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Interdiffusion in InGaAs/GaAs and InGaAs/GaAsP quantum wells

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Abstract

The shape of $In_{0.22}Ga_{0.78}As$ single quantum wells (SQW) grown by metal–organic vapour phase epitaxy (MOVPE) is changed by rapid thermal annealing (RTA). Samples with GaAs barriers were compared with strain-compensated ones with $GaAs_{0.82}P_{0.18}$ barriers using high-resolution X-ray diffraction (HRXRD), Auger electron spectroscopy (AES) and photoluminescence spectroscopy (PL). After annealing, the PL wavelength is decreased and the luminescence intensity increased. In bare strain-compensated layers, In diffusion is slightly reduced at 850°C annealing temperature. Encapsulation with SiO_2 leads to an increase of the In diffusion up to a factor of 10. In this case, the diffusion process is dominated by vacancies and strain compensation is no longer effective. © 1997 Elsevier Science S.A.

Keywords: Interdiffusion; Luminescence properties; Metal–organic vapor phase epitaxy; Single quantum wells

1. Introduction

Strained InGaAs single quantum wells (SQWs) are frequently used for GaAs-based devices such as laser diodes or transistors. In laser diodes the emission wavelength critically depends on the composition and thickness of the QWs. The luminescence properties can be affected by processes such as rapid thermal annealing (RTA) [1,2]. The observed changes are due to In–Ga interdiffusion. This interdiffusion is enhanced by dielectric encapsulation and can be used to create locally different bandgaps for monolithic integration of, for example, laser diodes and modulators [3]. One of the factors determining the amount of diffusion is strain. We have studied the effect of $GaAs_{1-y}P_y$ strain-compensating barriers on the interdiffusion in bare and SiO_2-coated samples under various annealing conditions. The strain-compensating barriers reduce the net strain in the SQW and thus allow for a higher In content to be incorporated without formation of misfit dislocations. In this way, the emission wavelength can be extended to the region longer than 1 μm.

2. Experimental details

Strained $In_xGa_{1-x}As$ SQWs, with thickness $t = 8$ nm and In content of $x = 0.22$ were grown by metal–organic vapour phase epitaxy (MOVPE) at 750°C on (001) oriented substrates. In sample A, this SQW was sandwiched by 100 nm thick GaAs layers. In the strain-compensated structure B, the same SQW was embedded in two 10 nm thick $GaAs_{0.82}P_{0.18}$ barrier layers. Here, the barriers were sandwiched by 120 nm thick $Al_{0.2}Ga_{0.8}As$ for reasons of carrier confinement. In sample C, additional GaAs spacer layers of 5 nm were inserted between the 6 nm $In_{0.25}Ga_{0.75}As$ SQW and the 10 nm thick $GaAs_{0.82}P_{0.18}$ barriers. One part of each sample was coated with 200 nm thick SiO_2 by PECVD (plasma enhanced chemical vapour deposition). Annealing was done in a RTA reactor under GaAs pressure at temperatures of 850 and 950°C for 20–60 s.

Composition and thickness of the compressively and tensively strained layers were determined before and after annealing using high-resolution X-ray diffraction (HRXRD). Coupled $\omega/2\theta$ rocking curves near the (004) reflection were collected using a Philips MRD and fitted with simulated ones. The obtained results were compared to In and P depth profiles determined by Auger electron spectroscopy (AES). Optical properties

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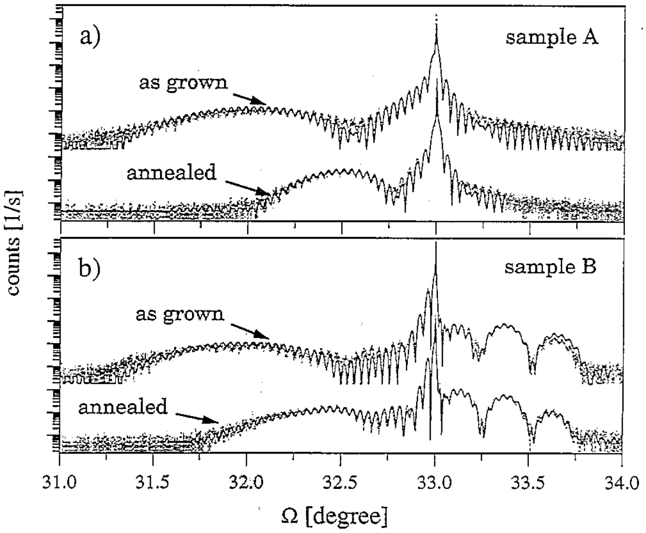

Fig. 1. Measured (- - -) and simulated (——) rocking curves of (a) InGaAs/GaAs SQW (sample A) and (b) InGaAs/GaAsP/AlGaAs SQW (sample B).

were studied by photoluminescence (PL) at 10 and 300 K. Plan view integral cathodoluminescence (CL) images of the QWs were taken at 300 K in a JSM 840 scanning electron microscope to yield information on defect generation.

