Microstructure Study on Heterostructures of AlInGaN/GaN/Al_2O_3 by Using Rutherford Backscattering/Channelling and XRD *

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(Received 13 June 2006)

A quaternary AlInGaN layer is grown by metal–organic chemical vapour deposition on a sapphire (0001) substrate with a thick ($> 1\,\mu m$) GaN intermediate layer. The compositions of In and Al are determined by Rutherford backscattering (RBS). The low ratio between the channelling yield and random yield according to the spectra of RBS/C ($\chi_{\min} = 1.44\%$) means that the crystal quality of the AlInGaN film is perfect. The perpendicular and the parallel elastic strain of the AlInGaN layer, $e^{\perp} = -0.15\%$ and $e^{//} = 0.16\%$, respectively, are derived using a combination of XRD and RBS/channelling.

PACS: 61. 10. Nz, 82. 80. Yc, 81. 05. Ea

In the past decade, InGaN-based ternary alloys attracted a great deal of interest because of their success in blue light emission diodes, in which the InGaN layer normally bears a compressive stress due to the lattice mismatch between InGaN and GaN crystals. The availability of AlInGaN quaternary alloy permits an extra degree of freedom by allowing independent control of the band gap and the lattice constant.[1] The value of this freedom is the ability to engineer lattice matched heterostructures or novel structures with different layers subjected to an adjustable degree of in-plane stress. Therefore, the growth and characterizations of AlInGaN films play a key role for the further application of GaN-based wide band-gap semiconductors. Some research results on the epitaxial growth and the optical and electrical properties of AlInGaN quaternary alloys have been published,[2−4] however there is not enough structural analysis on this kind of quaternary AlInGaN alloys.

Rutherford back-scattering (RBS) is a standard technique in the analysis of materials, and is used to determine the composition, the thickness and the interface of films.[5] If the ion beam is directed along a high-symmetry crystal direction, a phenomenon called the channelling occurs. The incident ion beam will undergo a series of correlated small angle scatterings and consequently the backscattering events significantly reduce compared to the backscattering events when the ion beam is directed in random direction. Here $\chi_{\min}$ is the ratio of the backscattered yield when aligned to a crystallographic axis Y_A to that aligned to the random direction Y_R, is a measure of the crystalline quality of the film, which is typically calculated behind the surface peak. RBS combined with channelling can provide useful information such as the crystalline quality and the defect density profile. Moreover, the angular scan around an off-normal axis can determine the tetragonal distortion e_T induced by the elastic strain in the epilayer.[6]

X-ray diffraction is a powerful tool to precisely determine to lattice constant of the thin film especially for the good crystal quality film. In order to compensate for the possible interlayer tilts, two scans were performed with rotating of the sample by 180°.

In this Letter, we first use the RBS/C to describe the thickness, composition and the crystalline quality of the AlInGaN/GaN/Al_2O_3 heterostructures, and then combining RBS/C and XRD, we present a quantitative analysis of the tetragonal distortion e_T and the elastic strain in the AlInGaN layer.

A quaternary AlInGaN layer was grown at 850°C by MOCVD on a sapphire substrate using a thick GaN layer as a template. For RBS measurements, a collimated 1.570 MeV He^+ beam was used with a backscattering angle of 167.8°. The sample was mounted on a high precision (±0.01°) three-axis goniometer in a vacuum chamber, so that the orientation of the sample relative to the He^+ beam can be precisely controlled. X-ray measurements were performed on a high resolution x-ray diffraction equipped with a four-crystal monochromator in Ge (220) configuration and one or two 200 μm slits before the detector. Monochromatic Cu $K_{\alpha 1}$ x-ray ($\lambda = 0.15406$ nm) was used as the incident light.

Figure 1 shows the random, ⟨0001⟩ aligned, and the simulated spectra of the AlInGaN/GaN/Al_2O_3 sample. The inset shows the geometry used in the backscattering measurements. The arrows (labelled

* Supported by the National Natural Science Foundation of China under Grant Nos 10375004 and 10575007.
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with In, Ga and Al) indicate the energy for backscattering from In, Ga and Al atoms at the surface respectively. The ⟨0001⟩ aligned spectrum of the Ga atoms indicates that the AlInGaN film has minimum yield $\chi_{\min} = 1.44\%$ and low dechannelling rate, showing that the AlInGaN layer has a perfect crystalline quality (the value of $\chi_{\min}$ from 1% to 2% indicates perfect crystalline quality and 100% an amorphous or polycrystalline material), which means that the density of defects in both layers and the interface between the AlInGaN and GaN is extremely low. A simulation of the random spectrum given by the RUMP program,[7] which is used to simulate the random RBS spectrum, reveals that the thickness of the AlInGaN and GaN layers is respectively 83 nm and 1050 nm, and the compositions of In and Al in the AlInGaN layer are 0.025 and 0.300.

