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Study on structure of AlGaN on AlN interlayer by synchrotron radiation XRD and RBS

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Abstract The AlGaN samples have been grown on AlN interlayer (IL) by metalorganic vapor phase epitaxy (MOVPE). The effects of AlN interlayer (IL) on improvement of crystalline quality of AlGaN and Al incorporation efficiency were investigated. The samples were characterized by synchrotron radiation X-ray diffraction (XRD) and MeV He ion Rutherford backscattering spectrometry (RBS). The AlN IL played a role in suppressing edge threading dislocations (TDs) and enhancing the screw ones. It also changed the state of stress in AlGaN from tension to compression. Crack-free AlGaN films were grown successfully by inserting AlN IL.

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Introduction

AlGaN is a key material for the fabrication of optoelectronic devices in the deep ultraviolet (DUV) and ultraviolet (UV) region such as UV LED and UV photodetector. AlGaN/GaN heterojunction field effect transistors (HFETs) are also attracting great interest due to their promising performance for high-voltage, high power, and high temperature microwave applications. However, the growth of thick crack-free AlGaN with high Al-composition is difficult due to the large lattice-mismatch between GaN and AlGaN. GaN epitaxial layer has typically been used as underlying layer to grow AlGaN. In this case, crack may be generated by the relaxation of tensile strain. AlN (or AlGaN) IL have been used to relieve stress between the GaN underlayer and the AlGaN layer on top, and crack-free AlGaN were grown successfully [1–6]. However, it is still under dispute about the mechanism of stress relaxation by AlN interlayer. In this paper, we report the growth and characterization of AlGaN on low temperature (LT) AlN IL.

Furthermore, the effects of AlN IL on improvement of crystalline quality of AlGaN and Al incorporation efficiency were investigated by synchrotron radiation X-ray diffraction and MeV He ion Rutherford backscattering spectrometry (RBS).

Experimental

The AlGaN samples with and without AlN IL were grown by MOVPE. The structures of the AlGaN samples are shown in Fig. 1. Three types of samples (AlGaN without IL, AlGaN on one IL and AlGaN with double ILs) were studied in this paper. The Al composition of the AlGaN samples ranges from 0.2 to 0.5.The thickness of AlN IL is 15 nm, which was grown at 600 °C. All samples were undoped. The samples were investigated by X-ray diffraction using synchrotron radiation and MeV He ion RBS. For RBS/channeling measurements, a collimated 1.57 Mev He^+ beam was used. XRD measurements were performed by a Huber five-circle diffractometer of Beijing Synchrotron Radiation Facility (BSRF). Synchrotron X-ray diffraction is a very effective tool to study the

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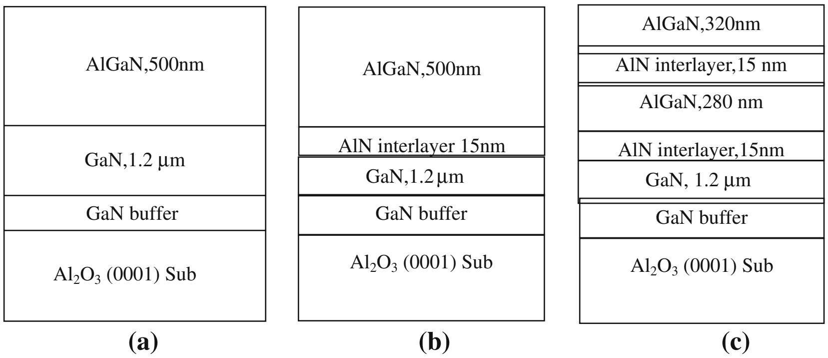

Fig. 1 Structures of AlGaN samples: (**a**) without interlayer, (**b**) with one AlN interlayer and (**c**) with two AlN interlayers

lattice parameter of AlGaN thin film due to its good monochromaticity and high sensitivity. The X-ray wavelength was set at 1.537 Å. The spot size of the incident beam is limited by a slit system to $0.3 \times 1.2\ mm^2$. The detector system, consisting of a scintillation counter and a 0.1 mm wide receiving slit, was located 35 cm away from the sample.

