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Lattice-matched $\text{Zn}_{1-y}\text{Cd}_y\text{Se}/\text{In}_x\text{Ga}_{1-x}\text{As}(001)$ heterostructures

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Abstract

$\text{In}_{1-x}\text{Ga}_x\text{As}$ buffer layers grown on $\text{GaAs}(001)$ wafers can be used as novel substrates lattice matched to the $\text{Zn}_{1-y}\text{Cd}_y\text{Se}$ active layers employed in blue–green lasers. Photoluminescence studies of $\text{Zn}_{1-y}\text{Cd}_y\text{Se}$ alloys ($x = 0.15$ and 0.25) grown by molecular beam epitaxy on such substrates show a dramatic reduction in the deep-level emission as compared to $\text{Zn}_{1-y}\text{Cd}_y\text{Se}/\text{GaAs}(001)$ heterostructures. The surface of the epilayers, however, exhibits a cross-hatched morphology as a result of ~ 10 nm deep surface corrugations oriented along perpendicular $\langle 110 \rangle$ directions. © 1998 Elsevier Science B.V. All rights reserved.

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1. Introduction

Recently, $\text{In}_x\text{Ga}_{1-x}\text{As}$ alloys have attracted interest as possible lattice-matched substrates for the

growth of II–VI based blue–green lasers [1,2]. For appropriate values of the In concentration x , $\text{In}_x\text{Ga}_{1-x}\text{As}$ alloys can be designed to match the lattice parameter of the $\text{Zn}_{1-y}\text{Cd}_y\text{Se}$ active layers in blue ($y \sim 0.15$) and blue–green ($y \sim 0.25$) lasers. However, high quality $\text{In}_x\text{Ga}_{1-x}\text{As}$ wafers with $x \geq 0.04$ are not available because of homogeneity problems in high- x bulk single crystals. We examined here the growth of $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer layers with optimized concentration and strain relaxation profile on GaAs and its implications for the quality of the $\text{Zn}_{1-y}\text{Cd}_y\text{Se}$ epilayers.

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2. Experimental procedure

All structures were grown by solid source MBE following the procedures described elsewhere [3] in a system which includes interconnected chambers for the growth of III–V and II–VI materials. 1 μm thick $\text{In}_x\text{Ga}_{1-x}\text{As}(001)$ 3×1 epilayers were grown at 500°C with V/III beam pressure ratios (BPRs) in the 15–30 range. The indium content in the alloy was calibrated in situ by means of XPS, and ex situ by X-ray diffraction (XRD) and Rutherford backscattering spectrometry (RBS) [4,5].

The backscattering yield ratio χ_{\min} between random and $\langle 001 \rangle$ channeling directions was used to quantify the overall structural quality of the near-surface region of the epilayers.

The residual strain in the epilayers was estimated from the measured angles between the different channeling directions, as illustrated in Refs. [4,5]. Throughout this paper the measured elastic deformation will be quantified in terms of the in-plane lattice strain $\varepsilon_{\parallel} = (a_{\parallel} - a_0)/a_0$, where a_0 is the free-standing equilibrium lattice parameter and a_{\parallel} is the measured in-plane lattice parameter in the epilayer.

On selected $\text{In}_x\text{Ga}_{1-x}\text{As}$ epilayers, $\text{Zn}_{1-y}\text{Cd}_y\text{Se}$ overlayers were deposited at 250°C with a Zn to Se beam-pressure ratio near unity. The Cd content in the alloy was also calibrated in situ by XPS and ex situ by RBS. The surface morphology of the different epilayers was probed by atomic force microscopy (AFM) in air, and we used photoluminescence spectroscopy (PL) to probe the optical quality of the II–VI epilayers. Optical excitation was provided by the 457.9 nm line of an

Ar^+ laser with a typical power density of 25 W/cm^2 and a sample temperature of 15 K.

3. Results and discussion

Graded composition $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer layers (type I) in which x varied from 0 to 0.33 with a parabolic composition profile were designed using a modification of Tersoff's model for strain relief in graded layers [7]. While Tersoff's [6] calculation employs the equilibrium density of misfit dislocations (MDs) computed by Matthew and Blakeslee [8], we used instead the experimentally-determined strain-release behaviour [4] in the calculation. This is essential since the $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ system shows higher residual strains and hence lower MD densities than predicted by the equilibrium theory [4].

