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# Lattice mismatch and surface morphology studies of $In_xGa_{1-x}As$ epilayers grown on GaAs substrates

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**Abstract.** $In_xGa_{1-x}As$ ($0.06 \le x \le 0.35$) epilayers were grown on GaAs substrates by atmospheric pressure metal organic chemical vapour deposition technique. Surface morphology and lattice mismatch in the InGaAs/GaAs films of different compositions were studied. Cross-hatched patterns were observed on the surface of the epilayers for bulk alloy composition up to $x \approx 0.25$. For $x > 0.3$, a rough textured surface morphology was observed.

**Keywords.** Epitaxial layer; metal organic chemical vapour deposition; InGaAs; lattice mismatch.

## 1. Introduction

InGaAs is an interesting material for opto-electronic applications in the range 0·9–3 μm and also for high speed device applications (Nagai 1974). The advantage of InGaAs/GaAs layers over AlGaAs/GaAs is that the concentration of deep levels which limit the device performance in the latter is reduced (Fitzgerald *et al* 1988a). However, in the case of $In_xGa_{1-x}As$ layers, lattice mismatch between the epilayer and the substrate creates undesirable lattice defects, especially misfit dislocations at the interface.

Frank and Merwe (1949) first showed that the lattice mismatch could be accommodated elastically until a critical layer thickness is reached and beyond that misfit dislocations are introduced. Matthews and Blakeslee (1974) developed a model for structural stability based on a specific mechanism for the formation of misfit dislocations. Halliwell *et al* (1984) reported that if the layer is thick and mismatch is large then mismatch dislocation network may be formed. This will lead to tetragonal distortion of the layer. The strain can be relaxed through introduction of misfit dislocations in a region which is electrically and structurally unimportant, generally called buffer layer. When the layer is step graded dislocation–dislocation interaction is large and the extent of relaxation is strongly limited and is not distributed evenly throughout the buffer layer. Here the misfit dislocations are forced to be close to the buffer–substrate interface so that maximum volume of the strained material can be relaxed. Here average distance between dislocations is very small.

Surface morphology of an epilayer is related to strain in the epilayer, which is influenced by defects at the interface. Olsen (1975) reported that mismatch ($\Delta a/a = \varepsilon \approx 2\%$) usually does not exhibit cross-hatching but leads to an irregular surface. He also reported that cross-hatch pattern is a signature of dislocation motion in which crystal growth occurs in a periodically increasing or decreasing manner rather than from an abrupt deformation. Chang *et al* (1990) reported that the strained layer which exhibits a clear cross-hatch pattern has an overall smoother surface than the film which does not show this pattern. Nishioka *et al* (1987) reported that clear recognizable cross-hatch pattern appears for GaAs/Si samples of thickness > 2 μm when the film has a relatively low etch pit density (EPDs) $\le 2 \times 10^7$ cm$^{-2}$. Strain relief in thick $In_xGa_{1-x}As$ layers has been studied by many authors (Maree *et al* 1987; Fitzgerald *et al* 1988b; Chang *et al* 1989) on MBE grown layers. Our aim is to study the origin of cross-hatch surface morphology in relaxed $In_xGa_{1-x}As$/GaAs layers grown by MOCVD technique using trimethylgallium (TMG) and trimethylindium (TMI).

## 2. Experimental

The MOCVD growth was carried out in a horizontal gas flow, atmospheric pressure reactor. The graphite susceptor was heated with rf heating coil and temperature measured by a thermocouple located inside the susceptor. The metalorganic sources were kept in temperature controlled baths. The bath temperatures were kept at – 12°C and 15°C for trimethylgallium and trimethylindium, respectively. 100% Arsine ($AsH_3$) diluted in hydrogen was used as the group V source. The carrier gas was

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palladium-diffused hydrogen with total flow rate of 4 l/min. The typical growth rate was about 2·5 μm/h. Semi-insulating GaAs substrates (100) oriented 3° off towards (110) were used. The substrates were organically cleaned using TCE, acetone, methanol and DI water and then etched in $H_2SO_4 : H_2O : H_2O_2$ (5 : 1 : 1) solution at 50°C, rinsed in DI water and finally dried in dry $N_2$ before introduction into the reactor. Change of indium composition in the epilayers was carried out by changing the flow rates of organometallic sources. Prior to growth, native surface oxides were removed by raising the substrate temperature to 750°C in $AsH_3$ ambient. 0·5 μm GaAs buffer layer was grown at 680°C on each substrate, followed by a layer of $In_xGa_{1-x}As$ grown at 625°C, with $x$ varying from 0·06 to 0·35. The epilayer thickness was ≈ 2 μm which was well above the critical layer thickness for all the compositions. Thickness measurement was carried out by an optical microscope using cleave-and-stain technique. Surface morphology of the epilayers was studied by Nomarski interference optical microscopy. Double crystal X-ray diffractometry (Bede QC1a) was used to measure the lattice constant and mismatch of the films perpendicular to the interface. Rocking curves were taken for (400) reflection using CuK$\alpha$ radiation at $\lambda = 1{\cdot}54051$ Å.

