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Strain relaxation in convex-graded $In_xAl_{1-x}As$ (x = 0.05–0.79) metamorphic buffer layers grown by molecular beam epitaxy on GaAs(001)

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ABSTRACT

This paper presents a study of structural properties of InGaAs/InAlAs quantum well (QW) heterostructures with convex-graded $In_xAI_{1-x}As$ (x = 0.05-0.79) metamorphic buffer layers (MBLs) grown by molecular beam epitaxy on GaAs substrates. Mechanisms of elastic strain relaxation in the convex-graded MBLs were studied by the X-ray reciprocal space mapping combined with the data of spatially-resolved selected area electron diffraction implemented in a transmission electron microscope. The strain relaxation degree was approximated for the structures with different values of an In step-back. Strong contribution of the strain relaxation via lattice tilt in addition to the formation of the misfit dislocations has been observed for the convex-graded InAlAs MBL, which results in a reduced threading dislocation density in the QW region as compared to a linear-graded MBL.

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1. Introduction

InGaAs/InAlAs heterostructures grown on strongly lattice-mismatched GaAs substrates via InAlAs metamorphic buffer layers (MBLs) are of great interest for high-speed and low power devices [1,2] because of its high electron mobility and small energy gap, which become higher and smaller, respectively, with increasing the In content in the InGaAs quantum well (QW) and the InAlAs barriers. To accommodate lattice mismatch in the InGaAs QW - GaAs system and filter threading dislocations (TDs), being the most harmful extended structural defects inherent to the MBL growth, different designs of MBLs including step- [2,3], linear- [4] and non-linear [5] graded layers are used. High electron mobility values were measured at low temperatures for the $In_xGa_{1-x}As/In_yAl_{1-y}As$ metamorphic structures with x,y > 0.7 grown on step- or linear-graded MBLs [2–4]. However, it is known that the using of the non-linear MBLs can lead to a stronger reduction of the TD density and improving the properties of the metamorphic structures. Indeed, it was shown that non-linear $In_xGa_{1-x}As$ MBLs with a maximum In content x_{max} ~0.35 provides the more efficient reduction of the TD density down to a value of 7×10^3 cm⁻² with a negligible increase in the surface roughness [6]. A convex-graded $In_xAl_{1-x}As$ MBL with the square root In content profile and $x_{max} = 0.55$ was demonstrated to be efficient in enhancing optical and electron transport properties of $In_{0.5}Ga_{0.5}As$ metamorphic layers

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grown on GaAs [5]. Recently, we have shown that the use of convex-graded $\ln_x Al_{1-x}$ As MBL with $x_{max} = 0.83$ instead of linear one in the samples with a top single 0.4 µm-In_{0.75}Al_{0.25}As layer grown on the MBL results in improvement of the sample crystallinity and at least three times reduction of the near-surface TD density down to a value of $(5 \pm 2) \times 10^7$ cm⁻² [7]. It should be noted that the minimum value of root mean square surface roughness (RMS) down to 2.3 nm (at an area of $10 \times 10 \ \mu\text{m}^2$) was also achieved in the samples with the convex-graded MBL. Moreover, much brighter photoluminescence has been observed in the InAs/In_{0.66}Ga_{0.34}As/In_{0.77}Al_{0.23}As/In_xAl_{1-x}As/GaAs QW structures when the convex-graded MBL was used instead of linear one, in good agreement with the improved structural properties [8].

X-ray reciprocal space mapping (RSM) is commonly used for characterization of MBLs and provides information on the lattice mismatch, residual strain, composition variation, crystallographic tilt, tilt azimuth as well as the rocking curve full-width-at-half-maximum (FWHM) [9–11]. To establish unambiguous correlation of the RSM angular profile to certain regions of the MBL, a transmission electron microscopy (TEM) technique was shown to be efficiently used in combination with the RSM [12,13]. Recently, a new sophisticated approach, combining x-ray RSM technique at different reflections and selected area electron diffraction (SAED) measurements by TEM, made along the growth axis at the structure cross-section, was proposed [14] and applied to elucidate the details of stress relaxation process in the $ln_xGa_{1-x}As$ ($x_{max} \sim 0.3$) MBL [15].