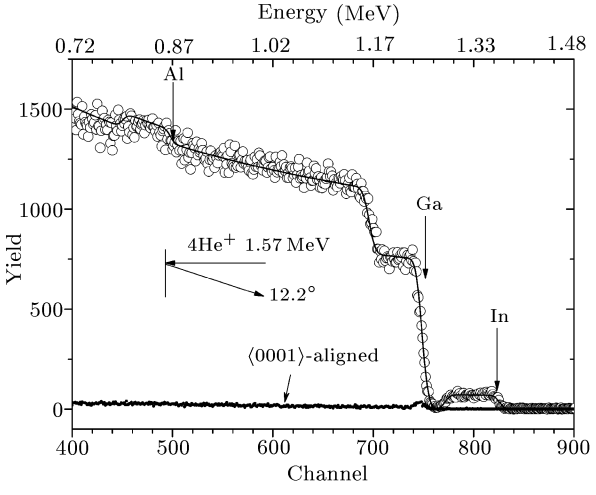


Fig. 1. Random (open circles), ⟨0001⟩ aligned (closed circles) and simulated (solid line) RBS spectra of the AlInGaN/GaN/Al_2O_3 sample prepared by MOCVD.

Figure 2 shows a symmetric XRD measurement of the sample. Taking the position of the Al_2O_3 (0006) peak as a reference, c_{epi} of AlInGaN epilayer is calculated to be 5.128 ± 0.001 Å. On the other hand, using Vegard's law and the lattice constants of InN ($a_b = 3.538$ Å, $c_b = 5.706$ Å), AlN ($a_b = 3.111$ Å, $c_b = 4.978$ Å) and GaN ($a_b = 3.189$ Å, $c_b = 5.185$ Å), $a_b = 3.174$ Å and $c_b = 5.136$ Å for bulk (fully relaxed) $Al_{0.300}In_{0.025}Ga_{0.675}N$ are obtained. Therefore, the perpendicular elastic strain $e^{\perp} = (c_{\text{epi}} - c_b)/c_b = -0.15\% \pm 0.02\%$ is deduced, indicating that the layer is under tensile strain in the parallel direction.

To measure the parallel elastic strain, an RBS angular scan (Figs. 3 and 4), similar to the study in Ref. [8], was carried out along the AlInGaN $\{10\bar{1}0\}$ plane by choosing a region of integration (channel 680–820 in Fig. 1) corresponding to the In and Ga atoms in the AlInGaN layer. Figures 3 and 4 show the dips of the angular scans along the AlInGaN ⟨0001⟩ axis and $\langle 1\bar{2}13\rangle$ axis. Gauss function fits are used to accurately determine the position of the dips (dotted line) respectively. The angle Φ_{epi} between the ⟨0001⟩ axis and $\langle 1\bar{2}13\rangle$ axis is determined to be 31.90°–0.10°=31.80°. The theoretical value of the angle is equal to $\tan^{-1}(a_b/c_b)$, which is $\Phi_b = \tan^{-1}(a_b/c_b) = 31.72°$ for bulk $Al_{0.300}In_{0.025}Ga_{0.675}N$. Therefore, $\Delta\Phi = \Phi_{\text{epi}} - \Phi_b = 0.08° \pm 0.005°$. The positive $\Delta\Phi$ value means that the AlInGaN layer is under tensile strain in the parallel direction, which is consistent with the XRD result. The tetragonal distortion deduced from the RBS/channelling study is $e_T = e^{//} - e^{\perp} = \Delta\Phi/\sin\Phi\cos\Phi = 0.31\% \pm 0.02\%$. Finally, the parallel elastic strain $e^{//} = 0.16\% \pm 0.02\%$ can be obtained. The result ratio $|e^{\perp}/e^{//}| = 0.94$ is larger than the value of 0.38 reported for the GaN[9] and also larger than the value of 0.40 reported for the $In_{0.18}Ga_{0.82}N$.[10] As compared to GaN and $In_{0.18}Ga_{0.82}N$, the lattice of $Al_{0.300}In_{0.025}Ga_{0.675}N$ is more elastic than the GaN and $In_{0.18}Ga_{0.82}N$. Due to the induced Al and In in the quaternary AlInGaN film, the lattice constant in plane ($a_b = 3.174$ Å) can be

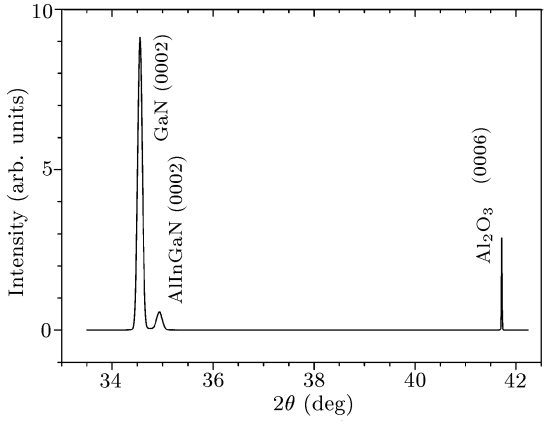


Fig. 2. XRD $2\theta/\omega$ scan of the sample with 2θ ranging from 33° to 42°.