Results and discussions

In the AlGaN alloy, Al fraction x is usually estimated by XRD using Vegard's law. When the strain in AlGaN layer cannot be neglected, the value of Al fraction x will be inaccurate [3]. In this case, the RBS measurement is a more reliable and accurate method because the RBS signal is mostly dependent on the atomic number and the composition of alloy. Figure 2 shows the RBS spectra of AlGaN sample with two AlN ILs. The simulation of the spectra reveals that Al composition is 0.5 for the AlGaN top layer, while Al composition is 0.4 for the underlying AlGaN layer. The thickness of AlGaN top layer is 320 nm and that of underlying AlGaN layer is 280 nm. The yield χ_{min} for different AlGaN samples was also evaluated from RBS spectra.

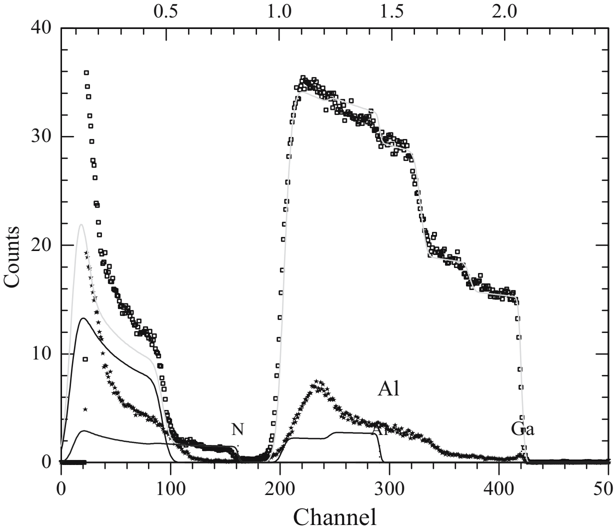

Fig. 2 Random (□), aligned (★), and simulated (solid line) RBS spectra of AlGaN sample with two AlN interlayer

Figure 3(a)–(c) show the SEM images of surface for the AlGaN with and without AlN IL. In the case of no interlayer, 500 nm thick $Al_{0.25}Ga_{0.75}N$ was grown directly on the GaN underlying layer. A lot of cracks can be observed from the top surface due to the large lattices-mismatch as shown in Fig. 3(a). The results calculated from the XRD show that the stress in $Al_{0.25}Ga_{0.75}N$ layer was tensile, which will be discussed later.

By inserting one AlN IL, crack-free AlGaN with the Al composition up to 0.35 can be obtained (Fig. 3(b)). In order to attain crack-free AlGaN with higher Al composition, the growth of AlGaN layer with two ILs was attempted. As result, crack-free AlGaN layer with Al composition up to 0.5 was obtained. The improvement of surface morphology is attributed to stress state in AlGaN layer. In this paper, the stress state in AlGaN layer with different Al composition was characterized by XRD and RBS measurements.

Crystalline quality of the AlGaN films grown on AlN IL was evaluated by XRD. To evaluate the crystalline quality of the AlGaN films grown on one AlN IL (Al composition x:0.22–0.35), a complete description of the mosaic structure requires both the out-of-plane and the in-plane misorientations to be fully specified [7]. Figure 4 shows the full width at half maximum (FWHM) of ω-scans around (104) and (002) AlGaN peaks as a function of Al composition for the samples with and without AlN IL. Comparing with the sample without AlN IL, the AlGaN grown on AlN IL exhibits an increase in FWHM of the (002) reflections. For GaN epilayers, the FWHM of (002) peak can be taken as a figure of merit for the tilt and consequently for the density of screw threading dislocations (TDs) [8]. Therefore, in our results, the insertion of AlN IL

