

Strain Analysis of Cubic AlGa_{1-x}N/GaN Grown on GaAs(100) Substrate by MOVPE

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Abstract We have grown cubic AlGa_{1-x}N films on the GaAs(100) substrates by metalorganic vapor-phase epitaxy. Photoluminescence and X-ray diffraction results indicate that high quality cubic AlGa_{1-x}N films have been obtained. And the Al molar fraction was achieved to be 0.38. For all the samples, the lattice strain in the AlGa_{1-x}N films exists and relaxes partly. And the unreleased lattice mismatch may vary with the change of Al molar fraction. The AlGa_{1-x}N lattices are unrelaxed for x up to 0.16.

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Group-III nitrides and their alloys are suitable for the application of the light emitting devices in the blue and Ultraviolet (UV) regions as well as of the high temperature/high power electronics devices^[1,2]. To date, most of the GaN devices have been made up of hexagonal phase crystal film^[3-7].

However, the cubic crystal of GaN offers several advantages over its hexagonal counterpart, including easy cleavage and no columnar growth, which make it suitable for a laser structure. In addition, according to theoretical predictions, the cubic GaN could possess the superior electronic properties for the certain device^[8]. It's also expected that the cubic nitrides may be an amendment to the p-type doping^[9]. The heterostructure cubic group-III nitride alloys have a large band-gap difference and can be cleaved by the GaAs. Therefore, they are promising for the application of the optical and electric device^[10]. Recently, we have achieved a cubic P-N junction GaN LED^[11]. To realize the high quality

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LED and LD, the heterostructure must be adopted. And it is necessary to improve the quality of the cubic nitrides alloys. However, only a few reports on the growth of cubic AlGa_{1-x}N^[10-12] and no discussion on the strain in the AlGa_{1-x}N films can be found.

In this paper, we described the growth of cubic Al_{1-x}Ga_xN and the improvement of the crystal quality. At the same time, we investigated the variation of the lattice strain in the AlGa_{1-x}N films. The achieved Al molar fraction was 0.38.

We grew a cubic Al_{1-x}Ga_xN on the GaAs (100) substrates with a low-pressure metal-organic vapor phase epitaxy (MOVPE) system. Triethylgallium (TEGa), trimethylaluminum (TMAI), NH₃ were used as the source materials. The growth consisted of a low-temperature buffer layer at 550 °C, a 600nm-thick cubic GaN at 850 °C, and a 100nm-thick cubic Al_{1-x}Ga_xN at 850 °C. The pressure in the reactor is 1×10^4 Pa during the growth. X-ray diffraction was used to strength the cubic structure. Photoluminescence (PL) was excited by the 325nm's line of He-Cd Laser. We measured the molar fraction of Al by photoluminescence and Auger electron spectroscopy (AES).

Several Al_{1-x}Ga_xN films with different Al molar fractions were deposited on the GaAs (100) by MOVPE. We changed the Al molar fraction by adjusting the flow ratio of TMAI to the sum of TEGa and TMAI. Atsushi Nakadaira and Hidenao Tanaka^[12] have determined the relationship between the PL peak energy and the Al fraction x : $E = 3.20 + 1.85x$. With this equation, we could determine the Al fraction of different AlGa_{1-x}N films. Figure 1 is the PL spectrum of a cubic AlGa_{1-x}N film at the room temperature. The only peak was at 359nm. Thus, we obtained the Al molar fraction to be 0.14. The FWHM of this peak was 17nm and the yellow emission was very weak, which indicated the good crystalline quality of the AlGa_{1-x}N. The Al molar fraction could also be measured by AES.

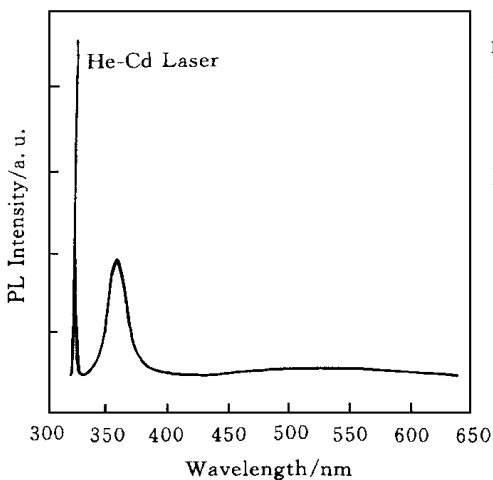


FIG.1 A room temperature photoluminescence spectrum of high quality cubic Al_{0.14}Ga_{0.86}N

The result from AES was in agreement with PL measurement. As what Atsushi Nakadaira and Hidenao Tanaka have reported^[12], the Al molar fraction was found to be proportional to the Al precursor ratio of the vapor phase.