The aim of this work is to study the strain relaxation mechanisms in metamorphic $In_{0.75}Ga_{0.25}As/InAlAs$ QW structures with convex-graded $In_xAl_{1-x}As$ MBLs (x_{max} up to 0.79) grown by molecular beam epitaxy (MBE) on GaAs substrates. The above mentioned RSM - SAED technique was employed for this study.

2. Experiment

The metamorphic InGaAs/InAlAs OW heterostructures were grown by MBE on semi-insulating GaAs (001) substrates via the convex-graded InAlAs MBL by using a RIBER 32P setup. Conventional solid source effusion cells were used to produce In, Ga and Al fluxes, whereas the As₄ flux was supplied from a VAC-500 valved cracking cell. A substrate temperature T_S was measured by IR pyrometer calibrated by using the well-known temperatures of oxides desorption from GaAs ($T_S = 580 \degree C$) and the (2×4) As-to-c (4×4) As transition of GaAs surface reconstructions during cooling under the As₄ flux ($T_{\rm S} = 510$ °C). monitored *in-situ* by reflection high energy electron diffraction (RHEED). To remove the native oxide layer from the GaAs substrate surface prior to the MBE growth, a special procedure of direct irradiation of the surface by a Ga molecular flux at much low $T_{\rm S} = 450$ °C [16] was used instead of the commonly exploited thermal oxide desorption at temperatures above 580 °C under an ambient As₄ flux. Then a 0.2 μ m-thick GaAs buffer layer was grown at $T_S = 590$ °C before the MBL starts. It was shown that the surface of such GaAs buffer consists of isotropic flat monolayer-thick islands and exhibits the RMS roughness as low as 0.16 nm at an area $10 \times 10 \ \mu m^2$ [7]. For the convex-graded In_xAl_{1-x}As MBL, the In content changed over the thickness (*l*) in accordance with the following equation $x = x_i + (x_{max} - x_i)(l/l_t)^{1/2}$, where x_i is the initial In content (0.05) and l_t is the total MBL thickness. To realize this complicated profile using standard thermo-controllers for effusion cells, the full temperature ranges of the In and Al cells temperature variation were divided into 19-20 intervals, with the optimal rates of linear changing of the cell temperatures being chosen for each of them [17]. The In and Al cell temperatures were changed during the MBL growth so as to keep constant the growth rate (0.6 ML/s) over the MBL thickness, which allows an easy control of the constant As₄/III ratio and provides much better reproducibility of the sample properties. The effective As₄ flux measured in the GaAs growth rate units equaled ~1 µm/h for all the structures at the used temperatures. The QW structures of various designs with MBL of different x_{max} and step-back were studied in the paper. The layer sequences of the typical samples studied are presented in Fig. 1. The samples contain a 24 nm-thick In_{0.75}Ga_{0.25}As QW embedded asymmetrically between

(a)		(b)	
			In _{0.75} Ga _{0.25} As, 4 nm
	In _{0.75} Ga _{0.25} As, 4 nm		In _{0.75} Al _{0.25} As, 68 nm
	In _{0.75} AI _{0.25} As, 76 nm		SL 2×(In _{0.7} Al _{0.3} As/InAs), 4/1 nm
	δ-Te doping		δ -Te doping
	In _{0.75} Al _{0.25} As, 8 nm		$SL 2 \times (In_{0.7}AI_{0.3}As/InAs), 4/1 nm$
	QW In _{0.75} Ga _{0.25} As, 24 nm		QW In _{0.75} Ga _{0.25} As, 24 nm
	In _{0.75} Al _{0.25} As, 40 nm		SL 4×(InAs/In _{0.7} Al _{0.3} As), 1/4 nm
	0.75 0.25 0.7 0.25		In _{0.7} Al _{0.3} As, 24 nm
	In _x Al _{1-x} As MBL		In _x AI _{1-x} As MBL
	x=0.05-0.79		x=0.05-0.75
	950 nm		850 nm
	GaAs, 200 nm		GaAs, 200 nm
	GaAs (001)		GaAs (001)
	substrate		substrate

Fig. 1. Design of the studied metamorphic InGaAs/InAlAs QW structures: sample A (a) and sample B (b).

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