Dislocation Density Estimation and Mosaic Model for GaN/SiC(0001) by High Resolution x-ray Diffraction

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ABSTRACT

High resolution x-ray diffraction and two dimensional triple axis mapping were used to characterize a group of GaN layers of about 1.1μm grown by direct current plasma molecular beam epitaxy technique on 6H-SiC(0001). A FWHM of 11.9 arcmins for an ω scan and 1.2 arcmins for an ω/2θ scan were observed. A careful study of the rocking curves showed there were some large mosaics in the GaN layer, and a tilt of 0.029° between the GaN layer and the SiC substrate was detected. The two dimensional triple axis mapping showed that the GaN mosaics were disoriented in the (0001) plane but rather uniformed in direction perpendicular to the plane. A mosaic model was deduced to explain the phenomenon, and the dislocation density was estimated to be about $\sim 10^9$ cm^{-2} according to the model.

1. INTRODUCTION

Recently, GaN has been paid much attention because of its large and direct bandgap, it has been regarded as one of the most potential candidate for new light sources and detectors in the short wave range, but the high dislocation density of more than 10^8 cm^{-2} in GaN is still a crucial kick for the short lifespan of GaN laser and the deterioration of GaN LEDs$^{(1-2)}$. Great efforts have been endeavored in looking for a suitable substrate for GaN epilayer and reducing dislocations in GaN layer, 6H-SiC is an attractive substrate and desirable for the realization of a GaN based injective laser due to his small lattice mismatch between SiC and GaN when compared to sapphire or GaAs substrates. 6H-SiC also has a high thermal and electrical conductivity as well as cleavage planes.

In this paper, we study the characterization of GaN crystalline quality and the estimation of dislocation density in GaN layers which are grown directly on 6H-SiC(0001) without insulating AlN buffer layer commonly used by plasma-assisted MBE.

The x-ray rocking curve combined with two dimensional triple axis mapping (TDTAM) is useful in determining dislocation densities, it is complementary to the transmission electron microscopy(TEM) and etch pit densities(EPDS) because of its nondestruction. Mosaic model theory is a generally accepted theory in calculating dislocation densities of crystal$^{(3)}$. In the following, it will be shown that there is some difference between the mosaic model for GaN and a common mosaic model.

2. EXPERIMENTS

The samples were grown on 6H-SiC(0001) by direct current plasma molecular beam epitaxy (DCP-MBE) technique, the growing rate was about 450Å/hour, resulted in the GaN layers of about 1.1μm thick.

X-ray diffraction was carried on Philips X'Pert MRD, whose goniometer had an accuracy of 0.0001°. The x-ray diffraction geometry was shown in fig.1, the double-crystal three-reflection analyzer in front of the detector resulted in a resolution of 12 arcseconds.

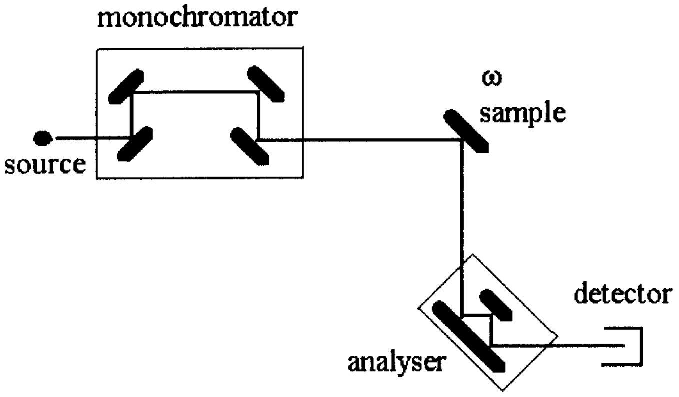

Fig. 1 The multi-crystal multi-reflection x-ray diffraction geometry. The double-crystal three-reflection analyzer in front of the detector resulted in a resolution of 12 arcseconds.

