

Structural properties, In distribution and photoluminescence of multiple InGaN/GaN quantum well structures

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A detailed electron microscopy and X-ray diffractometry (XRD) study of the structural properties of InGaN/GaN multiple quantum wells (MQWs) is presented. The influence of the growth temperature T_g for the GaN layers inside the MQW structure is investigated. The structural properties, in particular the measured In concentrations x_{In} and InGaN layer thicknesses, are correlated with photoluminescence spectra (PL) to contribute to the understanding of the key factors for the light emission which are essential for the fabrication of laser diodes in the blue/green spectral range.

The MQW structures were grown on $Al_2O_3(0001)$ by low-pressure metalorganic chemical vapor deposition (MOCVD) in an AIXTRON 2000G3 reactor with trimethylindium, trimethylgallium and NH_3 as precursors. A 2 μm GaN buffer layer was deposited at 1180 °C with H_2 as carrier gas at a total reactor pressure of 200 mbar. The InGaN/GaN MQW structures consist of 10 periods of InGaN with a nominal thickness $t_n = 10$ nm and GaN with $t_n = 15$ nm. The InGaN growth was always performed with N_2 carrier gas at 750 °C. The GaN was deposited at 950 (sample denotation according to the growth temperature s950), 850 (sample s850) or 750 °C (sample s750). H_2 carrier gas was used during the GaN growth for s950 and s850 while N_2 was supplied for s750.

The transmission electron microscopy (TEM) was carried out with a Philips CM200 FEG/ST electron microscope. Scanning electron microscopy (SEM) images were obtained in a field emission gun LEO 1530. The measurement of the local In concentration is based on the proportionality of the lattice parameter and the composition (Vegard's law). The details of the measurement of local lattice parameters in the InGaN by the evaluation program DALI (digital analysis of lattice images) are outlined in [1]. The PL was carried out at 6 K at an excitation wavelength of 315 nm with an excitation power of 42 mW/cm². The XRD analyses were performed according to [2].

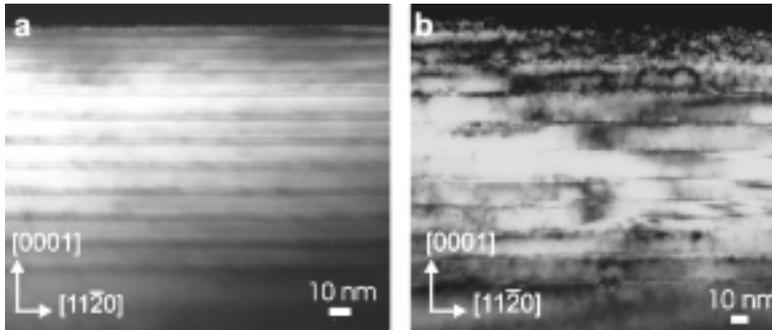


Fig.1: Cross-section TEM images taken under dark-field conditions with the $\vec{g} = (0004)$ imaging vector for (a) s950 and (b) s850.

Fig.1 shows overview cross-section TEM images of the MQW region of s950 (Fig.1(a)) and s850 (Fig.1(b)). Flat layers with a homogeneous thickness of (4.8 ± 0.8) nm (XRD: 3.9 nm) and a low defect density are observed for s950. The decrease of the GaN growth temperature for s850 induces a reduction of the structural quality. The average InGaN thickness rises to (6.8 ± 1.3) nm. The individual layer thicknesses increase from 5.3 nm for the bottom InGaN QW to 7.7 nm

for the top layer. In addition, the defect density (stacking faults and dislocations) in the MQW increases. Pinholes with the shape of an inverted hexagonal pyramid with diameters around 1 μm at the surface (similar to those shown in Fig.2 for s750) were occasionally found in s850. The properties observed by TEM agree reasonably with the results of the XRD analyses [2] demonstrating the homogeneity of the structures over macroscopic regions.

The structural quality is further degraded under the growth conditions of s750 which is visualized by the SEM image of the sample surface (Fig.2) showing a high density of pinholes which contain in some cases a filling (indicated by arrows in Fig.2). Energy

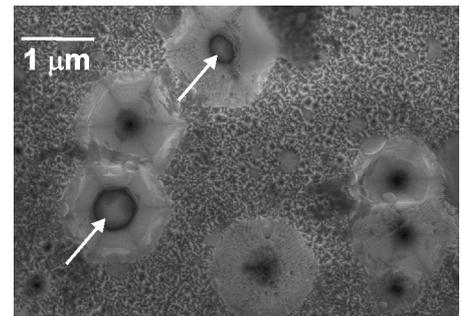


Fig.2: SEM image of the surface of s750.

dispersive X-ray microanalyses of the filling revealed an excess of indium compared to the surrounding region. Nanowires consisting of pure In were detected by XRD which could extend from the tip of the pyramids deeper into the structure. The results of the structure analyses show, that the decrease of the GaN growth temperature leads to a degradation of the MQW morphology.

