

The Dislocation Generation Mechanism of $\text{In}_x\text{Ga}_{1-x}\text{As}$ Epilayers ($0.32 \leq x \leq 1$) Grown on InP Substrates by Molecular-Beam Epitaxy

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The dislocation generation mechanism of the $\text{In}_x\text{Ga}_{1-x}\text{As}$ epilayers grown on InP substrates with $0.32 \leq x \leq 1$ were investigated. It was found that the growth mode is not only dependent on the lattice mismatch, the abundance of Ga atoms and the degree of cation disorder in the alloy composition also play important roles. In the negative mismatched range even with a medium lattice mismatch, InGaAs alloys with high degree of cation disorder and contain more Ga atoms ($x = 0.32-0.37$) trigger island growth and introduce high-density dislocations.

Introduction

The heteroepitaxy of $\text{In}_x\text{Ga}_{1-x}\text{As}$ epilayers on InP substrates has become important because they can be applied to the optical communication systems basing on novel fluoride fibers.¹ However, little attentions has been paid to study the dislocation generation mechanism of $\text{In}_x\text{Ga}_{1-x}\text{As}$ epilayers grown on InP substrates.²⁻³ Most of the previous studies concentrated their research in the $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ system,⁴⁻⁶ and concluded that the InGaAs grown on GaAs favors island growth when the lattice mismatch is larger than 2%. Recently, we have studied the dislocation generation mechanism⁷ of highly mismatched $\text{In}_x\text{Ga}_{1-x}\text{As}$ on GaAs. It was found that under the highly mismatched condition, the intermixing of cations must be taken into account and ternary InGaAs with a high degree of cation disorder (comparable In and Ga atoms) generates the highest density of vertical dislocations than any other composition. It is worthy of note that when the lattice mismatch of $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ increases, the indium composition and thus the degree of cation disorder also increase. So it is unclear that whether the onset of the island growth is mainly caused by the increase of the degree of cation disorder or lattice mismatch, especially at a medium mismatched condition.

Considering both the $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ and $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{InP}$ systems, the lattice matching condition between $\text{In}_x\text{Ga}_{1-x}\text{As}$ epilayers to the GaAs and InP substrates occurs at $x = 0$ and 0.53, respectively. If both systems are under small lattice-mismatched conditions, the former has a low degree of cation disorder (little In) but the latter has a very large one (In to Ga ratio close to 1). The investigation of the dislocation generation mech-

anism in the $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{InP}$ system may give some insight to the role that cation disorder plays in the heteroepitaxy. In this paper, we study this system by both the double-crystal x-ray diffraction (DXRD) and cross-sectional transmission electron microscopy (XTEM). The result also compares with the $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ case.

Experiments

All samples were grown on Fe-doped (100) InP substrates in a solid source VG V80H MK II molecular-beam-epitaxy system. Lattice matched $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ buffer layers with thickness 100 to 150 nm were first grown at 510 °C to smooth out the growing surface, then, 2- μm -thick undoped $\text{In}_x\text{Ga}_{1-x}\text{As}$ epilayers with $0.32 \leq x \leq 1$ were grown under the arsenic stabilized condition. The growth rates were kept around 1 $\mu\text{m}/\text{h}$ and the growth temperatures were 510 °C. XTEM studies were carried out in a JEOL 200 CX transmission electron microscope operating at 200 kV.

Results

A. DXRD Signals

Fig. 1 is the full width at half-maximum (FWHM) of (400) DXRD signals from $\text{In}_x\text{Ga}_{1-x}\text{As}$ epilayers with $0 \leq x \leq 1$ on InP. The FWHM reaches a minimum value of 20–30 arcsec when x is kept to around 0.53, and then increases as x deviates from the matching condition. In the positive mismatched region ($x > 0.53$), the FWHMs reach maximum values at x around 0.73–0.82, with 1.4%–2% mismatch with respect to the InP substrate. The FWHM decreases as x increases to 1, and is only 270 arcsec at $x = 1$. Meanwhile, it exhibits the same feature in the negative mismatched re-

gion, and the FWHMs reach maximum values at x around 0.32–0.37, with a corresponding mismatch ϵ of $(-1.5\%) - (-1.1\%)$. This result is in agreement with that reported by Tabuchi *et al.*⁸ and indicates that the material quality of InGaAs degrades most seriously as x is around 0.73–0.82 (compression) and 0.32–0.37 (tension).

