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Microstructure and formation mechanism of V-defects in the InGaN/GaN multiple quantum wells with a high in content

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InGaN/GaN heterostructures and multi-quantum well (MQW) structures have a wide range of applications such as the active layers in GaN-based light-emitting diodes [1] as it is possible to tune the optical band gap from visible to ultraviolet spectral range by controlling the In composition [2]. However, the initial GaN layer is usually grown on a sapphire substrate, and the high lattice mismatch between substrate and epilayer leads to highly defective material with high densities of threading dislocations (TD). These defects affect the structural and optical quality of the active layer composed of the InGaN/GaN MQW structure [3]. The so-called V-defects have been frequently observed in the InGaN/GaN MQW [4–6]. The origin of these defects and the role they play on the optical emission are still not clear though there are some studies focused on this issue [3, 4, 7].

All layers of this sample were grown on a c-sapphire (0001) substrate by using metal-organic chemical vapor deposition (MOVCD). Trimethylgallium (TMGa), trimethylindium (TMIn), and ammonia (NH_3) were used as the source precursors for Ga, In, and N, respectively. After thermal cleaning of the substrates in hydrogen ambient for 10 min at 1100 °C, a 25 nm thick GaN nucleation layer was deposited at 550 °C. Subsequently, an undoped GaN (u-GaN) layer and a n-type doped GaN (n-GaN) layer were grown on the low temperature GaN/sapphire at 1050 °C for 2 h with a V/III flux ratio of 1500. The InGaN/GaN MQW is composed of fifteen periods of 3 nm $In_{0.20}Ga_{0.80}N$ nominal composition wells and 13 nm GaN barriers. Finally, a GaN capping layer was deposited on the MQW.

The TEM diagram in Fig. 1 shows that the V defect begins at a TD, which runs through MQW from the high temperature GaN layer to the capping layer. During the MWQ deposition, the InGaN and GaN sidewall layers were epitaxially grown successively on the six $\{10\bar{1}1\}$ planes (marked with "s-QW"). The InGaN and GaN sidewall layers forming by the layer-by-layer growth similar to that on the (0001) planes (marked with "c-QW"). Because the thin InGaN layer is separated from the thin GaN layer, having almost the same composition with the main $In_{0.20}Ga_{0.80}N$ MQW, they might also work as another MQW, emitting undesirable long-wavelength weak extra lights. Therefore, the entire MQW has the (0001) surface and the $\{10\bar{1}1\}$ surfaces during the MQW deposition. The angle of connecting the $(10\bar{1}1)$ interface (or the $(\bar{1}011)$ interface) with the (0001) interface are not sharp (about an angle of 118°), but this corner is curved, as seen in Fig. 1.

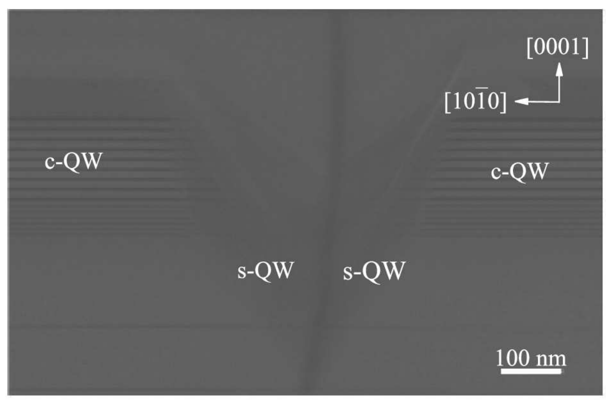

Fig. 1. Dark-field HRTEM images of V-defects in the InGaN/InGaN MQW

The InGaN and GaN crystals were formed by the layer-by-layer growth on the (0001) and $\{10\bar{1}1\}$ surfaces, where each monolayer on these surfaces would extend from the distant nucleation site toward the edge through the supply of atoms that adhere and migrate on the surface. With the growth of monolayers, the supply of atoms on both the (0001) and $\{10\bar{1}1\}$ surfaces may be

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gradually insufficient, especially in InGaN with growth rate less than GaN. Then, the monolayers on the (0001) and $\{10\bar{1}1\}$ surfaces stop growing before they meet with each other. This might be due to the low growth rate at the low temperature of 800 °C. Due to the continuous growth of these monolayers, at the corner a surface with step-wise lattices was formed.

Figure 2 shows the plot of the PL spectra for the InGaN/GaN MQW measured at room temperature.

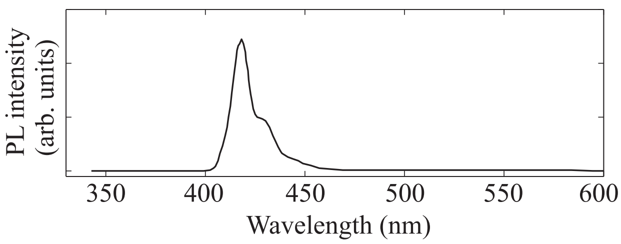

Fig. 2. Photoluminescence (PL) spectra of InGaN/GaN MQW

The emission peak is not symmetrical and there is a slight hump at the longer wavelength side. This broad dominant emission is observed in the region of 428 to 442 nm. This would be due to the inhomogeneous distribution of indium across the QWs or existence of localized states related transitions. Hence, the common-featured PL bands, peaking at 419 nm, is attributed to the excitons confined in the c-QW. In addition, the growth rate at the side $\{10\bar{1}1\}$ surfaces of the V-defects is indeed lower, than at the (0001) surface. Therefore, during the adatom diffusion, the growth rate and In-concentration increase at the lower (0001) surface of the overturned pyramid due to the well-known effect of the growth acceleration in the vicinity of reentrant angles. Therefore, the enhanced quantum confinement would increase the energy bandgap. Besides, owing to the decreased piezoelectric field in such tilted MQW, the reduced quantum confined Stark effect would also cause a much smaller bandgap [8]. Thus, the broad dominant emission bands of 428 to 442 nm are attributed to the MQWs grown on the $\{10\bar{1}1\}$ faceted sidewalls of the V-defects because of the above combined effects.

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