3. Results and discussion

The 8 nm thick $In_{0.22}Ga_{0.78}As$/GaAs SQW (A) has the highest effective strain. Fig. 1(a) shows the measured and simulated rocking curves before and after 20 s annealing at 950°C. The annealing causes an outdiffusion of indium from the SQW into the barriers. The maximum In content in the SQW is reduced to 12% and the thickness is nearly doubled. The In interdiffusion leads to a decrease of the PL wavelength λ from 1026 to 952.5 nm at 300 K (Table 1). The λ-shift corresponds with band structure calculations based on the In distribution determined by HRXRD and confirmed by AES. The full width at half maximum (FWHM) of the PL peak at 10 K decreases upon annealing. This is probably due to a homogenization of the upper QW interface that shows a slight roughness of some monolayers in the as-grown state [4]. Additionally, the luminescence intensity increases. CL investigations show that the as-grown sample is free of misfit dislocations (MD) and dark spot defects (DSD). After the annealing DSDs, but no MDs, are observed. Apparently, non-radiative point defects cluster into these microdefects and the luminescence properties of the surrounding areas are improved, leading to a higher PL and CL intensity.

Fig. 1(b) shows the rocking curves of sample B as-grown and annealed at 950°C for 20 s. In this case, quaternary layers are formed upon annealing. HRXRD does not allow for a determination of x and y in quaternary layers. AES profiles of the same samples (Fig. 2) confirm the results of HRXRD simulation made under the assumption of constant integral In and P content and independent diffusion. The PL wavelength reduction in sample B is somewhat higher than for sample A (Table 1). The FWHM of the PL peak at 10 K does not decrease as much as for sample A, indicating no improvement of the interfaces. In the CL image of the as-grown sample B, DSDs and cloudy areas are seen (Fig. 3(a)). The annealing process increases the number and size of the DSDs and homogenizes the luminescence (Fig. 3(b)). No MDs are observed. The third sample, C, has 5 nm GaAs spacers to avoid the formation of quaternary layers. In this case, the CL image is similar to that of sample A.

The In–Ga diffusion is described by Fick's law [5]. The one-dimensional solution of the In distribution $x(z, t)$ (z = growth direction, t = time) with the initial concentration x_0 confined in the region $-w < z < w$ is:

Table 1
PL wavelength (300 K) and peak width (10 K) for as-grown and annealed samples with and without SiO_2 caplayer (annealing time: 20 s)

Sample	InGaAs (nm)		GaAs (nm)	GaAsP (nm)		As-grown (nm)	
	d	x	d	d	y	λ: 300 K	FWHM: 10 K
A	8	0.22	100	—	—	1026	4.4
B	8	0.22	—	10	0.18	1021.5	4.0
C	6	0.25	5	10	0.18	1032	5.1

Sample	Annealed: 850°C (nm)		Annealed: 950°C (nm)		SiO_2: 850°C (nm)		SiO_2: 950°C (nm)	
	λ: 300 K	FWHM: 10 K	λ: 300 K	FWHM: 10 K	λ: 300 K	FWHM: 10 K	λ: 300 K	FWHM: 10 K
A	1016	3.9	952.5	2.6	995.0	3.8	929	5.0
B	1006	5.1	946	3.4	992.5	4.5	—	—
C	1020	4.9	953.5	5.0	994.5	4.9	916	9.2

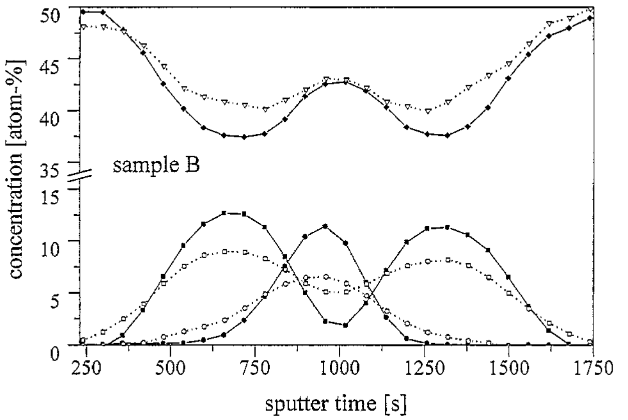

Fig. 2. AES depth profile from bevelled InGaAs/GaAsP/AlGaAs SQW (sample B): In (●, ○), P (■, □) and As (◆, ▽) (●, ■, ◆: as-grown; ○, □, ▽: annealed at 950°C for 20 s).

$$x(z,t)=\frac{1}{2}x_0\left[\operatorname{erf}\left(\frac{w-z}{L_D}\right)+\operatorname{erf}\left(\frac{w+z}{L_D}\right)\right] \quad (1)$$

where erf is the error function, L_D is diffusion length, $L_D=2\sqrt{Dt}$, and D is the diffusion coefficient.

