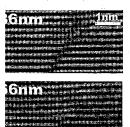
se models, Mg₃N₂ bricks are introduced in the



jected along $[10\overline{1}0]$ with experimental nm and defoci of 36, 56 and 66nm.



1nm



877

istallogr. 94, 340

jected along 1010 with experimental nm and defoci of 36, 56 and 66nm.

Unipress, Warsaw) for providing the bulk GaN contract HPRN-CT-1999-00040 (IPAM).

ory I, Weyher J L, Porowski S 1999 Proc. Xth) p 413 tin E, De Mierry P, Beaumont B, Damilano B, ⁷ I, Porowski S 1999 Phys. Rev. Lett. **83**, 2370 S, Perlin P, Robert J L, Contreras S, Wasik D, d. (b) 216, 567

Mierry P, Dalmasso S, Leroux M, Gibart M

tin E, De Mierry P, Beaumont B, Damilano B,

Indium distribution and influence of internal fields in InGaN quantum wells

F Rossi, N Armani, C Ferrari, V Grillo¹, L Lazzarini and A Passaseo²

CNR - IMEM Institute, Parco Area delle Scienze 37/A, 43010 Fontanini, Parma, Italy ¹ INFM-TASC, Basovizza SS 14, km 163.5, 34012 Trieste, Italy ² INFM National Nanotechnology Laboratory, via Arnesano, 73100 Lecce, Italy

ABSTRACT: A detailed structural and optical characterisation of InGaN/GaN multiple quantum wells with In content up to 6% is presented. High resolution X-ray diffraction was employed to determine with a good accuracy the In content in the wells. Transmission electron microscopy did not show significant In fluctuations in the wells, in agreement with X-ray diffraction results. SEM-cathodoluminescence spectroscopy measurements taken at different injection powers allowed us to obtain the screening of the internal fields, nearly restoring the flat band condition. The emission energy in the high injection limit confirmed the quantum confinement in the wells.

1. INTRODUCTION

The In_xGa_{1-x}N alloy is a very promising material as the active layer of light emitting diodes and laser devices due to the possibility of tuning the emission over a large wavelength range. In comparison with other III-V compounds the presence of a large spontaneous and strain induced polarisation generates strong electric fields in the wells (Ramakrisnan et al 2000). These fields are responsible of the quantum confined Stark effect (see for instance Chichibu et al. 1999), depending on the well thickness and In content, leading to a large red shift of the transition energies with respect to the energy gap of the material.

Moreover, due to the large difference in energy gap between GaN (3.501 eV at 77K) and InN (0.74 eV) and to the large and negative bowing of the energy gap vs composition curve in InGaN alloy (McCluskey et al 1998 and Davydov et al 2002), it has been suggested that a large contribution to the red shift can originate from local In composition fluctuations (Chichibu et al 1999).

This seems to be confirmed by spectroscopic and microscopic techniques in In rich InGaN wells (O'Donnell et al 1999). For instance by analysing the lattice displacements in high resolution TEM images of InGaN multi quantum wells (MQWs) with an average In composition of 17% Ruterana et al (2002) showed a local In content up to 45%.

In this work we present a detailed structural and optical characterisation of InGaN/GaN quantum wells by means of the complementary use of high resolution X-ray diffraction, TEM and cathodoluminescence techniques, in order to investigate the In composition homogeneity and its influence on the optical properties of this material system

2. EXPERIMENTAL

Four InGaN/GaN 5 period MQWs have been grown on (0001) oriented sapphire substrates using the MOCVD technique. The MQW thickness has been decreased from 7 to 1 nm with constant nominal 8% In content. The growth temperatures were 1100 °C and 740 °C for GaN and InGaN respectively.

Conventional diffraction contrast and high resolution TEM studies on cross sectional $(2\bar{1}10)$ and $(01\bar{1}0)$ samples have been carried out on a 2000 FX JEOL microscope working at 200 keV.

Spectrally resolved CL investigations have been performed between 6 and 300 K using a Gatan MonoCL2 system installed on a Cambridge 360 Stereoscan SEM.

3. RESULTS AND DISCUSSION

The samples have been characterised by High Resolution X-ray Diffraction techniques on a Philips Expert-Pro diffractometer using the (0002) and (0006) reflections and $(11\overline{2}\,0)$ transmission geometry. The symmetrical $(11\overline{2}\,0)$ rocking curve did not show any lattice mismatch along the interface demonstrating the complete pseudomorphic growth of InGaN/GaN MQWs.

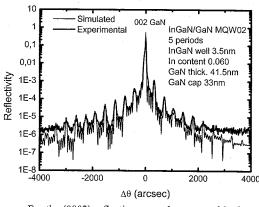


Fig. 1. Experimental and simulated HRXRD profile of (0002) reflection of sample MOW2.

For the (0002) reflection an analyser crystal in the ω -20 coupling of the scan axes was used to remove the peak broadening due to the crystal mosaicity. The measured curves were then simulated using a program based on the dynamical theory of X-ray diffraction and using well thickness as given by TEM. An example of such fitting is reported in Fig. 1.

