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Misorientation Effects on Al Composition in $Al_xGa_{1-x}As/GaAs$ Determined by High-Resolution XRD

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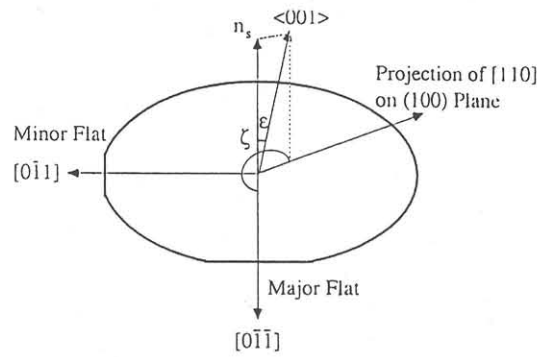
The degree of lattice mismatch and Al contents of $Al_xGa_{1-x}As$ epitaxial layers grown by LPMOCVD on (001) 2° off oriented GaAs substrates are detemined by four crystal x-ray diffractometry. The AlAs epitaxial layer grown on a misoriented GaAs substrate has a perpendicular strain of 0.27 % and epitaxial (001) plane was slightly tilted with respect to the (001) substrate plane. The Al contents was measured by (004) diffraction and its results were nearly the same as the PL measurements. The peak separation and the FWHM of the epitaxial layer peak showed periodical variation. The most accurate Al contents can be obtained, when the x-ray diffracted beam projection on (001) surface was aligned in the substrate tilting direction.

1. Introduction

The epitaxial layers grown on a (001) misoriented substrate has a better surface morphology and higher optical, electrical quality than layers grown on an (001) exact oriented substrate.[1 ~ 3] $Al_xGa_{1-x}As/GaAs$ heterostructures have been important materials for high speed electronic devices and optical communications. DCXRD measurement is an easy and nondestructive meathod with fast feedback for the determination of alloy composition. The AlAs has a lattice constant of only 0.16 % larger[4] than that of GaAs, indicating that epitaxial $Al_xGa_{1-x}As$ layer has no misfit dislocations within the thickness for device applications. The fact that epitaxial layer of $Al_xGa_{1-x}As$ grown on misoriented GaAs substrate has an epitaxial tilt plane with respect to the substrate plane is widely known.[5-6] In this work we qualitatively studied the azimuthal angle dependence of x-ray rocking curves of the epitaxial layer having tilt plane and determined the Al composition using only (004) diffraction and compared it to PL results.

2. Experiments

The sample studied was obtained by low pressure (60 torr) MOCVD at a substrate temperature of 630 °C. The GaAs substrate had a nominally 2° misorientation angle toward <011> direction, azimuthal 225° clockwise from $[0\bar{1}\bar{1}]$, as shown in Fig. 1. Without pre-cleaning, the GaAs substrate was loaded into the reactor via loadlock chamber after 3 times of N_2 purge. The epitaxial layer grown on misoriented GaAs substrate consists of initial 2-μm-thick AlAs layer follwed by $Al_{0.4}Ga_{0.6}As$ layer. To determine the alloy composition and lattice mismatch of the epitaxial layer, (004) and (115) x-ray rocking curves were measured using high-resoluion XRD at various azimuthal angle ζ, which represent the angle between the x-ray injected beam projection onto the (001) surface and $[0\bar{1}\bar{1}]$ direction.



n_s: Surface Normal of Substrate

ε : Misoriented Angle
; nominally (100) 2° ± 0.5° off toward <110>

ζ : Azimuthal Angle Clockwise from $[0\bar{1}\bar{1}]$ Direction
; nominally 225° in this substrate

Fig.1 Specification of a misoriented GaAs substrate.

The silicon single crystal was used as the first reference crystal with Cu $K\alpha_1$ radiation and CCC(channel cut collimator) was used to improve resolution. For comparison, single $Al_{0.3}Ga_{0.7}As$ epitaxial layer was also grown on misoriented GaAs substrate and the results of these samples were compared with photoluminescense (PL) measurements. PL measurements were performed at room temperature using 514.5 nm Ar+ laser as an exitation source.

3. Results and Discussion

The dependence of the peak separation and FWHM(full width at half maximum) between the substrate and AlAs epitaxial layer on the azimuth, obtained from (400) reflection, is represented in Fig. 2 for the AlAs/ $Al_{0.4}Ga_{0.6}As$ multilayer.