The FWHM of the DXRD signal is very sensitive to the crystal quality. Bennett and Alamo⁹ suggested that the broadening of the FWHM might be caused by the existence of both misfit dislocations and defects related to 3D growth. For the positively mismatched InGaAs on InP, samples with maximum FWHM values (e.g., $x = 0.73$) still have crosshatched surface features (2D growth).^{3,10} It is therefore not possible to directly relate the degradation of the crystal quality to the island growth, and XTEM images are necessary to distinguish the generation mechanism of dislocations.

B. XTEM Images

The [011] XTEM images with $\vec{g} = [400]$ for the $\text{In}_x\text{Ga}_{1-x}\text{As}$ epilayers grown on InP with $x = 0.66, 0.82, 0.88, 1$, (in compression) and 0.37 (in tension) are shown in Figs. 2(a), (b), (c), (d), and (e), respectively. The corresponding images with $\vec{g} = [022]$ are shown in Figs. 3(a)–(e). For $x = 0.66$ ($\epsilon = 0.9\%$), dislocations are almost confined at the $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ interface, no threading dislocations are detected. When x increases to 0.82 ($\epsilon = 2\%$), dislocations threading along the [100] growth direction with pyramid dislocation tangles (PDT) appear¹¹. The dislocation density is not high and the vertical-dislocations exist in both the (400) and (022) images.

For $x = 0.88$ ($\epsilon = 2.4\%$), more PDT defects

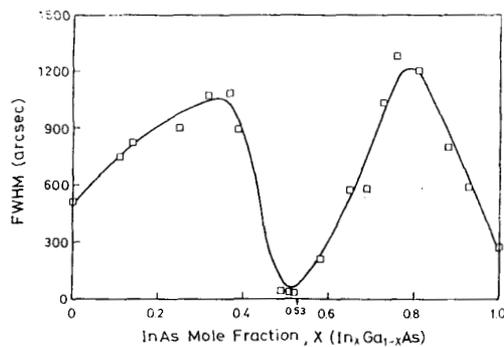


Fig. 1 The full width at half maximum (FWHM) of the (400) double-crystal x-ray diffraction signals from 2 μm thick $\text{In}_x\text{Ga}_{1-x}\text{As}$ epilayers ($0 \leq x \leq 1$) grown on InP substrates.

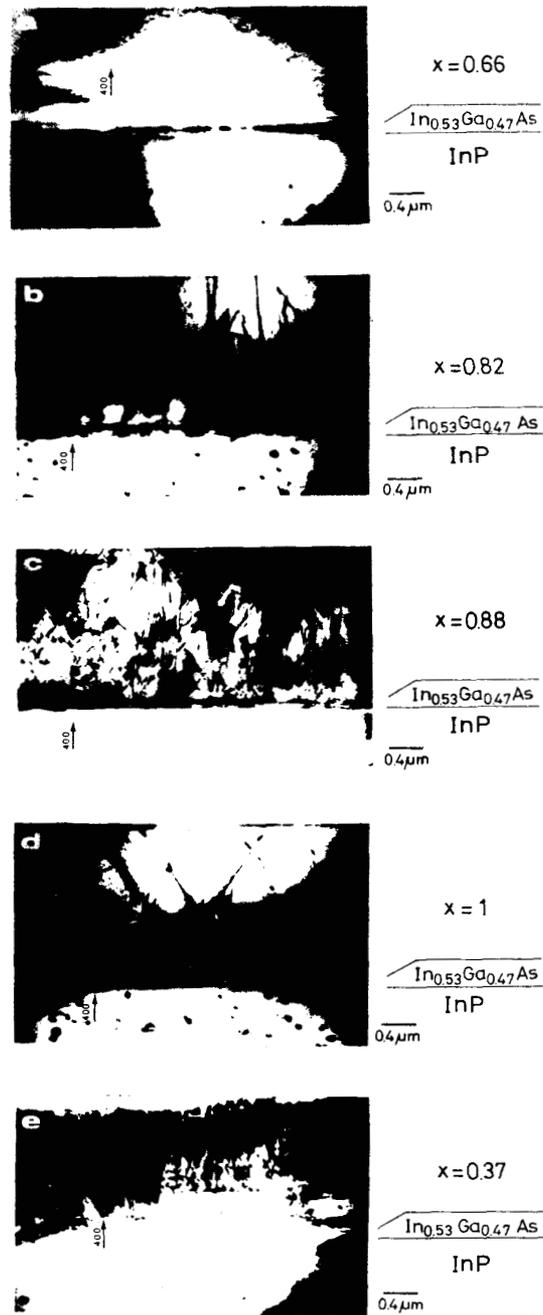


Fig. 2 Two-beam dark-field (400) XTEM images of $\text{In}_x\text{Ga}_{1-x}\text{As}$ epilayers grown on InP substrates for $x =$ (a) 0.66, (b) 0.82, (c) 0.88, (d) 1, and (e) 0.37, respectively. The $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ buffers are 100 to 150-nm-thick.

