Strain in GaN/Si<111> by RBS/Channeling

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Abstract GaN film grown on Si substrate was characterized by Rutherford backscattering/Channeling (RBS/C). The experimental results show that the thickness of GaN epilayer is about 2.5 μm and the GaN film has a good crystalline quality (χ_{min}=3.3%). By using channeling angular scanning, the 0.35% of average tetragonal distortion in GaN layer is observed. In addition, the depth profiles of strain in GaN film layer reveal that the strain in GaN film nonlinearly decreases with the increase of film thickness. The strain-free thickness (above 2.5 μm) of GaN film on Si substrate is far below that (150 μm) of GaN film on Sapphire.

Keywords RBS/Channeling, Strain, GaN/Si heterosystem

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1 INTRODUCTION

Wurtzite gallium nitride (GaN) and related III-nitride compounds have attracted widespread interest due to their applications in high brightness blue, green light emitting diodes and blue lasers.[1,2] Usually, GaN thin films are typically grown on sapphire or silicon carbide substrates using molecular beam epitaxy (MBE), metal organic chemical vapor deposition (MOCVD) or pulsed laser deposition (PLD).[3] The growth of GaN on Si substrate is another important technology in achieving novel optoelectronic integrated circuits. This heteroepitaxial technology has many advantages, such as low-cost, large-area substrate with high crystallinity, good surface quality, high mechanical strength and excellent thermal conductivity. The potential for integration between optoelectronics and microelectronics on a single wafer makes the epitaxy of a GaN layer on Si extremely important. However, due to large lattice mismatch (37.77%) and thermal expansion coefficient mismatch (41.16%) between Si and Wurtzite gallium nitride (GaN), the growth of high quality GaN film on Si aubatrate is very difficult. Therefore, many approaches, such as MOCVD,[4] vacuum reactive evaporation,[5] reactive magnetron sputtering,[6]

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MBE[7] and ultrahigh vacuum chemical vapor deposition[8] are explored to grow high quality GaN films on Si<111> substrate.

Recent progress in understanding GaN thin film growth revealed that strain is one of the key issues that engineers the growth and physical properties of the thin films, such as surface morphology, the size of the grains in the GaN films, bandgap and electrical or optical properties. However, until now the quantitative measurement of strain in GaN film grown on Si<111> substrate is not reported. In the present work, Rutherford Backscattering and Channeling (RBS/C) were used to characterize the strains in high crystalline GaN films on Si<111> substrate grown by MOCVD.

2 EXPERIMENTS

The gallium nitride films (GaN) were grown on Si<111> substrate by metal organic chemical vapor deposition (MOCVD). Detailed growth experiments were described elsewhere.[9]

The sample was characterized using RBS/Channeling for determining the thickness of GaN film, crystalline perfection and lattice distortion. A collimated 2 Mev He^+ beam was used for RBS/Channeling measurements. The detection angle was 165° and the energy resolution was 20 keV. The sample was mounted on a high-precision (±0.01°) three-axis goniometer in a vacuum chamber. RBS/Channeling angular scans through the $<1\bar{2}13>$ axes of GaN film and following a $\{10\bar{1}0\}$ planar direction were performed to determine the strain in the GaN epilayer. About 24 spectra were recorded changing the angle of incidence in step of 0.2°. Random spectrum was obtained with tilt angle of 38°, slightly out of the angular scan range to avoid the beam alignment with the $<1\bar{2}13>$ axis of the GaN epilayer. The aligned spectra were divided by the random spectrum to obtain the normalized yield data.

3 RESULTS AND DISCUSSIONS

Fig.1 shows the random, the $<0001>$ axe aligned and the simulation of random RBS spectra of the sample. The arrows labeled Ga and N indicate the energy for backscattering from these elements at surface. A simulation of the random spectrum reveals the composition of Gallium nitride films is fully close to stoichiometry and thickness of gallium nitride film (GaN) is equal to 2.45 μm. According to the simulation of random RBS spectrum, we can infer that the non-abrupt back edge of Ga signal is due to a 150 nm non-uniformity of the GaN layer thickness. The aligned spectrum shows that the minimum channeling yield χ_{min} (i.e., the ratio of the backscattering yields of the aligned and the random spectra in the near surface region) of the GaN film layer is

3.3%, which is close to that of perfect crystal,[10] indicating that the GaN layer has a good crystalline quality.

The $< 1\bar{2}13 >$ aligned spectrum and random spectrum of GaN film layer is shown in Fig.2. The normalized yields of $< 1\bar{2}13 >$ aligned spectrum with respect to random spectrum of GaN film layer are higher than those of $< 0001 >$ orientation due to the high Miller indices. The average strain stored in GaN film layer is determined according to the angular scanning curves shown in Fig.3. The scanning window (40–360 channel) shown in Fig.2 corresponding to the whole GaN film layer was chosen to obtain the channeling angular scanning dip along $< 1\bar{2}13 >$ axe in the $\{10\bar{1}0\}$ plane presented in Fig.3 (b). In order to accurately obtain the angle ϕ of the GaN epilayer between the $< 1\bar{2}13 >$ and $< 0001 >$ axis, channeling angular scanning dip along the $< 0001 >$ axis in the $\{10\bar{1}0\}$ plane is also presented in Fig.3(a). The positions (2.46°, 34.15°) of dip centroid in the angular scans for Fig.3 (a) and (b) were extracted using a cubic spline fit,[11] respectively. Therefore, we can infer that the angle ϕ of the GaN epilayer in our study between the $< 1\bar{2}13 >$ and $< 0001 >$ axis is 31.69°. For bulk GaN layer, the angle ϕ between the $< 1\bar{2}13 >$ and $< 0001 >$ axis is equal to 31.6° calculated from $\tan^{-1}$ (a/c), where a is 0.3189 nm and c is 0.5185 nm, respectively. The angle ϕ measured from channeling angular scanning is larger than that of bulk GaN, indicating that the GaN epilayer is compressively strained in the perpendicular direction, which is reasonable in view of Possion's effect for a GaN epilayer with a negative lattice mismatch relative to the Si substrate. As a measurement of the strain in GaN/Si epilayer, its average tetragonal distortion calculated by the formula[12] $\varepsilon_{\mathrm{T}} = \Delta\phi/\sin\phi\cos\phi$ is 0.35%, where ϕ is equal to 31.6°.