The DALI evaluation of HRTEM lattice fringe images yields the local In distribution. A representative example is shown in Fig.3 for s950. The black regions correspond to the GaN and increasing brightness of the gray shades to an rising x_{In} . An inhomogeneous In distribution is observed which is typical for s950 and also for s850. The

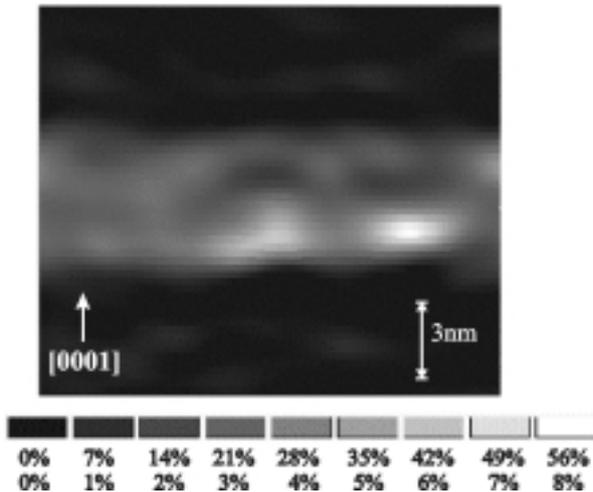


Fig.3: grayscale-coded maps of the local In concentration in the 9th InGaN quantum well of s950. The errors for the determined In concentrations are given by the numbers in the 2nd line.

PL spectra of s950 and s850 are presented in Fig.4. The spectrum of s750 is omitted due to its low PL intensity. A strong shift of the PL peak from 2.8 eV to 2.4 eV and a decrease of the PL intensity for s850 is observed. The bandgap energy E_g of bulk InGaN was calculated for the measured \bar{x}_{In} according to [5] to be 2.87 eV for s850 and 2.81 eV for s950. The PL peak energy of s950 corresponds to E_g while a strong red shift with respect to E_g is observed for s850 although the average In concentrations do not significantly differ. Since the properties of the small In agglomerations in the two samples are also similar, the localization of charge carriers does not appear to dominate the PL. The observed shift can be assigned to the quantum confined Stark effect induced by the piezoelectric fields [6]. Taking into account the measured \bar{x}_{In} and the increase of the InGaN layer thickness for s850 compared to s950, a large red shift of the PL peak energy appears to be plausible according to [7].

InGaN wells in both samples contain domains with a size of only a few nanometers with high x_{In} up to 60 % (white regions in Fig.3). The size and In concentrations of the In agglomerations did not significantly differ in s950 and s850. The composition inhomogeneity is most likely induced by phase separation due the large miscibility gap of the InGaN system [3]. An alternative origin of the small scale In agglomerations could be random alloy fluctuations which were theoretically predicted for cubic InGaN [4]. The local x_{In} can be averaged yielding 24 % in the InGaN QW depicted in Fig.3. However, areas with a significantly lower average In concentration were also found leading to an overall average In concentration \bar{x}_{In} of 16.7 ± 5 % (XRD: 12.5 ± 2.7 %) for s950 and 14.7 ± 5 % for s850 taking into account at least 30 different regions per sample in three different InGaN quantum wells. The given errors contain the standard deviations of the average In concentrations for the evaluated areas and reflect the compositional inhomogeneity on the size scale of the evaluated regions (20 nm).

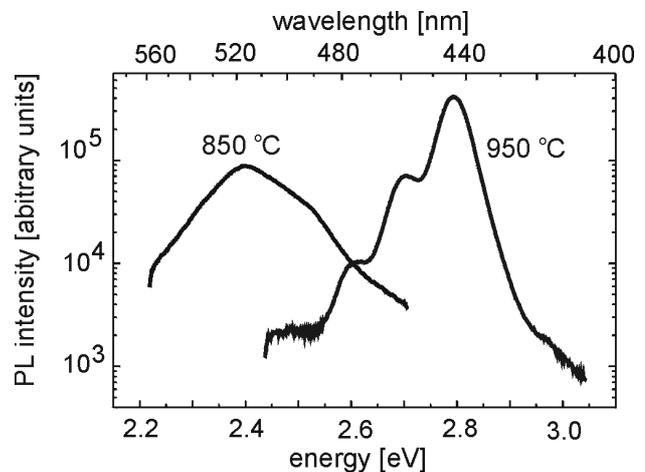


Fig.4. PL spectra of samples s950 and s850

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