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

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The degree of lattice mismatch and Al contents of Al$_x$Ga$_{1-x}$As epitaxial layers grown by LPMOCVD on (001) 2° off oriented GaAs substrates are determined 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 periodic 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.\cite{1-3} Al$_x$Ga$_{1-x}$As/GaAs heterostructures have been important materials for high speed electronic devices and optical communications. DCXRD measurement is an easy and nondestructive method with fast feedback for the determination of alloy composition. The AlAs has a lattice constant of only 0.16% larger\cite{3} than that of GaAs, indicating that epitaxial Al$_x$Ga$_{1-x}$As layer has no misfit dislocations within the thickness for device applications. The fact that epitaxial layer of Al$_x$Ga$_{1-x}$As grown on misoriented GaAs substrate has an epitaxial tilt plane with respect to the substrate plane is widely known.\cite{54} 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 ton) MOCVD at a substrate temperature of 630 °C. The GaAs substrate had a nominally 2° misorientation angle toward [011] direction, azimuthal 225° clockwise from [011], 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 followed by Al$_x$Ga$_{1-x}$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-resolution XRD at various azimuthal angle ζ which represent the angle between the x-ray incident beam projection onto the (001) surface and [011] direction.

![Projection of [110] on (100) Plane](image)

- $n_2$: Surface Normal of Substrate
- $ζ$: Misoriented Angle
- nominally (100) 2° x 0.5° off toward [110]
- $ξ$: Azimuthal Angle Clockwise from [011] in this substrate

Fig.1 Specification of a misoriented GaAs substrate.

The silicon single crystal was used as the first reference crystal with Cu Ka$_2$ radiation and CCC(channel cut collimator) was used to improve resolution. For comparison, single Al$_x$Ga$_{1-x}$As epitaxial layer was also grown on misoriented GaAs substrate and the results of these samples were compared with photoluminescence (PL) measurements. PL measurements were performed at room temperature using 514.5 nm Ar+ laser as an excitation 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 (000) reflection, is represented in Fig. 2 for the AlAs/AlGaAs/GaAs multilayer.

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 $\xi = 45^\circ$ and $\zeta = 165^\circ$ than in the other directions such as $\zeta = 165^\circ$. 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.

![Fig. 2 Peak separation and FWHM variation of rocking curve for AlAs epitaxial layer in AlAs/AlGaAs/GaAs heterostructure as azimuthal angle.](image)

![Fig. 3 (004) x-ray rocking curves of AlAs/AlGaAs/GaAs heterostructure measured at the azimuthal angle (a) $\xi = 45^\circ$, (b) $\zeta = 165^\circ$.](image)

![Fig. 4 Lattice tilting of AlGaAs epitaxial layer grown on a misoriented GaAs substrate.](image)
To compare the Al contents determined by x-ray rocking curve, the sample was characterized by another useful method of photoluminescence (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.

![PL spectrum data](image)

**Fig. 5** 300 K PL spectra of Al$_{0.4}$Ga$_{0.6}$As epilayer.

The average value of the Al contents in Al$_{0.4}$Ga$_{0.6}$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$_{0.4}$Ga$_{0.6}$As single layer grown on GaAs misoriented substrate was characterized by x-ray and PL, and we were able to obtain similar results. As seen in Fig. 2 and Fig. 3, both cases of angle separation variation and periodic rocking curve broadening were closely related to the substrate misorientation. The average value of Al contents for two tilting direction of $\zeta=45^\circ$, and $\zeta=225^\circ$ were found to be similar to the real value. The x-ray measurement for these two directions is most convenient 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 epilayer 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 epilayer tilting direction has shown to be the most accurate method to measure the Al contents.

5. References