In content was obtained assuming the Vegard's law for the InGaN alloy and taking the lattice parameters and the elastic constants given by Polyan et al (1996) and Wright (1997) for InN (see Table I).

Table I reports the results for all the samples investigated. The comparison between experimental and simulated diffraction curves demonstrated that:

- the negligible peak broadening in the experimental profile indicates a very good composition uniformity and stability along the MQW
- the broadening of the peaks observed using the ω -2 θ scan without analyser crystal is only due to the crystal mosaicity induced by dislocations .

| Sample | Period (nm) | Well thickness (nm) | Composition In _x Ga _{1-x} N | strain z | strain x | CL blue shift (meV) |
|--------|----------------|---------------------------|---|-----------------------|------------------------|---------------------------|
| MQW01 | 46.5 | 7.5 | $x = 0.060 \pm 0.002$ | | | 180 |
| MQW02 | 44.0 | 3.5 | $x = 0.060 \pm 0.004$ | 3.57×10^{-3} | -6.43x10 ⁻³ | 50 |
| MQW03 | 28.3 | 2 | $x = 0.060 \pm 0.005$ | | | 17 |
| MQW04 | 27.5 | 1÷1.5 | $x = 0.025 \pm 0.01$ | 1.41x10 ⁻³ | -2.53x10 ⁻³ | 0 |

Table I: summary of the structural and optical characterisation results

TEM observations in the (2110) crogood planarity of the interfaces and a unifo

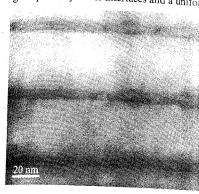


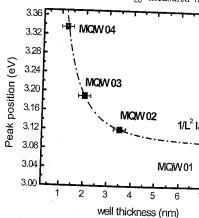
Fig. 2. Bright field (2110) projection TEM image of MQW01; g=(0002).

The well interfaces appear darker due shown in the (0110) projection. Finally, performed to investigate the presence of In content fluctuations in the nm range.

The influence of the spontaneous a evaluated by acquiring CL spectra at different the beam current by two orders of magnitude clearly observed, due to the screening mechan A typical curve showing the saturation trendshown in Fig. 3 for the MQW3 sample.

New software based on random walk N this conference) allowed us to calculate, for ear in the same screening of the field. The depi discriminated the role of each well and confirming a good in-depth homogeneity of In

The QW emission energy measured in



studies on cross sectional (2110) and ppe working at 200 keV. I between 6 and 300 K using a Gatan

on X-ray Diffraction techniques on a reflections and (1120) transmission how any lattice mismatch along the InGaN/GaN MQWs.

ig. 1. Experimental and simulated RXRD profile of (0002) reflection f sample MOW2.

) coupling of the scan axes was used to measured curves were then simulated ction and using well thickness as given

the InGaN alloy and taking the lattice 1996) and Wright (1997) for InN (see

vestigated. The comparison between

ile indicates a very good composition

1 without analyser crystal is only due to

| strain z | strain x | CL blue shift (meV) |
|-----------------------|------------------------|---------------------------|
| | -6.43x10 ⁻³ | 180 |
| 3.57×10^{-3} | | 50 |
| | | 17 |
| 1.41x10 ⁻³ | -2.53x10 ⁻³ | 0 |

l characterisation results

TEM observations in the $(2\bar{1}\bar{1}0)$ cross sectional projection using the (0002) reflection showed a good planarity of the interfaces and a uniform diffraction contrast in the wells (Fig. 2).

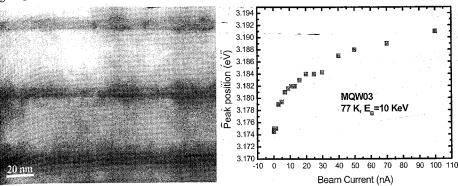


Fig. 2. Bright field (2110) projection TEM image of MQW01; **g**=(0002).

Fig. 3. Cathodoluminescence blue shift of the MQW3 sample as a function of the injected current.

The well interfaces appear darker due to the superimposed strain contribution that can be better shown in the (0110) projection. Finally, preliminary EELS and Z-contrast analyses have been performed to investigate the presence of In rich regions. These studies did not show significant In content fluctuations in the nm range.

The influence of the spontaneous and piezoelectric fields on the optical properties was evaluated by acquiring CL spectra at different temperatures and injection power densities. Increasing the beam current by two orders of magnitude up to 100 nA, a blue shift of the transition energy was clearly observed, due to the screening mechanism by the generated carriers (see the values in Table I). A typical curve showing the saturation trend when the flat band condition was nearly recovered is shown in Fig. 3 for the MQW3 sample.

New software based on random walk Montecarlo simulations on continuous space (Grillo et al, this conference) allowed us to calculate, for each penetration depth, the excitation conditions resulting in the same screening of the field. The depth resolved CL analyses performed using these values discriminated the role of each well and showed a substantially unchanged transition energy, confirming a good in-depth homogeneity of In composition.