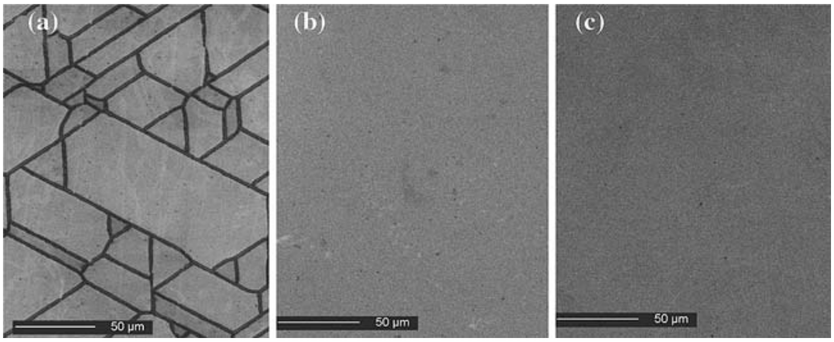

Fig. 3 SEM Images for AlGaN samples: (**a**) without interlayer, (**b**) with one AlN interlayer and (**c**) with two AlN interlayers

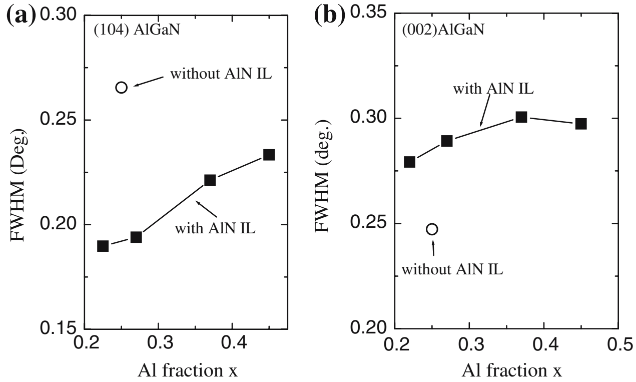

Fig. 4 FWHM of ω-scans around (**a**) (104), and (b) (002) AlGaN diffraction peak for the samples with and without AlN IL as a function of Al fraction x

leads to an increase in density of screw TDs. This result is opposite to that of Kashima et al. [9]. They have reported that the low temperature AlN IL acts as a filter against threading dislocations which have screw component [9]. However, the (104) reflections respond to both the edge and screw type TDs. In contrast with the sample without AlN IL, the FWHM of the rocking curve for the samples with AlN interlayer is reduced evidently. The result indicates that the AlN IL can reduce the threading dislocations, which have edge component. On the other hand, The increase in FWHM of ω-scan around AlGaN (104) plane with increasing Al fraction x was observed, Lafford et al. [4] have reported similar results, they attribute the increase in FWHM to an increase in the threading edge dislocation density associated with the smaller diffracting element boundaries.

To elucidate the stress state of AlGaN layers grown on AlN IL, the lattice constant of the samples used in this paper was measured by synchrotron radiation XRD.

Through Bragg's Law:

$$2d\sin\theta = n\lambda$$

$$d = \frac{1}{\sqrt{\frac{4(h^2+hk+k^2)}{3a^2}+\frac{l^2}{c^2}}}$$

AlGaN lattice constants c and a can be calculated from the θ–2θ scans on the (002) and (104) reflections. The relationship between the AlGaN lattice constants c and a, was shown in Fig. 5. The lattice constants of AlGaN according to Vegard's law are depicted as a dot line using those of stress-free AlN and GaN. With certain stress, for example, in-plane compressive stress makes a point move to the upper left from the line and vice versa [10]. It is found that the AlGaN layers are compressively stressed by the thin AlN IL, while the stress in AlGaN layer grown directly on GaN is tensile. The result exhibits that the AlN IL offers change in the in-plane lattice parameters [6]. The compressive stress is important for the growth of the thick AlGaN with