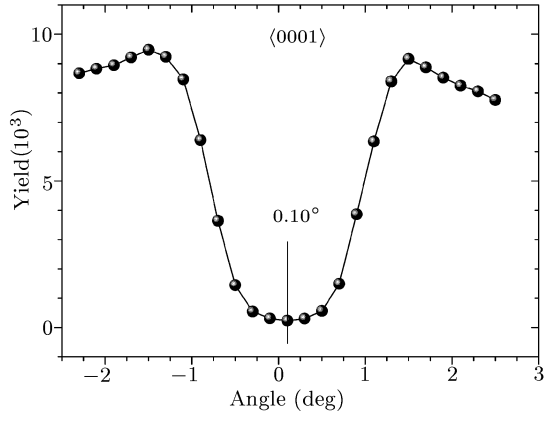


Fig. 3. Angular scan along the AlInGaN $\{10\bar{1}0\}$ plane showing the AlInGaN ⟨0001⟩ axis dip.

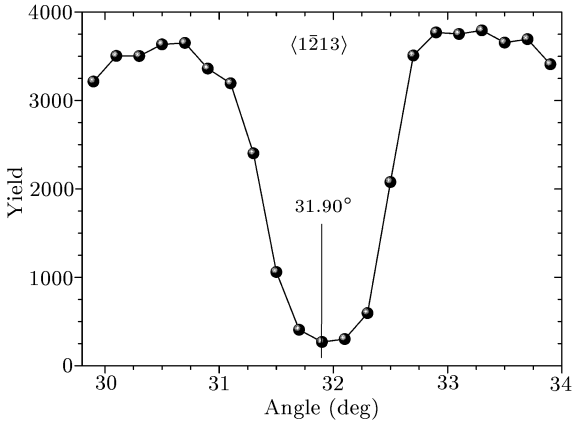


Fig. 4. Angular scan along the AlInGaN {10$\bar{1}$0} plane showing the AlInGaN ⟨1$\bar{2}$13⟩ axis dip.

adjusted very close to the in-plane constant of GaN($a_b = 3.189$ Å). Thus the strain in the parallel direction $e^{//}$ must be slightly smaller than that of GaN and $In_{0.18}Ga_{0.82}N$. That is why the value of $|e^{\perp}/e^{//}|$ is larger than the GaN and $In_{0.18}Ga_{0.82}N$.

In conclusion, an 83-nm $Al_{0.300}In_{0.025}Ga_{0.675}N$ with perfect crystalline quality has been prepared on GaN/Al_2O_3 by MOCVD at 850°C. The composition and the thickness of the AlInGaN layer are determined by RBS. Combined with XRD the strain in AlInGaN layer are determined as $e^{\perp} = -0.15\%$ and $e^{//} = 0.16\%$, respectively. The ratio $|e^{\perp}/e^{//}| = 0.94$ indicates that the lattice of $Al_{0.300}In_{0.025}Ga_{0.675}N$ layer is more elastic than GaN and $In_{0.18}Ga_{0.82}N$.

References

[1] Aumer M E, LeBouf S F, Bedair S M, Smith M, Lin J Y and Jiang H X 2000 *Appl. Phys. Lett.* **77** 821
[2] Kipshidze G, Kuryatkov V, Zhu K, Borisov B, Holtz M, Nikishin S and Temkin H 2003 *J. Appl. Phys.* **93** 1363
[3] Dong X, Huang J S, Li D B, Liu X L, Xu Z Y and Wang Z G 2003 *Chin. Phys. Lett.* **20** 1148
[4] Shakya J, Knabe K, Kim K H, Li J, Lin J Y and Jiang H X 2005 *Appl. Phys. Lett.* **86** 091107
[5] Chu W K, Mayer J W and Nicolet M A 1978 *Backscattering Spectrometry* (New York: Academic)
[6] Davies J A 1995 *Handbook of Modern Ion Beam Materials Analysis Materials* (Pittsburgh, PA: Pittsburgh Research Society)
[7] Doolittle L R 1985 *Nucl. Instrum. Methods* B **9** 344
[8] Wu M F, Vantomme A, Wach J De, Degroote S, Pattyn H, Langouche G and Bender H 1996 *J. Appl Phys.* **79** 6920
[9] Detchprohm T, Hairamatsu K, Itoh K and Akasnki I 1992 *Jpn. J. Appl. Phys.* II **31** L1454
[10] Wu M F, Vantomme A, Hogg S M, Langouche G, Van der stricht W, Jacobs K and Moerman I 1999 *Appl. Phys. Lett.* **74** 365