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Crystal quality and electrical properties of p-type GaN thin film on Si(111) substrate by metal-organic chemical vapor deposition MOCVD

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Properties

ABSTRACT

Purpose: In this paper, p-GaN samples have been grown on silicon substrates under various processing conditions. The effects of growth tenperature and thermal annealing on the crystal quality and strain were carefully investigated. The electrical properties such as hole concentration and mobility would be discussed.

Design/methodology/approach: GaN-based III–V semiconductors have become promising materials for short-wavelength optoelectronic devices because of their large and direct band gap energies. In this paper, p-GaN has been grown by metal-organic chemical vapor deposition (MOCVD) at 900°C, 950°C, 1000°C, and 1050°C with low temperature LT-deposited AlN/AlGaN buffer layer.

Findings: The mobility was achieved at 150 cm^2/Vs and the hole concentration was $8x10^{17}$ cm^{-3}. SIMS and XRD were used to measure and explain the relationships between hole concentration and the growth temperature. When the growth temperature was increased to 1000°C, the hole concentration was increased by ten times. According to the experimental results, the optimal growth temperature was 1000°C. After the thermal annealing process at temperature 850°C for 2 minutes, the FWHM of p-GaN was lowered to 617 arcsec. The effects of growth temperature were explained in the two temperature regions. From 900°C to 1000°C, the incorporation rate of Mg was slightly increased and the strain decreased with the growth temperature. Mg would provide holes and the lower strain would result in better crystal quality. The crystal quality and Mg concentration effects on hole concentration below 1000°C was thus beneficiary. On the other hand, when the growth temperature was further increased, the strain and FWHM increased while hole concentration decreased at 1050°C. At this high temperature, Si might become donor in GaN.

Research limitations/implications: It was suggested that the hole concentration reduced at 1050°C due to the Si diffusion and the strain caused by Mg dopant. According to the experimental data, the optimal growth temperature was 1000°C. After the annealing process, the FWHM of p-GaN was lowered to 617 arcsec.

Originality/value: Determination of crystal quality and electrical properties of p-type GaN thin film on Si(111) substrate by metal-organic chemical vapor deposition MOCVD.

Keywords: Mechanical properties; p-GaN; Strain; Hole concentration; FWHM; SIMS; Growth temperature

1. Introduction

GaN-based III–V semiconductors have become promising materials for short-wavelength optoelectronic devices because of their large and direct band gap energies [1-3]. The realization of high hole concentration p-type GaN layer has been a key factor to lead GaN to the successful commercial applications from the laboratory. GaN deposited on silicon (Si) substrates has great advantages including lower cost, excellent wafer quality, less hardness, and more design flexibility with current silicon electronic circuit system [4-7]. However, production of good quality p-type GaN on silicon substrate still encounters some problems that require further investigation, such as the high resistance ohmic contact of p-GaN and silicon diffusion to the epitaxial layer at high growth temperature from the Si substrate [8,9]. These could inevitably affect the electrical properties.

On the other hand, hydrogen can passivate magnesium in GaN by binding it with nitrogen and reducing the mobility. In order to overcome this problem, additional process would be necessary like the thermal annealing. With the growing potential in the newly developed illumination applications, much research works have focused on the electrical properties of p-GaN. Several researchers have tried to control the growth conditions to prevent the passivation [10]. The passivation affected hole concentration directly. S. Yamaguchi enhanced hole concentration by doping In to control the strain in GaN [11]. The strain in the epitaxy layer would depend on the growth temperature, dopant, and lattice mismatch [12]. It is also known that lattice mismatch on silicon substrate is higher than that on the sapphire [13].

In this paper, p-GaN samples have been grown on silicon substrates under various processing conditions. The effects of growth tenperature and thermal annealing on the crystal quality and strain were carefully investigated. The electrical properties such as hole concentration and mobility would be discussed. Secondary ion mass spectroscopy was used to reveal the in-depth elemental concentration profiles in silicon and magnesium.

2. Experimental

GaN thin film epilayers were grown on Si(111) substrates by metal-organic chemical vapor deposition (MOCVD) using an Aixtron AIX-200/RF-S reactor system. Si(111) was chosen due to its trigonal symmetry favoring epitaxial growth of the GaN(0001) plane. The substrate was cleaned by 5% HF solution prior to the epitaxial growth. Trimethylaluminum (TMAl), trimethylgallium (TMGa), trimethylindium (TMIn), bis-cyclopentadienyl magnesium (Cp_2Mg), and ammonia (NH_3) were used as Al, Ga, In, Mg, and N sources, respectively. A low temperature (LT) AlN/AlGaN buffer layer was deposited prior to the GaN epitaxy. The GaN experimental samples were grown at 900°C, 950°C, 1000°C and 1000°C. The thickness of GaN:Mg was 250 nm, and AlGaN/AlN bufer layer was 125nm/25nm. The contact of as-grown sample was deposited by e-gun evaporator. The annealing process was carried out at 850°C for 2 minutes to activate the sample and to provide the contact ohmic.