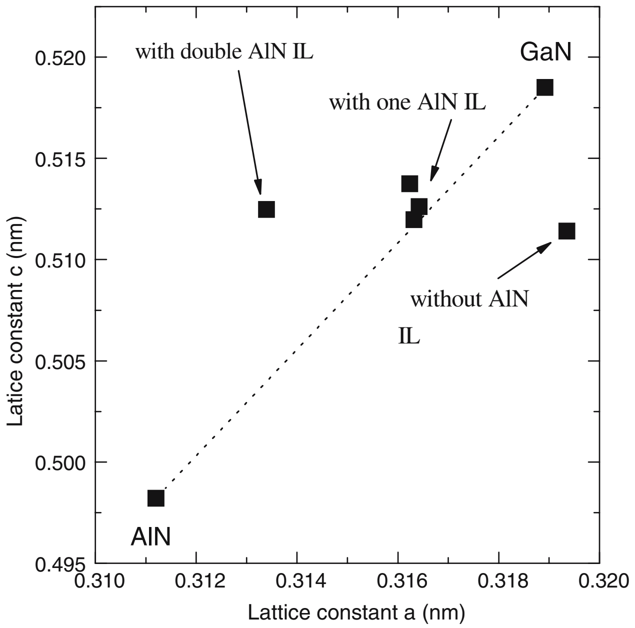

Fig. 5 Relationship between lattice parameter c and a for AlGaN samples grown with and without AlN interlayer

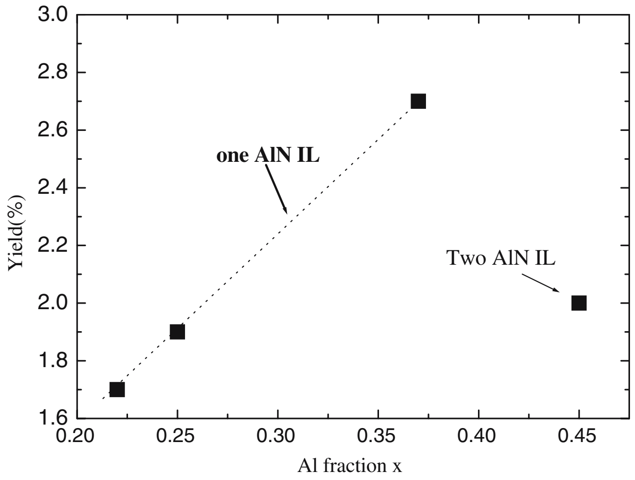

Fig. 6 Yield χ_{min} evaluated from RBS measurement as a function of Al composition x

high Al fraction x. After inserting AlN IL, the crack was reduced significantly, but still observed from the AlGaN grown on one AlN IL.

Comparing with AlGaN grown with one layer AlN IL, it is found that the AlGaN with two AlN layer shows higher Al incorporation efficiency, under same flow rate of TMAl. The Al composition x in AlGaN with two AlN ILs was significantly greater, by at least a factor of 1.6, than that of the AlGaN layer with one AlN IL. The improvement in Al incorporation may be due to the change in stress state during the growth of AlGaN on different AlN IL. The Al incorporation efficiency may also be related with the defect structure on the growing surface as reported for In incorporation in InGaN [11].

The yield χ_{min} evaluated from the RBS measurement is also a figure of merit for the crystalline perfection. Figure 6 shows the χ_{min} as a function of Al composition x. The χ_{min} increase with increasing Al fraction x, indicating that the crystalline quality of AlGaN on one AlN IL becomes poor with increasing Al composition x, this is consistent with the result of XRD as shown in Fig. 4. Through inserting two AlN IL, the $Al_{0.5}Ga_{0.5}N$ films with χ_{min} of 2.0% were obtained and the film is crack-free, indicating the crystalline quality is quite high. The results show that the insertion of two AlN ILs is an effective method to grow high quality and crack-free thick AlGaN with high Al composition x.

Conclusions

AlN IL was used to grow AlGaN layers by MOVPE. The effects of AlN IL on the improvement of crystalline quality of AlGaN and Al incorporation efficiency in AlGaN were investigated. AlN IL shows a role of suppressing edge dislocation defect but bring an increase in density of screw dislocation. Crack-free AlGaN films were obtained by inserting two AlN ILs. The stress in AlGaN layers is changed from tensile to compressive by the thin AlN IL.

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