developed and many vertical type dislocations were detected. Some of them are the V-shaped dislocations which appear in $(02\bar{2})$ but disappear under the (400) diffraction conditions in XTEM images.¹¹ For InAs grown on the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}$ ($\epsilon = 3.2\%$), in spite of the large lattice mismatch, threading dislocations are relatively scarce, similar to InAs grown on GaAs.⁷

$\text{In}_x\text{Ga}_{1-x}\text{As}$ on InP with a negative lattice mismatch is also observed. For $x = 0.37$ ($\epsilon = -1.1\%$) whose FWHM of the DXRD signal is within the range of maximum values, although this system only has a medium mismatch, a high density of threading dislocations appears and 3D growth occurs in this sample. Comparing the (400) and $(02\bar{2})$ type images as shown in Figs 2(e) and 3(e), we see that many V-shaped dislocations exist in this sample.

Discussion

Since the generation of threading dislocations has been attributed to the formation and coalescence of islands in the initial growth stage,⁷ the strain relaxation mechanism in the $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{InP}$ system can be understood from the analyses of the dislocation type and density in the XTEM images.

For $x = 0.66$ ($\epsilon = 0.9\%$), the XTEM images indicate that the heteroepitaxy is still under a 2D growth mode. It means that the onset of the island growth needs a larger lattice mismatch and the Ga atoms do not seem to be the island nucleation sources under such a medium mismatched condition, although a considerable intermixing of Ga and In atoms occurs at this composition. As x increases to 0.82 ($\epsilon = 2.0\%$), the growth mode changes to 3D and vertical-type dislocations are generated. Since V-shaped dislocations do not appear and the dislocation density is very low [Figs. 2(b) and 3(b)], large-sized and low-density quasi-2D relaxed islands must have formed in the initial stage.⁷ Gendry *et al.*³ have used plan-view TEM images to study the growth mode of an 80-Å-thick $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$ single quantum well grown on InP. They found that at higher growth temperature, very low-density and huge-size (e.g., $500 \times 250 \text{ nm}^2$) islands formed in the initial growth stage, and the islands exhibited moiré fringes which indicates islands were partially or totally relaxed. This initial growth mode observed in their case is consistent with what we predict from the analysis of the dislocations in the bulk epilayer. Considering the $\text{In}_x\text{Ga}_{1-x}\text{As}$ on GaAs systems with similar mismatch ($x = 0.28\text{--}0.3$), high density vertical dislocations appeared in the bulk epilayers⁷ and many small coherent islands (e.g., $30 \times 50 \text{ nm}^2$)