## 3. Results and discussion

X-ray diffraction patterns of the epilayers are shown in figures 1a–3a. The lattice mismatch ($\Delta a/a$) was determined using the relation,

$$(\Delta a/a) = \cot\theta\,\Delta\theta, \tag{1}$$

where $\theta$ is the Bragg angle and $\Delta\theta$ the peak position separation. Assuming completely relaxed layer, $\Delta a$ is equal to the lattice constant of $In_xGa_{1-x}As$ minus the lattice constant of GaAs (5·6534 Å). InAs mole fraction ($x$) was calculated using the relation given by (Stringfellow 1993)

$$a = 6{\cdot}0583 - 0{\cdot}405(1-x). \tag{2}$$

All the samples show epilayer peak on the lower $\theta$ side. The InAs mole fraction and mismatch of the films are shown in table 1. Samples are grown with uniform In concentration. The thickness of the layer is about 2 μm which is well above the critical layer thickness for all the values of In composition used. The compositions of the layer were also calculated using photoluminescence (PL) and electron microprobe analysis (EMPA) techniques which agreed well with the X-ray diffraction observation.

Surface morphologies of $In_xGa_{1-x}As$ layers are shown in figures 1b–3b. Cross-hatch pattern is observed in the layers in which In compositions are 0·12 ($\varepsilon = 0{\cdot}85\%$) and 0·21 ($\varepsilon = 1{\cdot}5\%$). Kishino *et al* (1972) proposed a model with regard to the growth mechanism of the aligned dislocation array to explain the origin of cross-hatch pattern. As the indium composition in the epilayer increases dislocations generated by the mismatch increase and cross-hatch pattern disappears gradually and textured surface morphology is observed. A rough textured surface morphology (figure 3b) is observed when $x = 0{\cdot}33$ ($\varepsilon = 2{\cdot}4\%$). A rough textured surface appears due to an irregular form in the image of dislocations because dislocations could not align along the line (Kishino *et al* 1972). The lattice strain might be too large to be

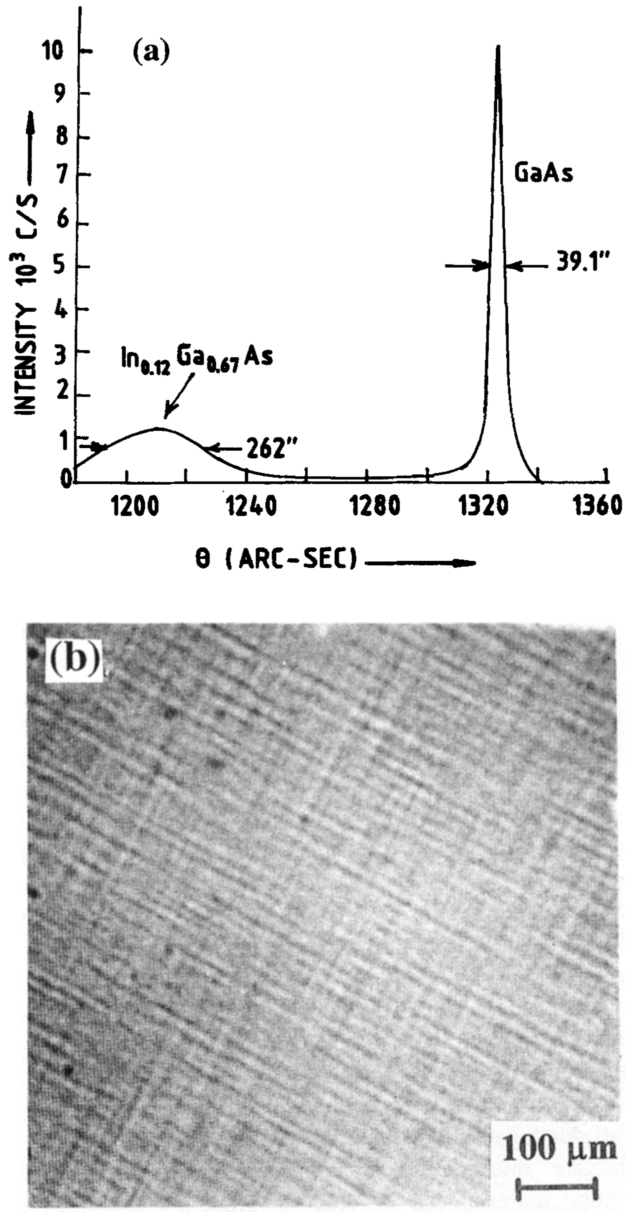


**Figure 1.** **a**. X-ray diffraction pattern of $In_{0.12}Ga_{0.88}As$ layer grown on GaAs and **b**. surface morphology of $In_{0.12}Ga_{0.88}As$ layer grown on GaAs.

