Correlations between Structural, Electrical and Optical Properties of GaN Layers Grown by Molecular Beam Epitaxy

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(Received July 4, 1999)

Screw and edge dislocation densities were estimated from X-ray diffraction profiles of GaN layers grown by molecular beam epitaxy. The results were confirmed by transmission electron microscopy. The layers had varying thicknesses or were deposited on differently nitridated sapphire substrates. It was found that the low temperature Hall mobility correlates with the screw dislocation density whereas the full width at half maximum of the donor bound exciton emission line changes similarly as the edge dislocation density.

1. Introduction

GaN layers are characterized by high defect densities primarily due to the heteroepitaxial growth on highly lattice mismatched substrates like sapphire or SiC. Besides threading dislocations with screw, edge or mixed character several other defects were found, like inversion domains, stacking faults or point defects [1, 2]. Different growth parameters were shown to influence the defect generation [3, 4]. Despite some existing studies on the scattering of electrons at dislocations [5 to 7] and their recombination activity [8], it is not yet very clear how these defects influence the electrical and optical characteristics of the layers. The goal of this paper is to find correlations between structural, electrical and optical properties in GaN layers. To exclude a dominant influence of point defects two sample series with expected constant point defect densities were chosen for the investigation. The effects of the layer thickness and the pregrowth nitridation procedure on the defect density, the Hall mobility and the full width at half maximum (FWHM) of the donor bound exciton (D0X) are investigated.

2. Experimental

The growth of the two investigated sample series was performed in a standard molecular beam epitaxy (MBE) system equipped with a radio frequency (rf) nitrogen plasma source. A nitridation step of the sapphire was performed before the growth start. For

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the layer thickness series the substrates were nitridated for 8 min at 750 °C, whereas for
the nitridation series containing 1 μm thick layers the nitridation temperature and time
were varied. Details of the growth procedure can be found elsewhere [9].

X-ray measurements were performed with a high-resolution diffractometer, equipped
with a Cu sealed anode, a fourfold Ge (220) monochromator and a slit in front of the
detector. For each sample, double axis scans were measured in ω mode for the GaN
(002) and (302) reflections. The (302) reflection was measured in skew symmetric dif-
fraction geometry. The Hall effect measurements were performed in a temperature
range between 20 K and 440 K at a magnetic induction of 0.85 T. Photoluminescence
(PL) spectra were recorded at 4 K with an excitation power of 12 mW using the 325 nm
line of a HeCd laser.

3. Results and Discussion

Using the procedure described in Ref. [10] screw and edge type dislocation densities
were estimated via double axis ω scans of the (002) and the (302) reflection for layers
with thicknesses of 100 nm, 400 nm, 1000 nm and 4000 nm and are depicted in Fig. 1.
Additionally, values obtained by cross sectional transmission electron microscopy
(TEM) are given which were extracted for a thick GaN layer grown with identical
growth parameters and should therefore be comparable to the layers investigated with
XRD. The dislocation types and densities at the corresponding thicknesses up to
4000 nm were determined with the aid of two beam experiments. Since the accuracy of
the TEM results depends on the estimation of the thickness of the investigated speci-
men area, the dislocation density may be uncertain by a factor of two.

Obviously, the results obtained with the two investigation methods show the same
tendency. The density of dislocations decreases by one order of magnitude with increas-
ing layer thickness. The densities obtained by TEM are identical for screw and edge
type dislocations suggesting a mixed character of the dislocations in this sample. On the
contrary, the edge type dislocation density determined with X-ray diffraction is by one
order of magnitude higher than the screw dislocation density in line with literature data.

![Fig. 1. Screw and edge dislocation densities vs. layer thickness determined by XRD and TEM. For details see text](image-url)
That the values obtained by TEM lie between the values resulting from XRD for screw and edge dislocations, is possibly a consequence of the high inversion domain density ($8 \times 10^9$ cm$^{-2}$) observed by TEM but not taken into account in the X-ray analysis. Additionally, the X-ray data give a mean value of the dislocation density in the whole layer, whereas the TEM results can be attributed to a distinct depth. Although the quantitative discrepancy between the results obtained by the two investigation methods is not fully understood, the identical behaviours for varying layer thickness are taken as justification for using X-ray diffraction FWHM as a figure of merit for dislocation densities.