The comparison of the solution with the results obtained by HRXRD for sample A yields $D=1.9\times 10^{-16}$ cm^2 s^{-1} for annealing at 850°C and the expected square root dependence of L_D on t. For the strain-compensated samples, the In diffusion coefficient was determined assuming the independence of the III- and V-sublattice, and is found to be slightly reduced at 850°C (Fig. 4). Nevertheless, the λ variation is not smaller, since the simultaneous P diffusion into the InGaAs QW reduces the effective QW width and thus causes an additional blueshift. The In diffusion in strain-compensated samples is more sensitive to the RTA temperature. For an exponential dependence of D on the temperature T, such that $D(T)\sim \exp(-E_a/kT)$, an activation energy E_a of 2.1 eV is found for sample A. Palfrey et al. [6] published a value of 2.6 eV. The activation energy E_a for the strain-compensated samples is 3.4 eV.

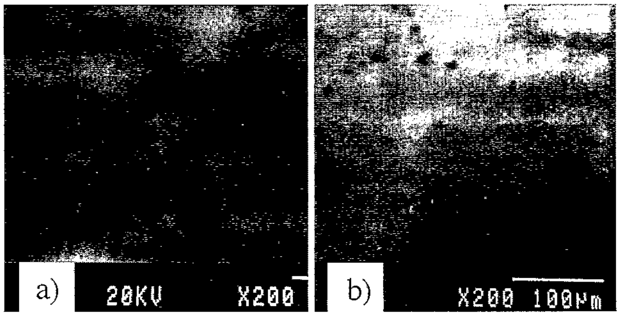

Fig. 3. CL plan view of the GaAs/GaAsP/AlGaAs SQW (a) as-grown; (b) annealed at 950°C for 20 s.

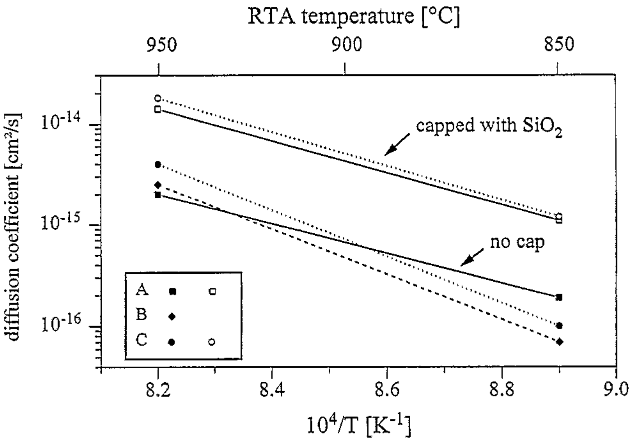

Fig. 4. Arrhenius plot of the diffusion coefficient vs. RTA temperature (annealing time 20 s): sample A (■, □); sample B (◆); sample C (●, ○) (■, ◆, ●: uncoated; □, ○: coated with SiO$_2$).

Several authors report on selective interdiffusion with different encapsulations during the annealing [1,7]. Coating of sample A with 200 nm SiO$_2$ increases D from 1.9×10^{-16} cm^2 s^{-1} to 1.1×10^{-15} cm^2 s^{-1} at 850°C. According to [8], the increased interdiffusion is caused by Ga outdiffusion into the caplayer. The formed Ga vacancies migrate into the bulk and enhance the intermixing rate. The annealing under encapsulation at 850°C effects the same reduction of the 10 K PL FWHM as in the uncapped case. The increase in FWHM at 950°C is not understood but could be related to sticking problems of the SiO$_2$ at 950°C and associated local variations of the In profile.

The coated strain-compensated samples show nearly the same diffusion coefficients and similar activation energies as the uncompensated ones (2.3 eV for sample A, 2.5 eV for sample C). The enhancement of diffusion by the cap layer masks the effect of strain compensation.

4. Conclusion

The insertion of GaAsP barriers with tensile strain, compensating the compressive strain in a GaInAs/GaAs QW, changes the interdiffusion behaviour during RTA. At lower temperature (850°C), strain compensation leads to a slightly slower diffusion. At higher temperature (950°C), the diffusion is slightly accelerated by the GaAsP layers, probably due to the fact that now P diffusion also becomes important. The activation energy for the diffusion process is 2.1 eV for InGaAs/GaAs and 3.4 eV for InGaAs/(GaAs)/GaAsP. Encapsulation with SiO$_2$ leads to a 10-fold increase of the diffusion coefficient. This accelerated diffusion is interpreted by the injection of Ga vacancies. These vacancies dominate the diffusion process and the effects of strain compensation.

Selective interdiffusion processes for monolithic integration of different optoelectronic devices can thus be used also for strain-compensated structures. Without encapsulation, these strain-compensated structures show a slightly higher stability against treatment at moderate temperatures (850°C).

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