Microstructure of defects in InGaN/GaN quantum well heterostructures

S-L Sahonta, Ph Komninou*, G P Dimitrakopoulos, Th Kehagias, J Kioseoglou, Th Karakostas, C Salcianu1 and E J Thrush1

Physics Department, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece
1Thomas Swan Scientific Equipment Limited, Buckingway Business Park, Swavesey, Cambridge, CB4 5FQ, UK
*E-mail: komnhnoy@auth.gr

Abstract. Defects in the active layers of MOCVD-grown InGaN/GaN blue-emitting multiple quantum well LED heterostructures on (111) silicon substrates are examined by conventional and high resolution transmission electron microscopy (HRTEM). The quantum wells contain small gaps, interfacial steps, sphalerite stacking and well thickness variations. No characteristic phase separation of the InGaN into In-rich clusters is observed within the wells. Despite the defective active layers and the absence of In clusters, the internal quantum efficiency of the device quantum wells is 23%, hence mechanisms by which carriers are localised in the quantum wells via the defects are considered. The roles of well gaps, thickness variations, stacking faults and sphalerite grains in exciton confinement are discussed.

1. Introduction
The brightest and most efficient III-nitride optoelectronic devices are those based on InGaN/GaN quantum well (QW) heterostructures [1], however the exact mechanism by which electron-hole pairs in InGaN recombine radiatively in spite of high threading dislocation densities is under debate. It is thought that excitons in InGaN QWs are isolated in local potential minima created by naturally-occurring In-rich regions within the QW, which act like quantum dots, isolating carriers from non-radiative traps such as threading dislocations that occur in large quantities throughout nitride films [2]. These quantum dot-like clusters within InGaN QWs have been characterized in many TEM studies [3], however it has been recently shown that phase separation in InGaN is enhanced considerably by TEM electron beam damage [4]. In addition, elemental studies involving non-damaging specimen preparation have shown that InGaN may in fact occur as a random alloy in QWs [5]. If phase separation does not occur in InGaN QWs, other mechanisms of carrier confinement must be considered. Narayan et al. reported that local QW thickness variations have a large effect on exciton confinement in wider regions of the QW [6]. Also, discontinuous QWs can present a mechanism for the isolation of carriers from threading dislocations, in that they resemble quantum box structures [7]. It is proposed that these features in combination are sufficient to prevent migration of carriers, resulting in the high emission efficiencies that we observe in InGaN devices.
This paper reports the presence of a variety of extended defects in working InGaN/GaN QW devices grown on silicon (111). No evidence of large-scale In segregation is observed in these QWs, thus it is proposed that the localisation of excitons in InGaN QWs is enhanced by the defective nature of the well, and not by InGaN phase separation.

2. Experimental
Blue light-emitting diode (LED) heterostructures consisting of five InGaN quantum wells of nominal 20% In alloy content were grown by MOCVD on silicon (111) substrates, using a combination of buffer layers and AlN/GaN superlattices in order to reduce the threading dislocation density arriving at the quantum well region. The dimensions of the QWs and barriers were chosen to minimize the characteristic red shift often observed in InGaN devices owing to the quantum-confined Stark effect, caused by large strain-induced internal electromagnetic fields in wurtzite GaN. Very thin wells, with a nominal thickness of 2 nm, were chosen to strongly confine the electron and hole wavefunctions within the well. Thick GaN barrier layers (of 18 nm nominal thickness) were deposited in between the wells to ensure that the carrier wavefunctions of adjacent QWs did not overlap. Finally, the high In alloy content of 20% was chosen to increase the depth of the potential barrier, in order to minimise thermionic migration of excitons out of the QW. Room temperature photoluminescence showed peak emission at 450 nm, with internal quantum efficiency (IQE) of approximately 23% (Figure 1). This value is relatively high for nitride-based devices grown on silicon (111) [8].

TEM specimens were prepared using tripod polishing and Ar+ ion milling. Specimens were studied using a JEOL 2011 TEM, with 0.19 nm point resolution and Cs = 0.5 mm, operating at 200 kV.

3. Results

The dislocation density measured at the device active layers, by the invisibility criterion when imaging in two-beam conditions using the g = 0002 and g = 11-20 reflections, is $5.5 \times 10^8 \text{ cm}^{-2}$. The QWs showed uneven interfaces and defective internal structure when viewed by conventional TEM methods (Figure 2). HRTEM imaging along the [11-20] zone axis revealed gaps in the QW, ranging from 5 nm to 50 nm in length. These gaps isolate regions of film of approximately these same dimensions, shown in Figure 3. Bragg filtering of the 0002 reflections, to display only basal lattice fringes, reveals extra half planes which terminate to indicate the positions of partial dislocations at the onset of the gaps in the QW (Figure 3). The separated regions of QW appear to be predominantly sphalerite in their structure, shown by characteristic stacking fault contrast (Figure 4a), analogous to a single InGaN...
zinc blende unit within the wurtzite matrix of the GaN barrier layers. Characterisation by the geometric phase analysis (GPA), placing a Gaussian mask of diameter g/4 over the 1-100 spot in the HRTEM diffractogram (inset Figure 4a), shows a region of high compression in the strain map (Figure 4b) corresponding to the position of the QW. A discontinuity is observed in the image phase profile on traversing the QW (inset Figure 4b). This phase shift is of 2/3π, corresponding to a displacement of the lattice by 1/3<1-100>, consistent with the I₁ type intrinsic basal plane stacking fault in GaN.