3. RESULTS AND DISCUSSION

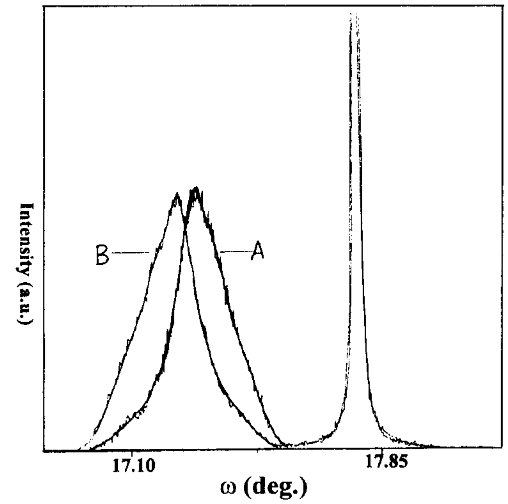

Fig. 2(a) The x-ray diffracting profiles under ω scan geometry (rocking curve) of a certain sample, curve (B) was the rocking curve measured by rotating the sample 180° around its [0001] compared to curve (A).

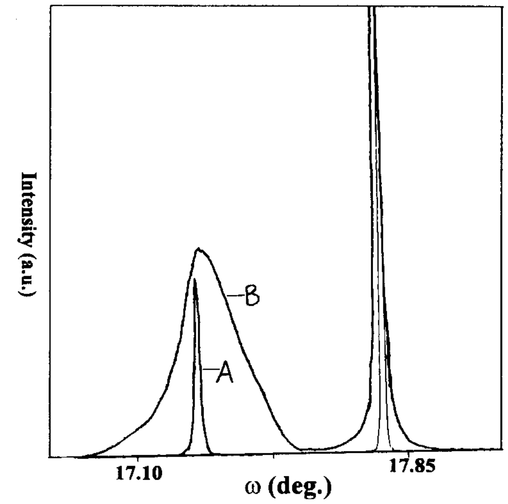

Fig. 2(b) The x-ray diffracting profile under ω/2θ scan geometry(curve A) compared with the profile under ω scan geometry(curve B).

Fig. 2(a) was the x-ray diffracting profiles under ω scan geometry (rocking curve) of a certain sample, curve (B) was the rocking curve measured by rotating the sample 180° around its [0001] compared to curve (A). In either case, a SiC(0006) reflection(right peak) and a GaN(0002) reflection(left peak) appeared, and the FWHM was 11.9 arcmins for either GaN(0002) peak, which could be compared with the results of a minimum FWHM 10 arcmins reported by Powell et al.(4). The shift of the GaN peaks between curve (A) and curve (B) showed that there was tilt between the GaN layer and the SiC substrate. By rotating the sample around its [0001] 90° by 90° and measuring the rocking curves, the tilt between the layer and the substrate was calculated after solid geometry to be 0.029°. Another character of fig. 2(a) was the asymmetry of the GaN (0002) peak. For curve (A), the left half was steep but the right half was rather flat ; while for curve (B), there was a reverse case. This showed that the asymmetry of GaN (0002) reflection was “fixed” on the sample and rotated with the sample, i.e., the asymmetry of GaN(0002) reflection was an intrinsic character. The reason for this phenomenon was that there was an extent of misuniformity in the {0001} planes, some large mosaics and many small ones in the sampling area caused the asymmetry of the GaN(0002) peak, if the mosaics, especially the few large mosaics, were asymmetrically distributed. The existence of large mosaics in GaN layer was convinced by ultra violet photoluminescence(UVPL) spectrum. It could be suspected that the misuniformity had a close connection with the nucleation of GaN on 6H-SiC(0001).