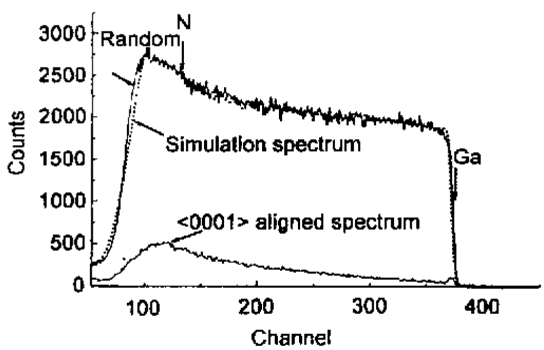

Fig.1 Random and $< 0001 >$ axe aligned spectra of GaN/Si$< 111 >$ sample

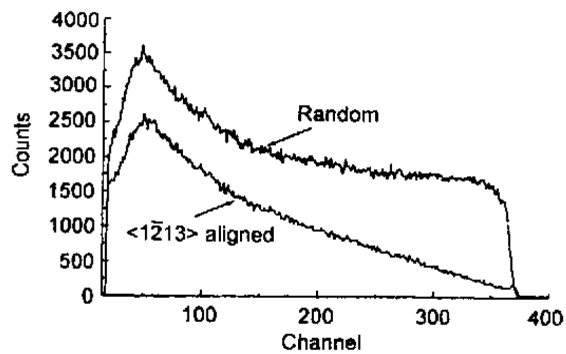

Fig.2 Random and $< 1\bar{2}13 >$ axe aligned spectra of GaN/Si$< 111 >$ sample

Detchprohm *et al*[13] have reported that the lattice constant of GaN film on Sapphire substrate varies with the film thickness of GaN and the strain in GaN film is almost completely relaxed at a film thickness above 150 μm. However, the quantitative information of strain distribution in GaN epilayer on Si substrate and the depth profile of the intrinsic strain in GaN epilayer are unclear. From the determined random and the $<1\bar{2}13>$ axe aligned RBS spectra shown in Fig.2 as well as strain calculated by Channeling angular scanning, the depth profiles of strain in GaN epilayer on Si substrate were derived and shown in Fig.4. The depth scale was converted from channel scale in Fig.2 by using stopping powers estimated by Trim code.[14] The open circle and broken line in Fig.4 denote the experimental values of tetragonal distortion at different depth of GaN epilayer and a polynominal-fitting curve, respectively. As is evident in Fig.4, the tetragonal distortions in GaN film on Si substrate nonlinearly decrease with the increasement of thin film thickness, and it also indicates that the strain in the GaN film is nearly completely relaxed at a film thickness above 2.5 μm, which is far below that of GaN grown on Sapphire.

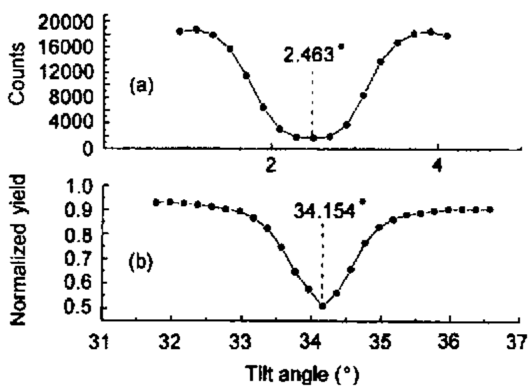

Fig.3 Channeling angular scanning for GaN/Si<111> sample were used to determine strain
(a) Channeling angular scanning along $<0001>$ axe in the $\{10\bar{1}0\}$ plane
(b) Channeling angular scanning along $<1\bar{2}13>$ axe in the $\{10\bar{1}0\}$ plane

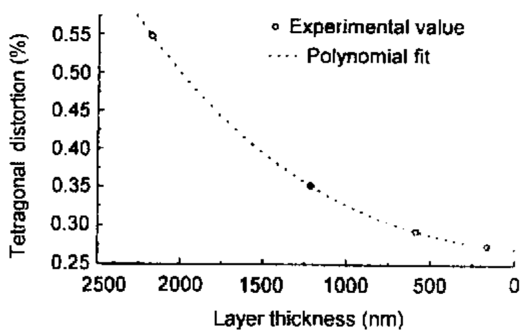

Fig.4 Strain depth profiles of GaN film on Si$<111>$ substrate

4 CONCLUSION

The crystalline perfection and the intrinsic strain in GaN film grown on Silicon substrates were investigated by Rutherford Backscattering and Channeling. The Channeling experiments demonstrate that the GaN film on Si substrate has a good crystalline quality (χ_{min}=3.3%). Channeling angular scanning shows the average strain in GaN film is equal to 0.35%, the strain in GaN film are nonlinearly decreased and strain-free GaN film will be observed at a film thickness above 2.5 μm.

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