Effect of nucleation layer morphology on crystal quality, surface morphology and electrical properties of AlGaN/GaN heterostructures*

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Abstract: Nucleation layer formation is a key factor for high quality gallium nitride (GaN) growth on a sapphire substrate. We found that the growth rate substantially affected the nucleation layer morphology, thereby having a great impact on the crystal quality, surface morphology and electrical properties of AlGaN/GaN heterostructures on sapphire substrates. A nucleation layer with a low growth rate of 2.5 nm/min is larger and has better coalescence than one grown at a high growth rate of 5 nm/min. AlGaN/GaN heterostructures on a nucleation layer with low growth rate have better crystal quality, surface morphology and electrical properties.

Key words: MOCVD; AlGaN/GaN; nucleation layer
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1. Introduction

Gallium nitride (GaN) and related III-nitride semiconductors have been demonstrated to be promising for a wide variety of optoelectronic and microelectronic applications[1, 2]. GaN has been grown on several substrate materials. Among these, sapphire is most widely used and GaN films on sapphire substrates have been successfully applied to blue light emitting diodes, laser diodes and high electron mobility transistors (HEMTs). However, GaN epilayers on sapphire substrates contain a high dislocation density of the order 10^9–10^{10} cm^{-2}[3], which is due to large crystal lattice mismatch and thermal mismatch between GaN and sapphire[4, 5]. The reduction of dislocation density is desirable for device performance and reliability. A two-step growth process utilizing a low temperature (LT) nucleation layer prior to high temperature (HT) GaN growth was established as the first breakthrough in obtaining device-quality smooth films. The role of the LT-nucleation layer has been widely studied and is now regarded as providing nucleation sites and controlling polarity in the subsequently deposited GaN layers[6].

Metal organic chemical vapor deposition (MOCVD) growth of GaN involves many variable growth parameters such as growth temperature, reactor pressure, V/III ratio, diluent gas, and input partial pressure of Ga species. It is very difficult to distinguish how each parameter influences the properties of GaN films. In this paper, we closely study the effects of LT nucleation layers with different growth rates on crystal quality, surface morphology and electrical properties of AlGaN/GaN heterostructures on sapphire substrates.

2. Experiment

Two samples were grown by a low-pressure MOCVD system on a (0001) sapphire substrate. Hydrogen was used as the carrier gas. Triethylgallium (TEGa), trimethylalumium (TMAl) and ammonia (NH_3) were used as precursors. Prior to epitaxial growth, the sapphire substrates were annealed at 1050 °C for 10 min in order to remove surface contamination. A 30 nm thick LT GaN nucleation layer was deposited at 480 °C with the chamber pressure at 40 Torr and the V/III ratio at 2500 for samples A and B. The LT-GaN growth rate, which was controlled by the flow rate of TEGa and NH_3, was 5 nm/min for sample A and 2.5 nm/min for sample B. Then, the susceptor temperature was ramped to 1020 °C and a 2 μm thick GaN buffer layer was grown, followed by a 24-nm-thick undoped AlGaN barrier layer. The reactor pressure remained at 40 Torr during growth. In order to investigate the effects of nucleation layer morphology on AlGaN/GaN heterostructures, an additional two samples C and D were grown using the same growth conditions of the LT GaN nucleation layer as samples A and B respectively. Then samples C and D were ramped to 1020 °C and annealed for 5 min.

The crystal quality was analyzed by high resolution X-ray diffraction (HRXRD) using a Bruker D8 diffract meter. The rocking curves at the symmetric (002) and asymmetric (102) planes were taken to evaluate the crystal quality. A 2theta–omega scan of the symmetric (002) plane was