The as-grown samples were characterized by secondary ion mass spectroscopy (SIMS) to determine the depth and the concentration of Mg and Si. To assess the crystal quality, the full width at half maximum (FWHM) data from X-ray diffraction (XRD) were measured. The evaluation of electrical properties was performed at room temperature using Hall measurement.

From the diffraction results, the lattice constant in the c-axis was also estimated. The strain along the c-axis between GaN thin film and the substrate was presented as $\frac{\Delta c}{c_0} = \frac{c - c_0}{c_0}$. The lattice constants c and c_0 were the measured value and the unstrained value. A negative value of $\Delta c/c_0$ corresponded to the tensile stress, while a positive value corresponded to the compressive stress.

3. Results and discussion

3.1. The enhanced crystal quality by annealing

The XRD θ/2θ spectra of the as-grown samples are shown in Fig. 1. The measured FWHM data from GaN(0002) are also shown with the spectra and they decrease with the growth temperature in general. Fig. 2 displays the XRD θ/2θ results after the annealing process. Fig. 3 summarizes the full-width-at-half-maximum (FWHM) results. It has been clearly evidenced that the annealing process was effective in reducing the FWHM and improving the xrystal quality. The FWHM reduced with the increasing growth temperature from 900°C to 1000°C. On the contrary, when the temperature was up to 1050°C, the FWHM was increased. Therefore, 1000°C was the optimal growth temperature. The lowest FWHM was about 600 arcsec, when the sample was grown at 1000°C and annealed at 850°C for 2 minutes.

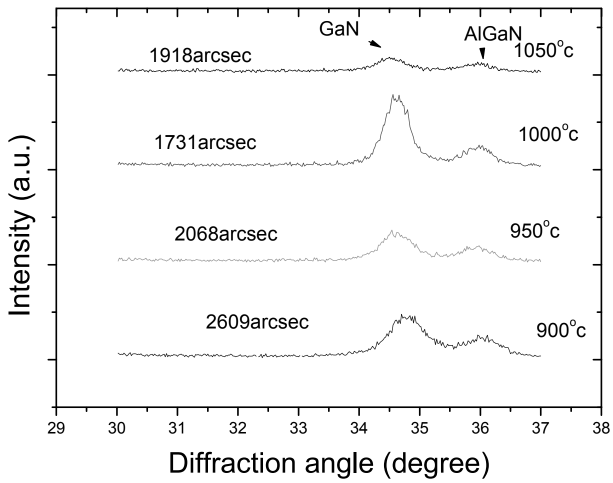

Fig. 1. XRD θ/2θ spectra of the as-grown samples

3.2. Strain and growth temperature

Fig. 4 shows the calculated strain from the X-ray results, both before and after the annealing process. The $\Delta c/c_0$ (tensile strain) decreases in 900°C ~1000°C. The annealing process also reduces the crystal strain. The growth temperature thus plays an important role in controlling the crystal quality. In addition, it was confirmed that the annealing process would reduce the FWHM and the residual stress.