In Table 1 the dislocation densities determined by XRD for the nitridation series are listed with the corresponding nitridation parameters. It can be clearly seen that the nitridation temperature has a remarkable influence on the screw dislocation density. As a result the sample nitridated at 200°C shows a screw type dislocation density of about $2 \times 10^7$ cm$^{-2}$ whereas the corresponding value for samples nitridated at a much higher temperature of 750°C is one order of magnitude higher, independent of the nitridation time. The edge dislocation density increases by a factor of two when extending the nitridation time from 8 min to 90 min at a temperature of 750°C.

In Fig. 2 the peak Hall mobility and the mobility at 20 K are shown in dependence on layer thickness. A clear increase of both values can be stated with the increase of layer thickness. This improvement goes hand in hand with the reduction of the dislocation density, but it is not possible to separate the contributions of screw and edge type dislocations. For the nitridation series the peak Hall mobility and the mobility at 20 K

<table>
<thead>
<tr>
<th>$T_{\text{nitr}}$ (°C)</th>
<th>$t_{\text{nitr}}$ (min)</th>
<th>$\rho_{\text{screw}}$ (cm$^{-2}$)</th>
<th>$\rho_{\text{edge}}$ (cm$^{-2}$)</th>
<th>max. $\mu_H$ (T) (cm$^2$/Vs)</th>
<th>$\mu_H$ (20 K) (cm$^2$/Vs)</th>
<th>FWHM D$^0!X$ (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>90</td>
<td>$2 \times 10^7$</td>
<td>$1 \times 10^{10}$</td>
<td>195</td>
<td>97</td>
<td>10.8</td>
</tr>
<tr>
<td>750</td>
<td>8</td>
<td>$5 \times 10^8$</td>
<td>$1 \times 10^{10}$</td>
<td>162</td>
<td>14</td>
<td>10.8</td>
</tr>
<tr>
<td>750</td>
<td>90</td>
<td>$6 \times 10^8$</td>
<td>$2 \times 10^{10}$</td>
<td>212</td>
<td>2</td>
<td>13.3</td>
</tr>
</tbody>
</table>
can be found in Table 1. No correlation between the peak Hall mobility and the varying dislocation densities can be found. At low temperatures the reduction of the screw dislocation density for the layer nitridated at 200 °C for 90 min is reflected in the highest mobility. Additionally, it can be seen that the sample with the highest edge and thus highest total dislocation density is characterized by the lowest mobility.

In Fig. 2 also the FWHM of the D0X emission line is plotted versus the layer thickness. The FWHM becomes smaller with increasing layer thickness pointing to the improved structural quality also reflected in the reduced overall dislocation density. As can be seen in Table 1, the change in screw dislocation density within the nitridation series has no influence on the FWHM of the D0X line, whereas the sample with the highest edge dislocation density shows the broadest D0X line. For almost all the investigated samples the carrier concentration is in the range of 10^{17} cm^{-3} at room temperature. Therefore it is sure that the D0X emission and not a band to band recombination was investigated. Only in the sample with a thickness of 100 nm the Mott limit is exceeded and we cannot exclude effects correlated with this phenomenon.

In conclusion, we demonstrated the applicability of X-ray diffraction for the determination of dislocation densities and found a correlation between the screw dislocation density and the low temperature Hall mobility for all investigated samples. Furthermore the FWHM of the D0X peak is found to vary similarly as the edge dislocation density. The peak mobility is not a good indicator for variations in the dislocation density.

Acknowledgements The authors would like to thank K.-H. Vennen-Damm and S. Hesselsmann for technical assistance. The work was supported by the Deutsche Forschungsgemeinschaft (Contract No. Ho 1388/10-1).

References

[10] H. Heinke, V. Kirchner, S. Einfeldt, and D. Hommel, see this volume.