For comparison, we also employed $\text{In}_{0.27}\text{Ga}_{0.73}\text{As}$ buffer layers with homogeneous composition (type II). The free-standing lattice constant of $\text{In}_{0.27}\text{Ga}_{0.73}\text{As}$ alloys ($a_0 = 5.7627 \text{ \AA}$ [9]) would match that of $\text{Zn}_{0.75}\text{Cd}_{0.25}\text{Se}$, but the partial character of the $\text{In}_x\text{Ga}_{1-x}\text{As}$ strain relaxation on GaAs for a 1 μm thick type II buffer is expected to provide a less than ideal lattice match to the II–VI active layer. The excess indium concentration at the surface of the graded $\text{In}_x\text{Ga}_{1-x}\text{As}$ type I buffer ($x = 0.33$) was calculated precisely to compensate for the partial character of the strain relaxation in the buffer.

In Table 1 we summarize the RBS-derived structural parameters for two different type I $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffers. The measured values of the backscattering yield ratio χ_{\min} between random and

Table 1

Structural parameters of two different graded composition $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffers grown by molecular beam epitaxy on GaAs(001) wafers. Nominal value of the sample thickness was 1 μm in both cases. In the nominal composition profile the In concentration varied from $x = 0$ at the wafer surface to $x = 0.33$ at the free surface with a parabolic composition profile. All parameters listed were determined by means of Rutherford backscattering spectrometry (RBS). Column 1: sample number. Column 2: sample thickness. Column 3: In atomic concentration at the surface. Column 4: backscattering yield ratio χ_{\min} between random and $\langle 001 \rangle$ channeling directions. Column 5: measured in-plane strain

Sample	t (nm)	x_s	χ_{\min} (%)	ε_{\parallel} (%)
C18	858 ± 50	0.320 ± 0.004	12 ± 1	-0.38 ± 0.04
C88	915 ± 50	0.340 ± 0.004	10 ± 1	-0.48 ± 0.04

$\langle 001 \rangle$ channeling directions (10–12%) provide a qualitative indication of a relatively high crystal-line quality of the near-surface region [10]. Substantially higher values of χ_{\min} ($\sim 18\%$) were observed in type II buffers. As a rule, the $\text{Zn}_{0.75}\text{Cd}_{0.25}\text{Se}$ overlayers were found to exhibit the same value of χ_{\min} within experimental uncertainty as the underlying $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer.

The measured residual strain in the buffers indicate that – as expected – only partial strain relaxation can be achieved in a $1\ \mu\text{m}$ thick buffer. For sample C18 (C88) the measured -0.38% (-0.48%) residual compressive strain corresponds to $a_{\parallel} = 5.761\ \text{\AA}$ ($5.763\ \text{\AA}$). The in-plane lattice mismatch between $\text{Zn}_{0.75}\text{Cd}_{0.25}\text{Se}$ ($a_0 = 5.764\ \text{\AA}$ [11,12]) and C18 (C88) is therefore only 0.05% (0.02%). The implication is that the model employed to design the type I buffers was successful in predicting the excess surface concentration of indium required to compensate the partial character of strain relaxation.

In Fig. 1 we compare the PL at 15 K from 300 nm thick $\text{Zn}_{0.75}\text{Cd}_{0.25}\text{Se}$ epilayers grown in identical conditions on a GaAs buffer (Fig. 1a) and on a type I $\text{In}_x\text{Ga}_{1-x}\text{As}$ graded buffer (Fig. 1b). All spectra displayed a sharp (10–20 meV FWHM) near-band-edge (NBE) emission feature at 2.46 eV, and deep-level-related emission features in the gap.

The II–VI epilayers are expected to grow pseudomorphically on the lattice-matched $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffers, while they are expected to be mostly relaxed with the formation of a large MD density when grown directly on GaAs, since the expected critical thickness of $\text{Zn}_{0.75}\text{Cd}_{0.25}\text{Se}$ on GaAs is only 25 nm [13]. The results in Fig. 1 clearly indicate that the related deep-level emission intensity is decreased by at least a factor of 30 when the epilayer is grown on lattice-matched $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffers as opposed to GaAs.

The obvious improvement in the optical quality of II–VI epilayers grown on lattice-matched $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffers comes at a cost. In Fig. 2 we illustrate AFM studies of the surface morphology of type II (top) and type I (bottom) $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffers on GaAs. The corresponding results for 300 nm thick $\text{Zn}_{0.75}\text{Cd}_{0.25}\text{Se}$ epilayers grown on the two types of buffers are illustrated in Fig. 3. A comparison of the results in Figs. 2 and 3 clearly indicate that the surface morphology of the II–VI epilayers mirrors that of the III–V buffers.

