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Structural study of a GaN layer grown on (001)GaAs by MOCVD

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1. Introduction

Recently GaN has attracted much interest. GaN epilayers on sapphire substrates, which have a wurtzite structure, are being used for blue-light-emitting devices. On the other hand, to form a coherent heterostructure of GaN and other Ⅲ-Ⅴ semiconductors GaN must have a cubic(zincblende) structure, i.e., β-GaN. The cubic structure is crystallographically isotropic, which results in some advantages in optical and electrical applications, In case of GaAs substrate, the large lattice mismatch between these two materials can introduce many defects which cause serious problems, although lots of available specification, the easy cleavage and the cost of substrate, are fascinating. For understanding of this results, it is necessary to investigate the atomic scale structure using TEM.

In this paper we performed cross-sectional TEM observation to analyze the microstructure of the GaN on GaAs prepared by MOCVD

2. Experiments

The GaN on (001)GaAs heterostructure was grown by MOCVD. Prior to the deposition of GaN, a GaAs substrate was thermally cleaned at 580 ℃ and NH_3 was supplied 3min at 580 ℃ for surface nitridation. Subsequently TMG(560sccm at -15 ℃) and NH_3(560sccm at room temperature) were supplied simultaneously to deposit a GaN epilayer at 580 ℃. The TEM specimen preparation of the GaN layer was done by mechanical prethinning and final argon ion milling using a specimen cooling unit. The observation was carried out using a JEM-2010 electron microscope operated at 200kV.

3. Results and Discussion

Fig.1 represents a transmission electron diffraction(TED) pattern taken from the <110> cross-sectional sample of GaN/(001)GaAs structure showing the superposition of diffraction spots from the GaN and GaAs lattices. This reveals that the GaN layer has a zincblende structure(β-GaN) and the same crystal orientation as the GaAs substrate. It is found that the pretreatment of surface nitridation plays an important role in producing nuclei of β-GaN. During the pretreatment, arsenic atoms on the surface of substrate are replaced by nitrogen atoms altering GaAs to β-GaN pseudomorphologically. Subsequently GaN layer formed from TMG and NH3 can grow homoepitaxially in a zincblende structure on it. From the spots marked by arrows, One can notice the existence of α-GaN whose c-axis is inclined 5° to the <111>direction of GaAs substrate. The distance between GaN spots were measured to calculate the lattice parameter of β-GaN using GaAs spots as references. We obtained the value of 0.452 $\pm$ 0.001nm as the lattice parameter of β-GaN, which is in good agreement with the values of values of 0.451-0.454nm in literature. We found that the interface between GaN and GaAs is made up of {111} facetting from high resolution image. The SFs are thought to be formed to relieve strains which are generated by the lattice mismatch of 20% between β-GaN and

GaAs. The local region with many SFs has 2H-like(a wurtzitelike) stacking mode and that with few SFs has 3R(a zincblend) structure. The occurrence of a wurtzitelike stacking mode is expected because α-GaN is more stable than β-GaN. Fig.2 is a (110) cross-sectional dark field(DF) image which shows the existence of α-GaN which is embeded in the entire width of GaN layer. The observation described above demonstrates that the SFs, which is caused by lattice mismatch near interface, can be seeds of the α-GaN. Actually, α-GaN is considered to the more stable phase. Therefore very small factors like SFs can induce the growth of α-GaN during the growth procedure, though the energy difference between them is small. From the TED pattern taken from the same area as Fig.2 We observed the streaks which is due to α-GaN. It is found that c-axis of α-GaN is inclined 36° to <111> direction of GaAs and that [110] GaAs is parallel to the $[2\bar{1}\bar{1}0]$ α-GaN. We have done convergent beam electron beam diffraction to confirm whether the zone axis is [110] or $[1\bar{1}0]$.

4. Conclusion

From the cross-sectional TEM observation., the following results concerning the structure of GaN were obtained.

(1) The GaN grown at 580 ℃ using TMG and NH3 has a zincblend structure containing small amount of wurtzite structure embeded in local region.

(2) The c-axis of α-GaN which is embeded in the β-GaN is inclined 36° to the <111>direction of GaAs and [110] direction of GaAs is parallel to the $[2\bar{1}\bar{1}0]$direction of α-GaN.

(3) SFs, which occur near interface to relieve lattice mismatch of 20%, is running to the top surface and most of them grow along one of two <111>directions. In addition, these SFs can be the seeds of α-GaN.

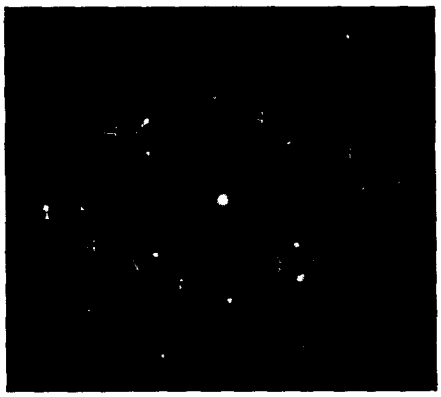

Fig.1. <110> cross-sectional TED pattern of the sample of GaN on (001)GaAs.

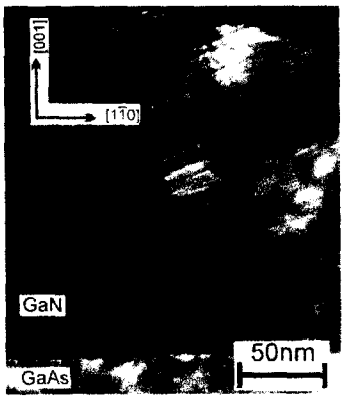

Fig.2. [110] CS DF image of the sample of GaN on (001)GaAs whch shows the existence α-GaN