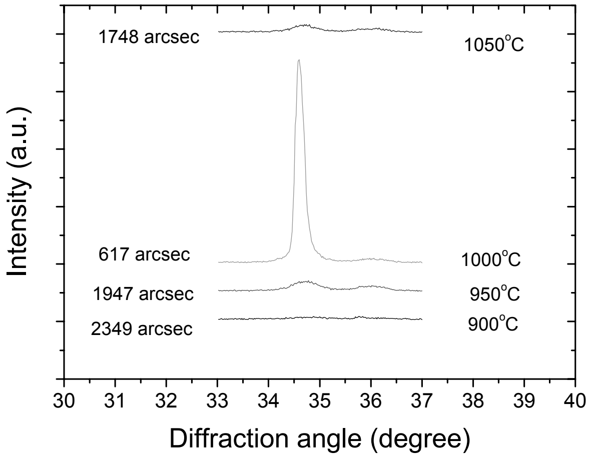

Fig. 2. XRD θ/2θ spectra of the annealed samples

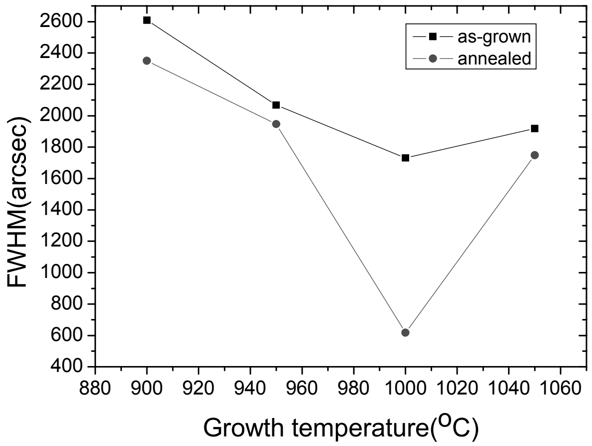

Fig. 3. The variation of FWHM in c-axis with the growth temperature from 900°C to 1050°C

The hole concentration data measured by Hall measurement are shown in Figure 5 for the annealed GaN samples. It has been observed that the hole concentration increased with the growth temperature. The hole concentration was increased by ten times to about $8x10^{17}cm^{-3}$. The strain data were also shown for the annealed samples for the purpose of comparison. A low temperature buffer layer and the increased temperature seem to be effective up to about 1000°C. This step could enhance crystalline mosaicity through strain relief with increasing growth (anneal) temperature. The degree of relaxed strain increased with the growth temperature until 1000°C. It was about $6x10^{-5}$/°C.

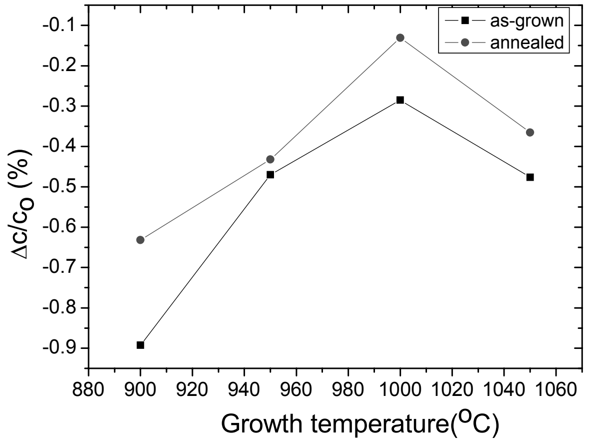

Fig. 4. Strain in c-axis of the samples, both before (as-grown) and after the annealing process

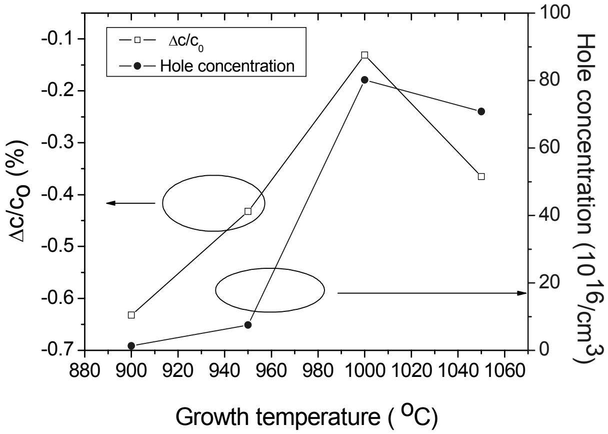

Fig. 5. Hole concentration and strain versus the growth temperature

3.3. Hole concentration below 1000°C

The hole concentration and the mobility of p-GaN samples are shown in Fig. 6. The mobility was increased with the growth temperature up to 150 cm^2/Vs. The effects of the growth temperature on the p-GaN crystal quality and the electrical properties were discussed in the two temperature regions. In 900°C~1000°C, the hole concentration increased, FWHM reduced, and strain reduced with the growth temperature. The SIMS results on Mg are given in Fig. 7. The Mg atom incorporation rate increases with the growth temperature. More Mg atom would provide more opportunities for more holes in GaN. In this experiment, temperature was employed to control the strain. While the strain and the FWHM decreased, the hole concentration was also enhanced. The crystal quality and Mg concentration could affect the hole concentration very effectively below 1000°C. The hole concentration that was provided by Mg exceeded the reduction in hole caused by the strain.