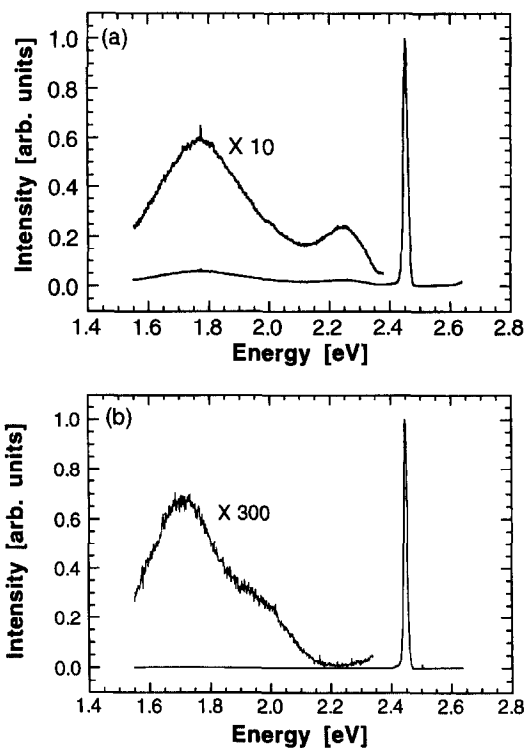


Fig. 1. Photoluminescence spectra at 15 K from 300 nm thick $\text{Zn}_{0.75}\text{Cd}_{0.25}\text{Se}$ epilayers grown on GaAs buffer layers (a) or on graded-composition $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer layers (type I) in which x was varied from $x = 0$ to 0.33 (b). All buffers were fabricated by molecular beam epitaxy (MBE) on GaAs(0 0 1) wafers. The spectra have been normalized to the intensity of the near-band-edge emission feature at 2.46 eV.

Depending on the value of the In concentration x , the surface morphology of $\text{In}_x\text{Ga}_{1-x}\text{As}$ epilayers on GaAs is known to reflect either the high-roughness deriving from a largely three-dimensional (3D) growth mode (in the high- x range), or a characteristic cross-hatched pattern of surface corrugations parallel to the MD network established at the $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ interface (in the low- x range).

The results in Fig. 2 show that type II buffers exhibit the former type of surface morphology, while type I buffers show the latter type of morphology. In particular, the surface of the type I buffer (Fig. 2b) is characterized by surface corrugations with an amplitude of $\sim 10\ \text{nm}$ (peak-to-valley $\sim 20\ \text{nm}$) oriented along perpendicular $\langle 110 \rangle$ directions and spaced by $\sim 0.5\text{--}1\ \mu\text{m}$. With a corresponding

rms roughness of 5 nm, type I buffers are some 35% smoother than type II buffers, which show the random roughness deriving from the 3D growth mode (Fig. 2a) and a typical rms roughness of ~ 8 nm.