compensated by making the misfit dislocation array. Chang *et al* (1990) performed detailed experiments on several $In_xGa_{1-x}As$ layers grown by MBE. They have concluded that surface cross-hatch pattern is seen on the surface of layers if the misfit strain is smaller than 2%. For values of misfit strain > 2%, a rough textured surface is obtained. This is in accordance with our experimental observations. The FWHM of bare GaAs substrate is 12 arc-sec. The FWHM of the epilayer increases and that of the substrate also increases as the In composition of the film increases. Lattice mismatch also increases accordingly. The presence of threading dislocations in the epilayer as well as in the substrate was explained by Krishnamoorty *et al* (1991) using balance of force model. Our results are also consistent with their observation. The epilayer having cross-hatch pattern was determined to be high in quality from the half width of the rocking curve. Noad and SpringThorpe (1980) also observed similar type of results by resistively heated MOCVD technique using triethylindium (TEI) as indium source. Halliwell *et al* (1984) have studied the effect of mismatch on the broadening of the substrate peak in double crystal X-ray diffraction due to lattice mismatch, the substrate assumes an overall curvature which leads

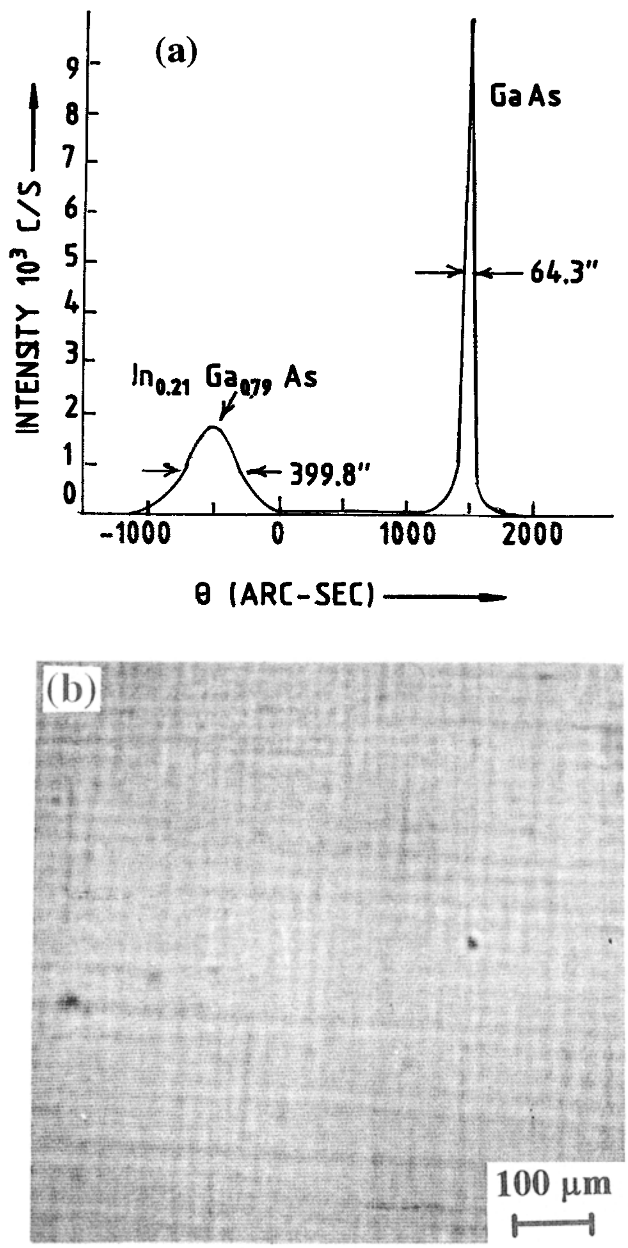


**Figure 2.** **a**. X-ray diffraction pattern of $In_{0.21}Ga_{0.79}As$ layer grown on GaAs and **b**. surface morphology of $In_{0.21}Ga_{0.79}As$ layer grown on GaAs.