The QW emission energy measured in the limit of nearly flat band conditions is plotted in

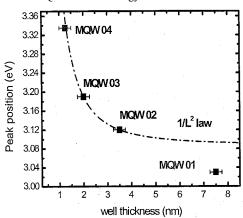


Fig. 4. Experimental dependence of the cathodoluminescence peak position as a function of the well thickness in the four quantum wells. The 1/L² law is reported.

Inst. Phys. Conf. Ser. No 180 Paper presented at Microsc. Semicond. Mater. Co ©2003 IOP Publishing Ltd

Fig. 4 as a function of the well width L.

The experimental data followed the L² dependence expected for emissions related to carriers confined in a QW, except for the thickest sample. This behaviour demonstrated the presence of the confinement in our InGaN samples, for QW thickness lower than 4 nm. The curve cannot fit the emission energy of the 7.5 nm thick QW, in agreement with Bernardini and Fiorentini (2000), who rule out the possibility of achieving a complete field screening in wells with thicknesses well beyond the effective screening length of 2 nm. Their uncompensated red shift in GaN wells of 7 nm is comparable with our experimental result.

From the QW related transition energy in the high injection limit we could estimate a value of the bowing parameter at least higher than 3.0 in these InGaN wells with x (In) <7%.

4. CONCLUSIONS

By the complementary use of structural and optical characterisation techniques a very accurate study of InGaN/GaN MQWs was performed. The recombination energies of the QWs were obtained by the CL technique at high injection levels under almost completely screened built-in electric fields. The results are consistent with the L^{-2} dependence, except for wells larger than a few nm, as expected from the theory. Thus the data obtained for the present set of low In concentration samples demonstrate a uniform In distribution in the wells. This is also consistent with the TEM results which did not show significant lateral and in-depth In fluctuations.

The marked difference of In content fluctuations with previous data concerning InGaN QWs with higher In content also suggests the role of strain as a driving force in the formation of In rich zones.

ACKNOWLEDGEMENTS

Thanks are due to Dr S Frabboni from University of Modena and Dr R Balboni from IMM-CNR for EELS and Z-contrast studies. Thanks are also due to Prof M Albrecht for useful discussions.

REFERENCES

Bernardini F and Fiorentini V 2000 Appl. Surf. Sci. 166, 23

Chichibu S F, Sota T, Wada K, DenBaars S P and Nakamura S 1999 MRS J. Nitride Semicond. Res. 4S1, G27

Davydov V, Klochikhin A A, Emtsev V V, Kurdyukov D A, Ivanov S V, Vekshin A V, Bechstedt F, Furthmuller J, Aderhold J, Graul J, Mudryi A V, Harima H, Hashimoto A, Yamamoto A and Haller E 2002 Phys. Stat. Sol. (b) 234, 787

Fiorentini V, Bernardini F, Della Sala F, Di Carlo A and Lugli P 1999 Phys. Rev. B60, 8849

Grillo V, Armani N, Rossi F, Salviati G and Yamamoto N this conference

McCluskey M D, Van de Walle C G, Master C P, Romano R T and Jonson N M 1998 Appl. Phys. Lett. **72**, 2725

O'Donnel K P, Martin R W, Middleton P G, Bayliss S C, Fletcher I, Van Der Stricht W, Deemester P and Moerman I 1999, Mat. Sci. and Engineering B59, 288

Polyan A, Grimmsditch M and Grzegory I 1996 J. Appl. Phys. 79, 3343

Ramakrishnan A, Wagner J, Kunzer M, Obloh H, Kohler K and Johs B (2000) Appl. Phys. Lett. 76, 79

Ruterana P, Kret S and Poisoon M A 2002 Mat. Sci. and Engineering B93, 185 Wright A F 1997 J. Appl. Phys. 82, 2833

Electrostatic fields in InGa variation with indium co energy filtered TEM

J S Barnard, M J Kappers, E J Thru

Department of Materials Science and Cambridge CB2 3QZ

¹ Thomas Swan Scientific Equipment Ltd,

ABSTRACT: The III-V nitride system of their class. Using a combination (EFTEM) and high-resolution imagi concentration and width of a set of growth temperatures. We have thus make the content and compared this to those theoretically calculated values of the primary of the primary of the primary content.

1. INTRODUCTION

The III-nitrides are the subject of m properties, even with threading dislocat luminescence mechanism of the strained I controversy because of the role of the electhave the highest piezoelectric constants in have much in common with the II-VI oxid degree of lattice mismatch between InN (10⁸ Vm⁻¹) exist and offset the conduction wolt.

Much effort has been spent in measur optical techniques, such as the temperate dependent PL and Franz-Keldysh oscillation measured the electric field strength using an potential difference and the width of the QW

2. THEORY

The theory of off-axis electron hologr is important to note that the phase shift of at V(r), can be written as:

 $\Delta \phi(\mathbf{R}) = \mathbf{C}$

where R is the in-plane coordinate of the spectral extension of the field both inside and outs