4. Discussion

It has been shown that the IQE of an InGaN QW LED grown on Si (111) substrate is not hindered by regions of sphalerite stacking, nor by gaps permeating the active layer. It is expected that these defects in fact encourage the localisation of carriers within the well, preventing them from being trapped by threading dislocations. The regions of sphalerite stacking in the InGaN are not detrimental to the device efficiency, due to the fact that stacking faults are not known to induce deep electronic states in the band gap, however it has been suggested that they temporarily pin excitons, encouraging radiative recombination at a slightly red-shifted energy, thus broadening the peak emission of the device [9]. The small monolayer variations in the QW thickness due to extra basal atomic half planes also may contribute to carrier confinement by relegating carriers to the wider regions of the quantum well, where they may recombine radiatively instead of drifting to defects [6]. The most dramatic effect on the carrier localisation however may relate to the gaps in the well. These gaps isolate strained regions of InGaN of approximately three monolayers’ thickness, which can be envisaged as quantum boxes, in which carrier wavefunctions are physically separated from threading dislocations in the surrounding heterostructure. It is expected that these quantum boxes have the greatest effect on the prevention of non-radiative recombination in this device, however the high measured IQE value is likely to be due to a combination of all of these mechanisms.

An interesting observation is the absence of contrast relating to In-rich regions within the QWs, which have been reported in TEM studies by other groups. Images were taken using only low dosage electron beam exposure for 30 seconds, following recent reports suggesting that the electron beam
induces phase separation in InGaN, which on analysis appears as false quantum dot-like clusters [4]. Although this study does not rule out the presence of small-scale fluctuations in In concentration within the QWs that are undetectable by mass-thickness contrast in HRTEM, no characteristic contrast attributable to In-rich clusters within the well were observed. Additionally, GPA analysis showed no contrast fluctuations corresponding to lattice distortions within the well, which are usually characteristic of In clustering in TEM specimens. It is therefore proposed that the formation of In-rich clusters is not a necessary requirement for carrier localization in InGaN, but that extended defects in combination of the type seen here are essential.

Figure 4. (a) HRTEM image of a QW with atomic contrast characteristic of $I_1$ stacking faults. (b) GPA basal plane strain map formed by masking the 1-100 spot (inset (a)) of the diffractogram of image 4a. The phase profile of the boxed region in image 4a shows a discontinuity of $2/3\pi$ (inset (b)), corresponding to a basal lattice shift of $1/3<1-100>$, consistent with the $I_1$ basal plane stacking fault.

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References
[1] R W Martin, P R Edwards, R Pecharroman-Gallego, C Liu, C J Deatcher, I M Watson, K P O'Donnell., J. Phys. D: Appl. Phys. 35 604–608 (2002)
[2] S Nakamura, Science 281 956-961 (1998)
[3] F A Ponce, S Srinivasan, A Bell, L Geng, R Liu, M Stevens, J Cai, H Omiya, H Marui, S Tanaka, Phys. Stat. Sol. (b), 240 2 273-284 (2003)
[4] T M Smeeton, C J Humphreys, J S Barnard, M J Kappers, J. Mat. Sci. 41 9 2729-2737 (2006)
[5] M J Galtrey, R A Oliver, M J Kappers, C J Humphreys, D J Stokes, P H Clifton, A Cerezo, Appl. Phys. Lett. 90 6 61903-61903 (2007)
[6] J Narayan, H Wang, J Ye, S-J Hon, K Fox, J C Chen, H K Cho, J C C Fan, Appl. Phys. Lett. 81 5 841-843 (2002)
[7] P Lefebvre, A Morel, M Gallart, T Taliercio, B Gil, J Allègre, H Mathieu, N Grandjean, B Damilano, J Massies, Mat. Res. Soc. Symp. Proc. Vol. 639 G10.1.1-G10.1.12 (2001)
[8] Y P Hsu, S J Chang, W S Chen, J K Sheu, J Y Chu, C T Kuoc. J. Electrochem. Soc. 154 3 H191-H193 (2007)
[9] C Stampfpl and C G Van de Walle, Phys. Rev. B, 57 24 R15 052-R15 055 (1998)