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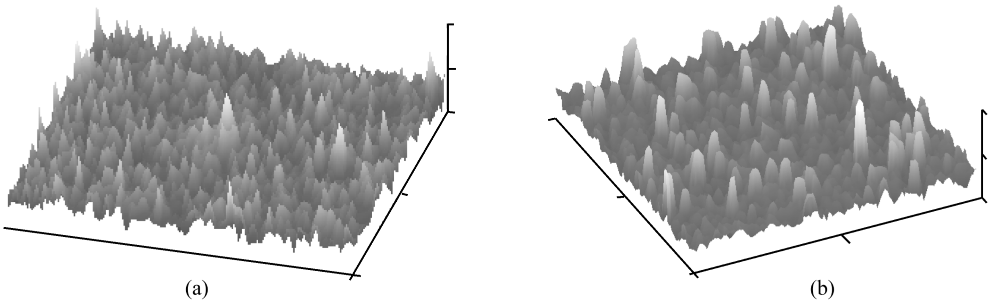
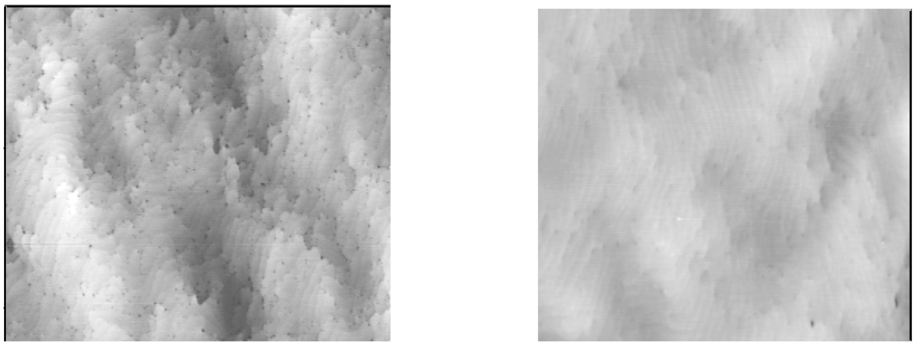


(a) (b)

Fig. 1. AFM images of the LT GaN nucleation layer of (a) sample C and (b) sample D.



(a) RMS = 1.5 nm (b) RMS = 0.4 nm

Fig. 2. AFM images of AlGaN/GaN heterostructures of (a) sample A and (b) sample B.

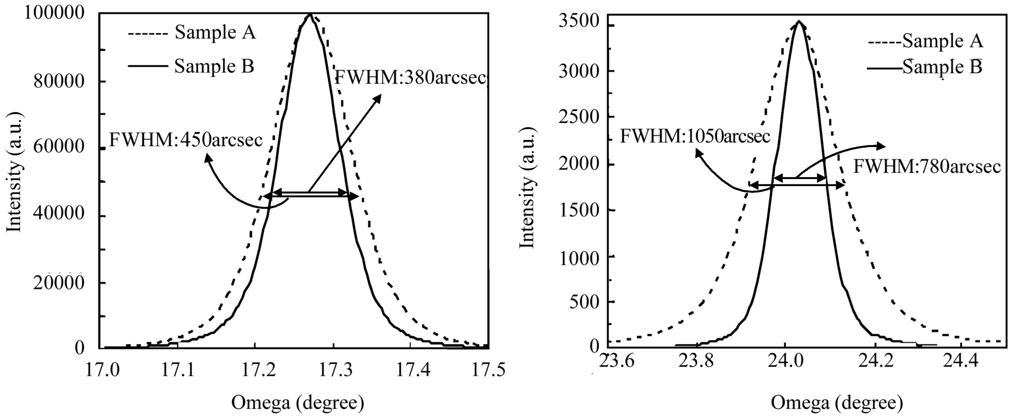


Fig. 3. Full-width at half-maximum of rocking curves of AlGaN/GaN heterostructures.

performed to evaluate the strain of the GaN layer. The surface morphology of the LT nucleation layers and AlGaN/GaN heterostructures was characterized by atomic force microscopy (AFM). The carrier concentration and mobility were analyzed by Hall measurement.

3. Results and discussion

Figure 1 shows the surface morphology of samples C and D with the LT GaN nucleation layer. The nucleation islands of sample D are larger and sparser than those of sample C. The island height of sample C is 36 nm, and that for sample D is 21 nm. The average island sizes of samples C and D are 10 and 17 nm, respectively. The different NL layer growth rates caused this difference. The RMS of samples A and B are 1.5 and 0.4 nm, respectively, as shown in Fig. 2. The surface of sample A with a nucleation layer growth rate of 5 nm/min is rougher than that of sample B. It can be seen that the larger size of nucleation islands is conducive to better coalescence of GaN.

