the 2DEG density degradation.

3.3. Relation between time-dependent degradation and surface oxidation

In order to analyse the surface variation of sample B in depth, it was characterized by XPS and EDX after the Hall effect measurement of 200 hours. Figure 4 presented the XPS curves before and after Ar-ion surface cleaning. Before Ar-ion surface cleaning, it can be clearly seen from Fig.4(a) that there were two obvious peaks of the elements C and O, except the peaks of elements Al, Ga and N. It is seen from Fig.4(b), that after 10min Ar-ion surface cleaning, the element C peak disappeared, but the element O peak was not changed. It can be explained that the element C peak originated from the surface contamination and the element O peak was from surface oxide.

The EDX measurement was done near the surface hexagonal defects of sample B. The element composition was analysed in the four points, including the inner (point 1), the side face (points 2 and 3) and the outer (point 4) of the hexagonal defect, shown in Fig.5. Table 1 lists the element composition in the four points. In the inner point (point 1) of the defect, only the elements Ga and N exist, this reveals that the surface hexagonal defects formed in the AlGaN barrier layer, not in GaN buffer layer. The element O was observed only in the two points (points 2 and 3) located on the side face of the defects. It is concluded that surface oxidation always occured in the side face of the surface hexagonal defects.
Fig. 5. The EDX measurement point distribution of the sample B.

Table 1. The surface element composition obtained by EDX.

<table>
<thead>
<tr>
<th></th>
<th>Ga</th>
<th>Al</th>
<th>N</th>
<th>O</th>
</tr>
</thead>
<tbody>
<tr>
<td>point 1</td>
<td>50.99%</td>
<td>49.01%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>point 2</td>
<td>28.81%</td>
<td>18.34%</td>
<td>46.97%</td>
<td>5.88%</td>
</tr>
<tr>
<td>point 3</td>
<td>28.17%</td>
<td>18.65%</td>
<td>45.39%</td>
<td>7.79%</td>
</tr>
<tr>
<td>point 4</td>
<td>27.90%</td>
<td>18.45%</td>
<td>53.65%</td>
<td></td>
</tr>
</tbody>
</table>

In conclusion, the above experimental and analytical results show that many surface hexagonal defects are formed by strain relaxation of high Al-content AlGaN barrier layer for high Al-content AlGaN/GaN heterostructure. The surface oxidation always occurs in the side face of these hexagonal defects, and causes reduction of surface states, which leads to the time-dependent degradation of 2DEG density.

4. Conclusion

We have investigated a time-dependent degradation mechanism of high Al-content AlGaN/GaN heterostructures. The 2DEG density of high Al-content AlGaN/GaN heterostructures exhibits a time-dependent degradation that varies from days to weeks. It is found that surface oxidation is the main reason for the degradation. The high in-plane tensile-strains of high Al-content AlGaN barrier layer were relaxed to form many hexagonal defects during the growth. When exposing the sample to air, surface oxidation occurred in the side face of the surface hexagonal defects in high Al-content AlGaN/GaN heterostructures, which resulted in the degradation of 2DEG density.

References