Figure 2(a) and 2(b) show the X-ray diffraction profiles of two Al_{1-x}Ga_xN samples with different Al molar fractions. The Al molar fraction of the sample in Fig.2(a) is 0.16 and that in Fig.2(b) is 0.38. They both have one peak of $2\theta = 39.97^\circ$ and the other at a higher angle.

We assigned the peak of $2\theta = 39.97^\circ$ to the (002) diffraction of the cubic GaN and the other peak at a higher angle to the (002) diffraction of the cubic Al_{1-x}Ga_xN. With the increase of the Al molar fraction, the (002) diffraction of AlGa_{1-x}N

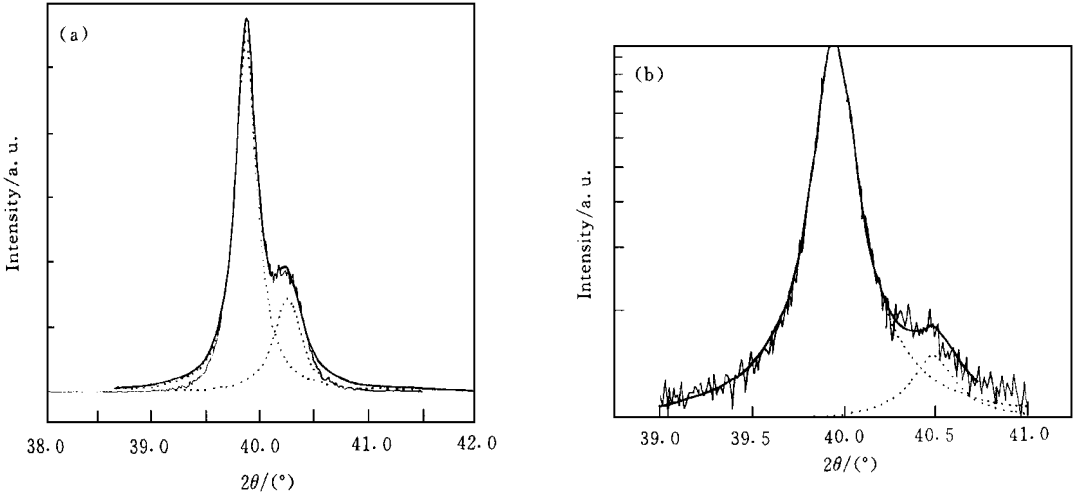


FIG. 2 X-ray diffraction profile of cubic AlGaIn with different Al concentrations
 (a) $x = 0.16$ (b) $x = 0.38$

drifted to a higher angle. We dotted the curves by using the Lorentzian function to determine the diffraction peaks of AlGaIn. The diffraction peaks of AlGaIn in Fig. 2(a) and 2(b) are 40.27° and 40.46° , respectively. Wu and Yaguchi have ever used X-ray diffraction to determine the Al molar fraction of AlGaIn^[10]. They assumed that the lattice in AlGaIn was relaxed completely and then used the unstrained AlN lattice constant of 0.44nm. However, in our samples, it is more believable that the lattice didn't completely relax.