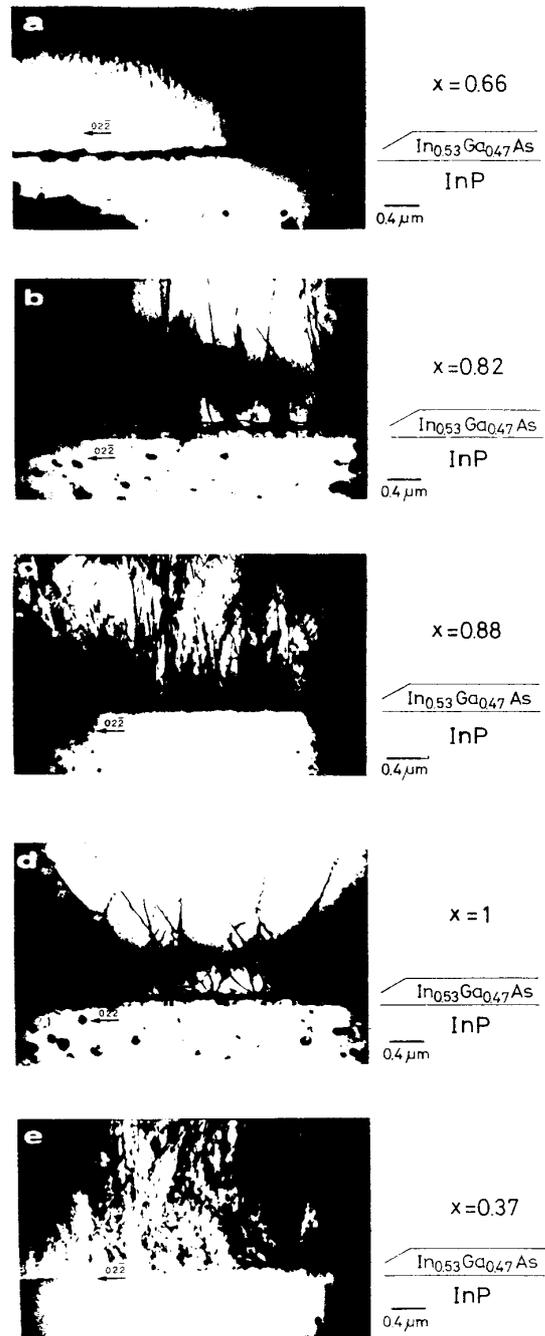


Fig. 3 Two-beam dark-field $(02\bar{2})$ XTEM images of $\text{In}_x\text{Ga}_{1-x}\text{As}$ epilayers grown on InP substrates for $x =$ (a) 0.66, (b) 0.82, (c) 0.88, (d) 1, and (e) 0.37, respectively.

formed in the initial stage.⁶ The reason that under the similar 2% positive mismatched conditions, the InGaAs grown on GaAs and InP show different dislocation features is the following: In_xGa_{1-x}As with $x = 0.3$ has a higher degree of cation disorder and contains more Ga atoms (the island nucleation sources) than that with $x = 0.82$, so these two materials develop different island features and introduce different dislocation types in the bulk epilayers.

As x increases continuously to 0.88 ($\epsilon = 2.4\%$), more PDT defects and vertical dislocations appear, a higher island density than that of $x = 0.82$ must have appeared in the initial stage. Meanwhile, since the percentage of Ga atoms in this alloy is low, the corresponding island nucleation sources should also decrease, and each island can grow larger and thus easily to relax before coalescence, as proved by the fact that not many V-shaped dislocations are observed. Comparing the difference of XTEM images between $x = 0.82$ and 0.88, the growth mode is weak 3D in the former but 3D in the latter; the difference in dislocation densities indicates that $x = 0.88$ has a higher island density than $x = 0.82$, although the former has a lower percentage of Ga atoms. This result shows that the increased lattice mismatch also favors island growth. For $x = 1$ (InAs), the dislocation type indicates that the strain relaxation mechanism is similar to that of InAs grown on GaAs.⁷

For InGaAs on InP with a negative lattice mismatch, the XTEM images indicate that island growth occurs even under a medium mismatch of -1.1% for $x = 0.37$ [Figs. 2(e) and 3(e)]. Most of the islands in the initial stage must be strain free because high-density V-shaped dislocations are observed in this case. We explain this phenomenon as follows: both the degree of cation disorder and Ga concentration in this composition are large and there are thus many island nucleation centers even at such a medium mismatched range. This high density of islands limits the island size and the medium mismatch hampers the relaxation of islands. As a result, coherent islands appear. The importance of cation disorder and alloy composition in the heteroepitaxy can be seen in this case.

Conclusion

The dislocation generation mechanism of the In_xGa_{1-x}As epilayers grown on InP has been investigated. In the negative mismatched range even with $\epsilon = -1.1\%$ ($x = 0.37$), threading dislocations

are generated because both the considerable cation disorder and the higher Ga concentration trigger island growth. For In_xGa_{1-x}As grown on GaAs and InP substrates, the appearance of high density of V-shaped dislocations, which indicates the formation of coherent islands at the initial growth stage, is only found at $x = 0.3-0.5$ when grown on GaAs and at $x \approx 0.37$ when grown on InP, both of them have a high degree of cation disorder and contain higher Ga concentrations. For the growth of In_xGa_{1-x}As on InP with positive mismatch, although island growth occurs at $x \approx 0.82$, few V-shaped dislocations were generated. These results indicate that lattice mismatch is not the only factor to determine the growth mode, the cation disorder and the corresponding Ga concentration of the InGaAs alloy also play important roles in the InGaAs/InP system.

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