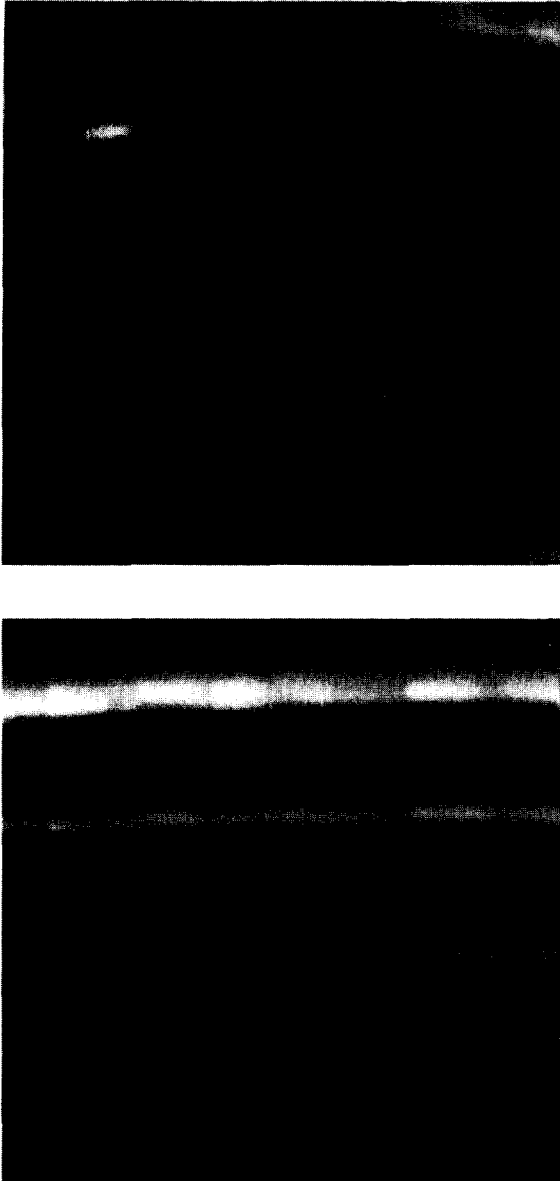


Fig. 2. Atomic force microscopy (AFM) studies of the surface morphology of type II (upper image) and type I (lower image) $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer layers. The 2D rms roughness in the two images was 8 and 5 nm, respectively. The sampled area was $5\ \mu\text{m} \times 5\ \mu\text{m}$ in size in both cases.

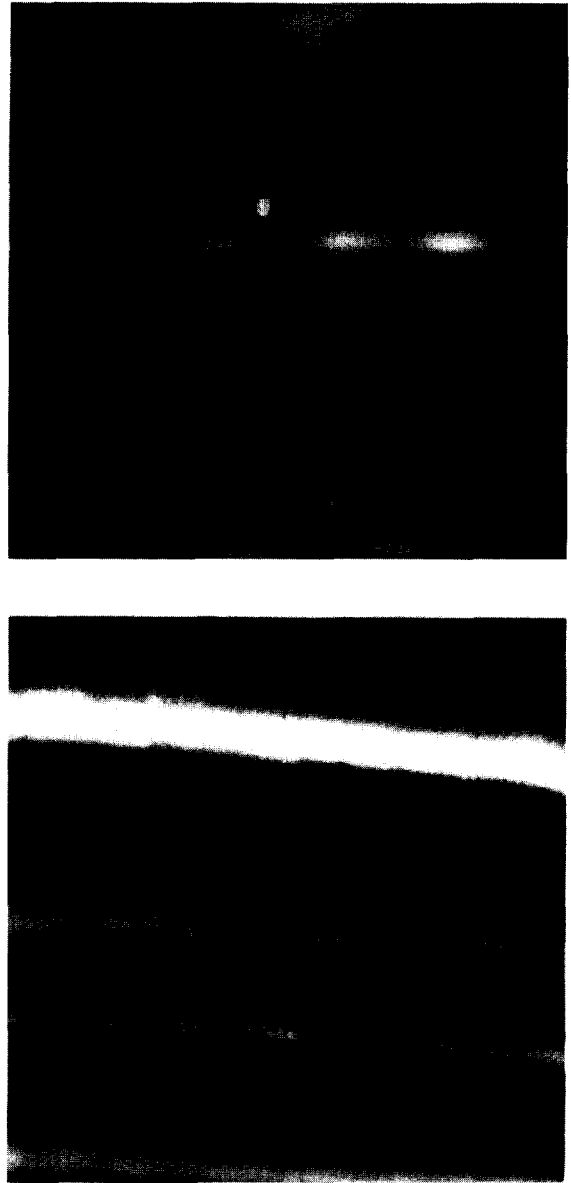


Fig. 3. AFM studies of the surface morphology of 300 nm $\text{Zn}_{0.75}\text{Cd}_{0.25}\text{Se}$ layers grown by MBE on type II (upper image) and type I (lower image) $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer layers. The 2D rms roughness in the two images was 7 and 5 nm, respectively. The sampled area was $5\ \mu\text{m} \times 5\ \mu\text{m}$ in size in both cases.

4. Conclusions

The optical quality of $\text{Zn}_{0.75}\text{Cd}_{0.25}\text{Se}$ epilayers grown on lattice-matched, graded-composition

$\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer layers showed a marked improvement as compared to II–VI epilayers grown on GaAs, with a decrease by at least a factor of 30 in the deep-level emission intensity relative to the NBE emission.

The surface morphology of the $\text{Zn}_{0.75}\text{Cd}_{0.25}\text{Se}$ epilayers was found to mirror that of the underlying III–V buffers, with analogous morphological features and rms roughness.

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