It is clearly seen from Fig. 3 that the X-ray rocking curve (XRC) FWHM of sample B is less than that of sample A. It has been demonstrated that the XRC for the symmetric (002)-reflecting plane is related to screw and mixed dislocations, whereas the XRC for the asymmetric (102)-reflecting plane is directly influenced by all threading dislocations, including edge dislocations[7]. Therefore, a smaller FWHM represents better crystal quality. Consequently, a nucleation layer grown at a lower growth rate is helpful for achieving a higher crystal quality of the subsequent layer.

Also, the two-dimension electron gas (2DEG) mobility of AlGaN/GaN heterostructures was measured by the Hall effect at room temperature. The mobility of sample A is 950 $\mathrm{cm^{-2}/(V{\cdot}s)}$, and the mobility of sample B is 1420 $\mathrm{cm^{-2}/(V{\cdot}s)}$.

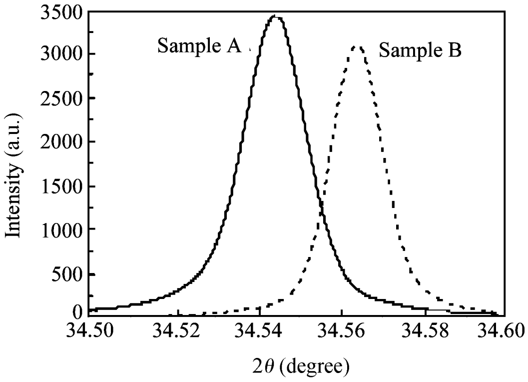


Fig. 4. HRXRD 2theta-omega scan curves of samples A and B.

As mentioned above, the GaN film grown on the lower growth rate nucleation layer had good crystal quality and surface morphology. In terms of 2DEG, the dislocation scatting and surface roughness scattering decreased, and high 2DEG mobility could be achieved.

The residual stress of the GaN epitaxial layer was analyzed to determine the relationship between nucleation layer morphology and the properties of AlGaN/GaN heterostructures. The 2theta–omega scan of HRXRD can determine the lattice parameter accurately. Consequently, the type of strain can be determined, and the values of the stress can even be calculated. Diffraction angles of the (002) allow us to obtain the c-axis lattice constant and c-axis strain. As shown in Fig. 4, the c-axis lattice constants of samples A and B are 0.51926 and 0.51859 nm, respectively. The c-axis strains of sample A and B are 1×10^{-3} and 5.7×10^{-5}.

It is believed that the residual stress in GaN can affect all aspects of AlGaN/GaN materials. A nucleation layer grown at low growth rate is helpful in that it suffers less stress for HT-GaN. And there is a lower dislocation density induced by stress release, which is helpful for achieving better crystal quality, better surface topography and higher mobility of AlGaN/GaN heterostructures. A high nucleation growth rate resulted in the deterioration of surface morphology and crystal quality of AlGaN/GaN heterostructures. The reason for these differences is probably that the lower growth rate of the nucleation layer could enhance the surface mobility of Ga atoms, and improve the nucleation layer's crystal quality. This better quality of nucleation is helpful for increasing the crystal quality, surface morphology and electrical characteristics of AlGaN/GaN heterostrutures.

4. Conclusion

The effects of nucleation layer morphology with different growth rates on crystal quality, surface topography and electrical characteristics of AlGaN/GaN heterostructures were analyzed. A nucleation layer with lower growth rate enhanced the surface mobility of Ga atoms and improved the nucleation layer's crystal quality. Consequently, smoother morphology, larger size of nucleation islands and better coalescence can be obtained. The residual stress of the HT-GaN was reduced and high crystal quality was achieved. The surface morphology and electronic characteristics of the AlGaN/GaN heterostructures were improved.

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