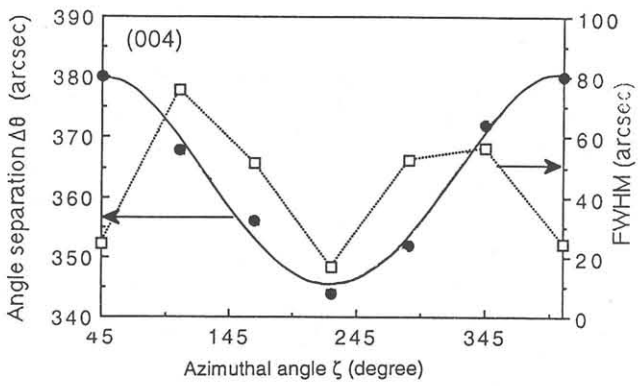


Fig. 2 Peak separation and FWHM variation of rocking curve for AlAs epitaxial layer in AlAs/$Al_{0.4}Ga_{0.6}As$/GaAs heterostructure as azimuthal angle.

The results in Fig. 2 calculated follow a sinusoidal function of 362 + 18 cos (45 - ζ), indicating that (001) epitaxial plane was 18 arcsec tilted with respect to the (001) substrate plane. The epitaxial layer had perpendicular mismatch of 0.27 % and parallel mismatch of 0.01 % from (115) diffraction measurement which indicated that it was a fully strained layer. In Fig. 2, we could predict the tilting orientation of the substrate which represents minimum peak separation at azimuthal angle of 225 degree.

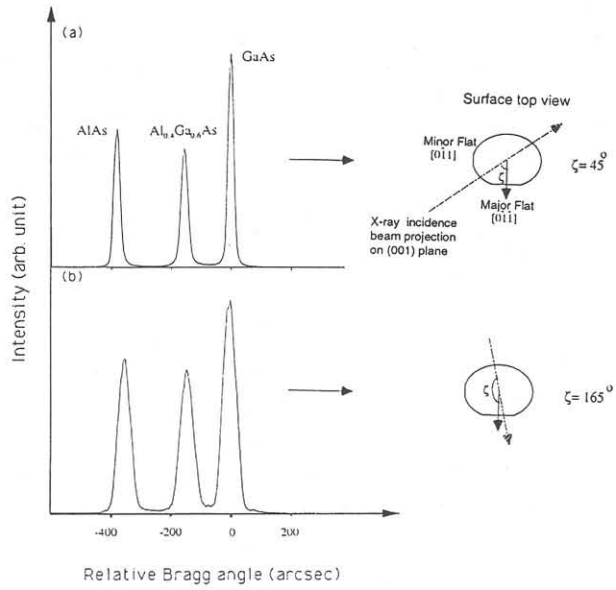


Fig. 3 (004) x-ray rocking curves of AlAs/$Al_{0.4}Ga_{0.6}As$/ GaAs heterostructure measured at the azimuthal angle (a) ζ = 45°, (b) ζ = 165°.

As shown in Fig. 2 and Fig. 3, the narrowest and highest intensity of x-ray peak were observed when the x-ray beam projection on the (001) surface was aligned in these tilting direction of ζ = 45° and ζ = 225° than in the other directions such as ζ = 165°. Interestingly, we found that the FWHM of the substrate as well as of the epitaxial layer also showed periodical variation. It is most likely that periodical variation of the FWHM and intensity is originated from the non-uniform distribution of surface steps and kinks. It is predicted that the step growth causes epitaxial tilt in the strained layer as seen in Fig. 4.[7-8]

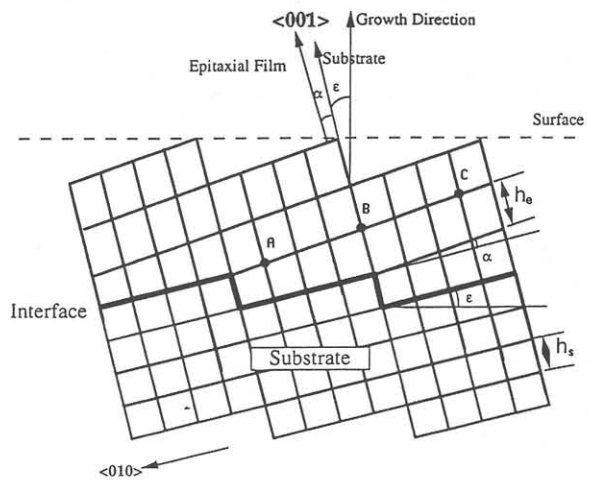


Fig. 4 Lattice tilting of $Al_xGa_{1-x}As$ epitaxial layer grown on a misoriented GaAs substrat.