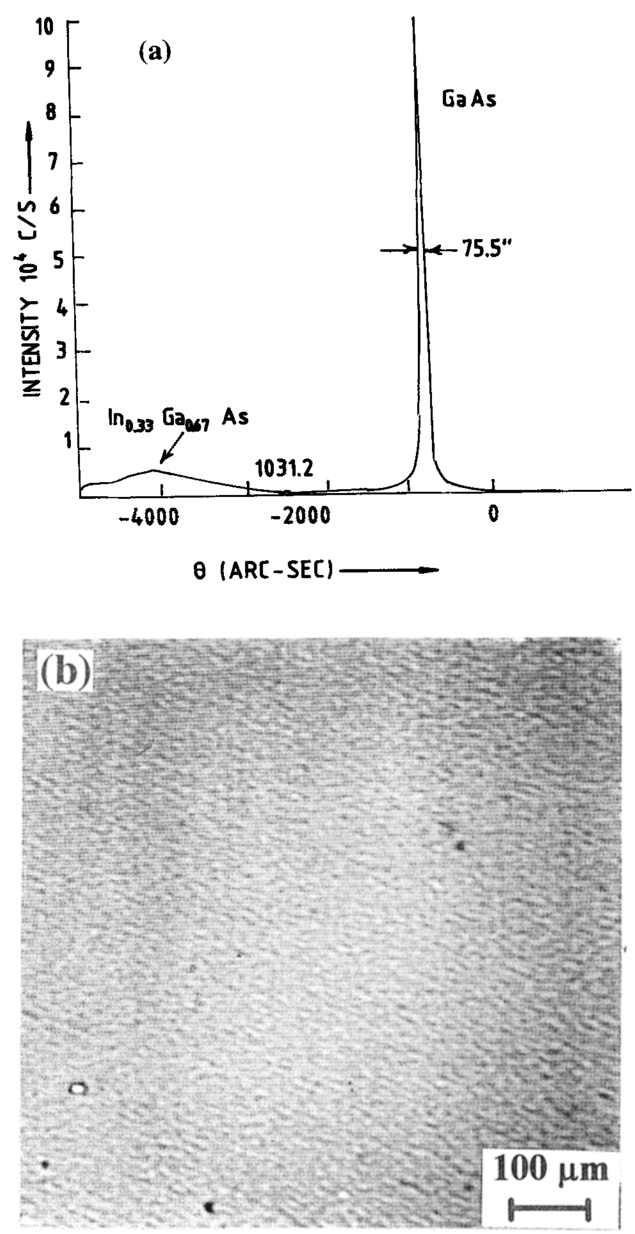


**Figure 3.** **a**. X-ray diffraction pattern of $In_{0.33}Ga_{0.67}As$ layer grown on GaAs and **b**. surface morphology of $In_{0.33}Ga_{0.67}As$ layer grown on GaAs.

**Table 1.** Lattice mismatch of $In_xGa_{1-x}As$ layers grown on GaAs substrate.

| Sample no. | FWHM (arc-sec) Sub. | FWHM (arc-sec) Layer | Thickness (μm) | ($\Delta a/a$) ($10^{-2}$) | Lattice constant (Å) | InAs mole fraction |
|---|---|---|---|---|---|---|
| 1. | 39·1 | 262·0 | 2·0 | 0·85 | 5·7015 | 0·12 |
| 2. | 64·3 | 399·8 | 2·0 | 1·47 | 5·7369 | 0·21 |
| 3. | 75·5 | 1031·2 | 2·0 | 2·36 | 5·7869 | 0·33 |

to peak broadening. The etch pit density of these layers was calculated by chemical etching technique. The pits were revealed by 1AB : 4HF solution at room temperature and were counted in a calibrated area using a Zeiss Optical microscope at magnification $\times 200$. The EPD obtained was $\approx 2\times 10^7\,cm^{-2}$ and $\approx 5\times 10^8\,cm^{-2}$ for $Ga_{0\cdot21}In_{0\cdot79}As$ and $Ga_{0\cdot33}In_{0\cdot67}As$ layers, respectively.

If the peak broadening is solely attributed to the dislocation density, the average dislocation density $N_d$ can be calculated by using the relationship (Murlidharan and Ploog 1989)

$$N_d = (\Delta W/4b)^2, \tag{3}$$

where $\Delta W$ is the FWHM obtained from double crystal X-ray diffraction measurement and $b$ the Burger vector. For textured sample ($x = 0\cdot33$), the dislocation density is found to be $\approx 10^8\,cm^{-2}$ while for cross-hatch pattern sample ($x = 0\cdot21$) the EPD is $4\times 10^7\,cm^{-2}$.

## 4. Conclusions

Surface morphology of lattice mismatched MOCVD grown $In_xGa_{1-x}As$/GaAs heterostructure has been studied by Nomarski optical microscopy. When the misfit strain in the epilayers is smaller than 2%, threading dislocation density in the layer is low and cross-hatch patterns are observed. Thus cross-hatching provides a convenient method to determine the misfit dislocations via optical microscopy. Therefore, devices can be made in the range 0·9–1·2 μm with ungraded $In_xGa_{1-x}As$ epilayers with small In compositions ($0 < x < 0\cdot25$).

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