We can use Bragg law to obtain the diffraction lattice parameter a_{AlGaIn} of (001) planes along the substrate axis. a_{AlGaIn} in Fig. 2(a) is 0.448 nm and that of 2(b) is 0.446. The unstrained lattice parameter of epitaxial AlGaIn layer was calculated by Vegard's law. In terms of the lattice constant of AlN at 0.44nm and that of GaN at 0.452nm, the AlGaIn unstrained lattice parameters for the samples in Fig. 2(a) and 2(b) were 0.45nm and 0.447nm, respectively. Since the diffraction lattice parameter is not equal to the unstrained lattice parameter, a tetragonal distortion must present. According to a tetragonal distortion model, the a_{AlGaIn} and a_u can be related by^[13]

$$a_{AlGaIn} = a_u \times (1 + \epsilon) \tag{1}$$

$$\epsilon = \frac{a_{AlGaIn}}{a_u} - 1 \tag{2}$$

and

$$a_{AlGaIn} = a_u \times (1 + \epsilon) \tag{3}$$

$$\epsilon = \frac{a_{AlGaIn}}{a_u} - 1. \tag{4}$$

Here, ϵ is the perpendicular strain while ϵ being the parallel stress. a_u is the unstrained AlGaIn lattice parameter. ϵ and ϵ can be related via the elasticity theory^[14]

$$\epsilon = \frac{-2 \times \nu}{1 - \nu} \times \epsilon \quad (5)$$

For a majority of the materials, the Poisson's ratio ν lies in the range 0.25~0.35. Now, we take ν as 1/3, so that $2\nu/(1-\nu)$ is equal to 1, and the unit-cell volume can be only approximately conserved. Table 1 gives the measured and calculated parameters of these two cubic Al_{1-x}GaN samples. The $a_{\text{AlGaIn}}/a_{\text{AlGaIn}}$ ratio can reflect the strain in the AlGaIn films. As is shown in table 1, the $a_{\text{AlGaIn}}/a_{\text{AlGaIn}}$ ratio in the sample of Fig. 2 (a) is 1.0089 and that of Fig. 2 (b) is 1.0045. The ratio then seems to decrease for large values of the misfit. It indicates that some misfits relief mechanisms (e.g., dislocation) have been introduced and thus lower the ratio. Also, the relaxation of the lattice strain can be determined by the value of $(a_{\text{AlGaIn}} - a_{\text{GaN}})/a_{\text{GaN}}$. The value of $(a_{\text{AlGaIn}} - a_{\text{GaN}})/a_{\text{GaN}}$ reflected the extent of how a_{AlGaIn} lattice matched the GaN lattice. As we all know, the GaN lattice and the Al_{1-x}GaN lattice are different. If the a_{AlGaIn} matched with the GaN lattice, there must be the lattice strain in the parallel direction of AlGaIn. Given $x=0.16$, this value is zero. It means that AlGaIn films were under the tensile stress and extended to match the GaN. If the a_{AlGaIn} completely matched GaN lattice, the lattice strain in the AlGaIn is completely unrelaxed. While for $x=0.38$, AlGaIn does not match GaN at all. But ϵ would not equal to zero, so we could conclude that the lattice strain in this AlGaIn film just relaxed partly. For the lower-Al-concentration samples, we could not clearly resolve the two peaks so that it is difficult to study the lattice strain for a lower Al concentration.

Table 1 The measured and calculated parameters of two cubic Al_{1-x}GaN films

| Sample | x | $2\theta/(\circ)$ | a_{u}/nm | $a_{\text{AlGaIn}}/\text{nm}$ | $a_{\text{AlGaIn}}/a_{\text{AlGaIn}}$ | ϵ | $(a_{\text{AlGaIn}} - a_{\text{GaN}})/a_{\text{GaN}}$ |
|--------|------|-------------------|--------------------------|-------------------------------|---------------------------------------|-----------------------|---|
| A | 0.16 | 40.27 | 0.450 | 0.448 | 1.0089 | -4.4×10^{-3} | 0 |
| B | 0.38 | 40.46 | 0.447 | 0.446 | 1.0045 | -2.2×10^{-3} | -8.8×10^{-3} |

In summary, cubic Al_{1-x}GaN ($0 < x < 0.38$) films have been grown on the GaAs (100) substrates by MOVPE. It is found that, for all the samples, the lattice strain in the AlGaIn films exists but doesn't completely relax. And the unrelieved lattice mismatch might vary with the change of the Al molar fraction. The Al_{1-x}GaN lattices are unrelaxed for x up to 0.16. X-ray and photoluminescence indicate that we obtained almost a complete phase of cubic AlGaIn. The Al molar fraction is achieved to be 0.38.

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