Fig. 2(b) was the x-ray diffracting profile under ω/2θ scan geometry(curve A) compared with the profile under ω scan geometry(curve B). The FWHM of GaN(0002) diffraction under ω scan geometry was 11.9 arcmins., while it was only 1.2 arcmins. under ω/2θ scan geometry. It should be noted that ω scan characterized the crystalline quality in the reflecting plane and ω/2θ scan characterized the crystalline quality perpendicular to the reflecting plane, information could be obtained that the GaN layers were well orientated in the [0001] direction but rather disorientated in the (0001) plane.

Fig. 3 was a TDTAM for GaN(0002) reflection, an obvious character was that the layer reciprocal lattice point(rlp) in fig.3 had a big elongation perpendicular to the diffracting vector, and in fig. 3 the mapping had a much larger FWHM (0.0192°) in the ω axis direction than that of in ω/2θ axis direction(0.0186°). The asymmetry of the mapping in the ω axis direction coincided with the x-ray diffracting profiles. From the TDTAM principle, the great elongation in the ω axis direction showed that the mosaics perpendicular to the [0001] direction were much more disoriented than those parallel to this direction. From the above, a simple mosaic model for GaN on 6H-SiC(0001) was deduced: along the [0001] direction, the mosaics were uniformed to be regarded as a perfect column, the columns were separated by single dislocation walls. The mosaic model would be published elsewhere in details.

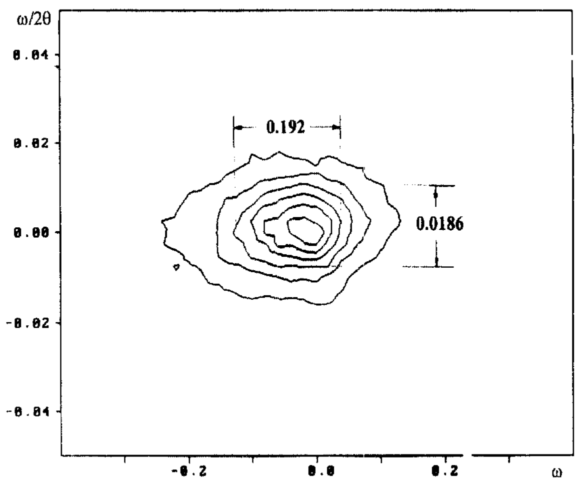

Fig. 3 A TDTAM for GaN(0002) reflection.

Assuming the size of the column was t, h was the spacing of dislocations in the walls, and the orientations of the mosaics had a Gaussian distribution(5), after mathematical deduction one had

$$D_B = \frac{\beta_\alpha}{\sqrt{2\pi \ln 2} \cdot st}$$

with β_α the x-ray diffraction FWHM under ω scan and s the Burgers vector. Finally one had $D_B \sim 10^9$ cm^{-2} .

The dislocation density we got was expressed as $D_B = \dfrac{\beta_\alpha}{\sqrt{2\pi \ln 2} \cdot st}$ according to the above mosaic model, while for a general mosaic model, the expression was $D_B \approx \dfrac{\beta_\alpha}{4.36t^2}$ (6). The reason for the difference between the two formula was that we had deduced from the TDTAM that along the [0001] direction, the small mosaics formed nearly perfect columns, while for a general mosaic model, all the mosaics were disoriented.

4. CONCLUSION

A series of GaN layers of about 1.1μm were grown by direct current plasma molecular beam epitaxy technique on 6H-SiC(0001), high resolution x-ray diffraction and two dimensional triple axis mapping were used to characterize the GaN layers. A FWHM of 11.9 arcmins for an ω scan and 1.2 arcmins for an ω/2θ scan were observed. The careful study of the rocking curves showed there were some large mosaics in the GaN layer, and a tilt of 0.029° between the GaN layer and the SiC substrate was detected. The two dimensional triple axis mapping showed that the GaN mosaics were disoriented in the (0001) plane but rather uniformed in direction perpendicular to the plane. A mosaic model was deduced to explain the phenomenon, and the dislocation density was estimated to be about ~10^9 cm^{-2} according to the model.

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