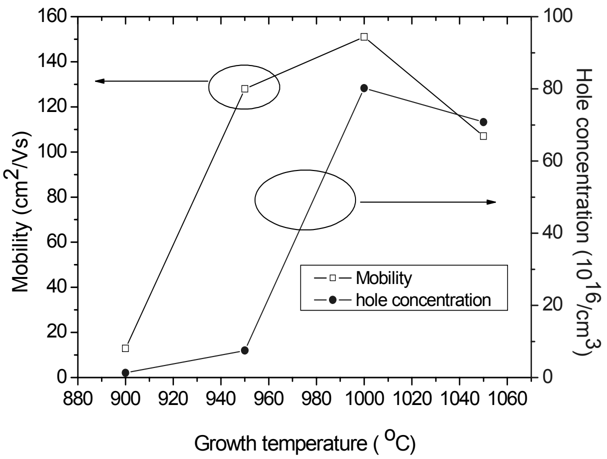

Fig. 6. Hole concentration and mobility of p-GaN as functions of the growth temperature

3.4. Silicon atoms diffusion above 1000°C

It has been shown that Mg concentration increases with the growth temperature. The relationship between the dopant concentration and the strain can be realized from the following equation [14]:

$$\varepsilon = \frac{c - c_0}{c_0} = bC$$

Here, C is the dopant concentration, b is a factor of proportionality, and ε is the strain. It is believed that dopant and temperature are the two dominant factors in affecting the strain. In 900°C -1000°C, growth temperature dominated the variation of hole concentration. However, when the dopant concentration increased dramatically, the hole concentration depended on Mg concentration.

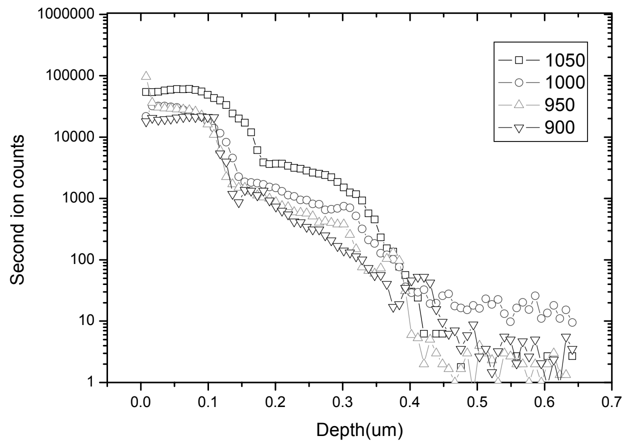

Fig. 7. SIMS analysis of Mg depth profile of the sample grown at different temperatures

Above 1000°C, the hole concentration decreases. In addition, the strain and FWHM increase as well, while the hole concentration decreases. The results of Si distribution by SIMS are shown in Fig. 8. It has been observed that a part of silicon atoms diffused in GaN epitaxial layer. The diffusion of Si atoms would increase the residual stress and could reduce the hole concentration. Thus, Si atoms play the role of donors in GaN. This might result in hole and electron compensation in GaN. Therefore, FWHM increased again due to Si atom diffusion in GaN. The hole concentration increased with the growth temperature through strain relaxation and incorporation of Mg increased below 1000°C. The results above 1000°C depend on crystal characteristics and on diffusion of Si atoms.

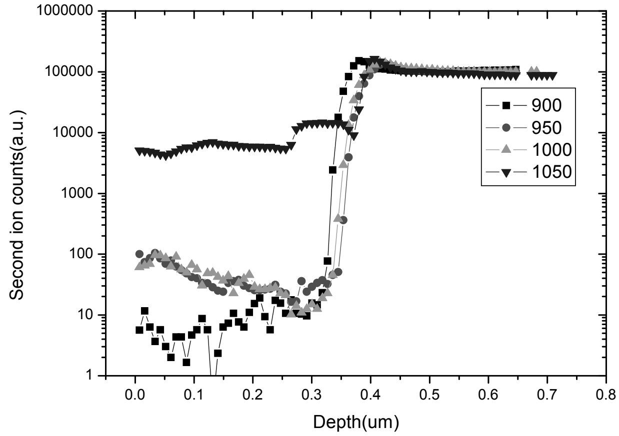

Fig. 8. Si depth profile analysis by SIMS of the samples grown at different temperatures

4. Conclusions

In this report, p-GaN has been grown by metal-organic chemical vapor deposition (MOCVD) at 900°C, 950°C, 1000°C, and 1050°C with low temperature LT-deposited AlN/AlGaN buffer layer. Both the crystal quality and the electrical properties were investigated. The hole concentration increases with growth temperature in 900°C~1000°C. When the growth temperature was optimal at 1000°C, the hole concentration was improved by ten times up to about a value of $8x10^{17}cm^{-3}$. In addition, the effect of process temperature was explained in two ranges. In 900°C-1000°C, the hole concentration increased due to the incorporation rate of Mg and the released stress increased with the growth temperature. However, at 1050°C, the hole concentration reduced owing to the Si diffusion and the strain caused by Mg dopant. According to the experimental data, the optimal growth temperature was 1000°C. After the annealing process, the FWHM of p-GaN was lowered to 617 arcsec.

Acknowledgements

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