In Fig. 4 the epitaxial layer of $Al_xGa_{1-x}As$ grown on misoriented GaAs substrate has a triaxial strain near the interface (site A, B) having asymmetrically distorted shape. In the distance place(site C), the epitaxial lattice has only the biaxial strain with tetragonal shape eventualy result in epitaxial tilt plane with respect to the substrate plane. The Al contents in $Al_xGa_{1-x}As$ layer can be determined conventionally by using Vegard's law. The lattice constants of strained $Al_xGa_{1-x}As$ layer grown on GaAs substrate must be corrected by the Poisson ratio. However, the accurate Poisson ratio of AlAs is not established up to date because of its unstable material properties in the oxygen environment. However in this work, the AlAs epitaxial layer grown prior to the growth of $Al_{0.4}Ga_{0.6}As$ epitaxial layer was used as a 100 % Al reference in the x-ray measurement of this sample. The vertical lattice mismatch of AlAs layer grown between $Al_{0.4}Ga_{0.6}$ As and GaAs layer was same as the mismatch of AlAs single layer grown on GaAs substrate. The Al contents can defined by;

$$Al(\%) = \frac{\left(\frac{\Delta a}{a}\right)_{\perp}^{AlGaAs}}{\left(\frac{\Delta a}{a}\right)_{\perp}^{AlAs}} \times 100$$

To compare the Al contents determined by x-ray rocking curve, the sample was characterized by another useful meathod of photoluminescense (PL) at room temperature. Figure 5 shows the PL spectrum data of the band edge transition in $Al_{0.4}Ga_{0.6}As$ layer at room temperature.

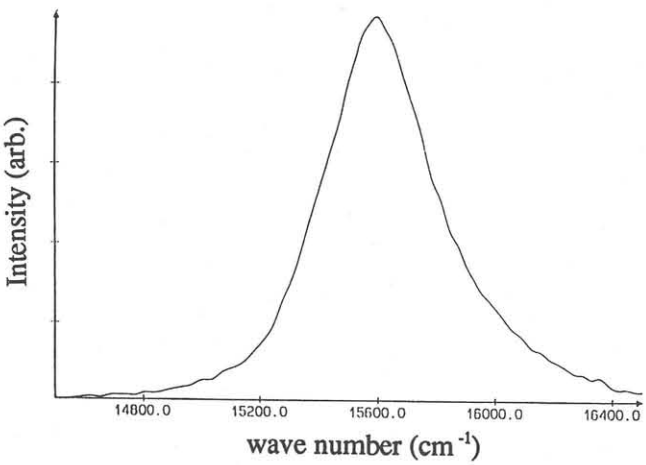


Fig. 5 300 K PL spectra of $Al_{0.4}Ga_{0.6}As$ epitaxial layer.

The average value of the Al contents in $Al_xGa_{1-x}As$ layer for various (004) diffraction angle was 40.6 % which is identical to the results of (115) asymmetric diffraction and PL data. To confirm the results, the other sample of $Al_{0.3}Ga_{0.7}As$ single layer grown on GaAs misoriented substrate was characterized by x-ray and PL, and we were able to obtain similiar results. As seen in Fig. 2 and Fig. 3 , both cases of angle separation variation and periodic rocking curve brodening were closely related to the substrate misorientation. The average value of Al contents for two tilting direction of $\zeta=45^0$, and $\zeta=225^0$ were found to be similiar to the real value. The x-ray measurement for these two directions is most convienient and reliable than any other directions because at these tilting direction the shape of the rocking curve becomes clearer and sharper.

4. Summary

From the calculation of the various directional data, the AlAs epitaxial plane was found to be 18 arcsec tilted with respect to the GaAs substrate plane having a perpendicular strain of 0.27 %. We have observed that both cases of angle separation and the FWHM of the strained epitaxial layers have shown periodical behavior when measured in the various azimuthal direction. The x-ray measurement along the epitaxial tilting direction has shown to be the most accurate method to measure the Al contents.

5. References

1. H. Z. Chen, A. Ghaffari, H. MorKoc and A. Yariv, Appl. Phys. Letters, 51, 2094 (1987).
2. R. K. Tsui, G. D. Kramer, J. A. Curless and M. S. Puffley, in Growth of Compound Semiconductor, SPIE. Vol. 796, 10 (1987).
3. A. S. Brown, U. K. Mishra, J. A. Henige and M. J. Delaney, J. Appl. Phys. 64, 3476 (1988).
4. M. S. Goorski, T. F. Kuech, M. A. Tishler, and R. M. Potemski, Appl. Phys. Letters, 59(18), 2269 (1991).
5. A. Leiberich and J. Levkoff, J. Crystal Growth, 100, 330 (1990).
6. A. T. Macrander, G. P. Schwarz and G. J. Gualtieri, J. Electrochem. Soc. 134, 578C (1987).
7. P. Maigne and A. P. Roth, J. Crystal Growth, 118, 117 (1992).
8. P. Auvray, M. Baudet and A. Regrency, J. Crystal Growth, 95, 288 (1989).