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Microstructural characterization of V-defects in InGaN/GaN multiquantum wells

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GaN-based materials have wide bandgap and good thermal stability, which are widely used in photoelectric and microelectronic devices, such as light-emitting diodes, laser diodes, detectors, high electron mobility transistors, etc [1, 2]. But, owing to the lattice mismatch and thermal mismatch between GaN and substrate in heteroepitaxy, there are high density defects in GaN materials, such as V-defect, dislocation, point defect and so on. In the InGaN multi-quantum well (MQW) structure, the so-called V-defects are often observed [3, 4]. These defects have a hexagonal inverted pyramidal appearance with $\{10\bar{1}0\}$ walls, and they are limited by a hexagon in the basal plane [4]. The V-defects often nucleate on threading dislocations (TDs), and crossed with the MQW just above the underlying layer. Several suggestions, such as strain release, low surface mobility of the adatoms on the InGaN layer and/or reduced Ga incorporation on the $\{10\bar{1}1\}$ planes in comparison to the $\{1000\}$ surface, have been proposed to explain the generation of this V-defect [5, 6]. The model established by Northrup and Neugebauer [7] using the first principle calculation shows that indium is a kind of differential surfactant. The indium reduces surface energy of $\{10\bar{1}1\}$ relative to $\{1000\}$, which promotes the V-shaped defect with $\{10\bar{1}1\}$ opening from the threading dislocation.

All layers of the samples were grown on a c-sapphire (0001) substrate by MOVCD. During the MOCVD growth, trimethylgallium, trimethylindium and ammonia were used as precursors of gallium, indium and nitrogen. Biscyclopentadienyl magnesium and disilane were used as p- and n-type dopant sources, respectively. After thermal cleaning of the substrates in hydrogen environment at 1100 °C for 10 min, 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 at 1150 °C for 2 h with a V/III flux ratio of 1500. Then, thirteen pairs of InGaN (2.7 nm)/GaN (11.5 nm) MQW were grown at 860 °C. The MQW were capped with 900 Å of $Al_{0.06}Ga_{0.94}N$. Cross-section-view transmission electron microscopy (TEM) samples were prepared by wedge polishing followed by Ar^+ ion milling. TEM measurements were carried out by a Philips CM200 high-resolution transmission electron microscope at an operating voltage of 200 kV.

Low magnification dark field TEM (Fig. 1) showed a number of threading dislocations in the MQW. On the left side of the image we can see a threading dislocation reaching the MQW, and it does not go out from the top of the defect, instead of stopping at the quantum well. Nevertheless, on the right side of the image, a threading dislocation enters the GaN overlay from the last quantum well. In the micrograph a mixed-type threading dislocation (labeled with M) and a pure-edge TD (labeled with E) can be seen. The mixed-type threading dislocation was decomposed into an a-type and a c-type dislocation. The a-type component dislocation bends to an

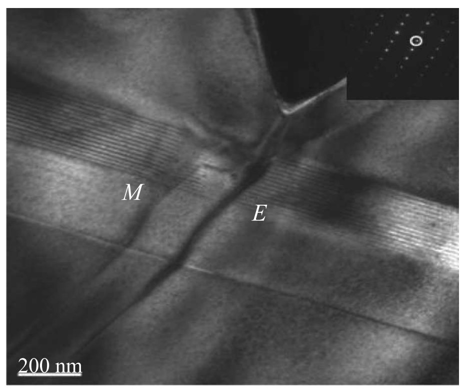

Fig. 1. Cross-section dark field TEM images of the InGaN/GaN MQW. The diffraction spot was marked in upper right corner

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interface direction contributing to a misfit dislocation in the InGaN/GaN interface, afterwards from an interface to another threading dislocation. Due to the $g \cdot b = 0$ invisibility criterion, the c-type component dislocation is not seen, because this decomposition reaction is an energetically neutral reaction [8]. This dislocation has a Burgers vector $b = 1/3\langle 11\bar{2}0\rangle$ in the $\{0001\}$ sliding surface, which alleviates the mismatch in this region. Due to the poor compatibility between GaN and InN, In-rich clusters have been found in InGaN quantum wells, which are caused by the fluctuation of indium composition [9]. The fluctuation of the In components in the quantum well may cause the decomposition reaction of the threading dislocation, which results in the mismatch strain-induced dislocation. The threading dislocations associated with this defect have different characteristics. When the dislocations have c-component, the possibility of nucleation increases.

In Figure 2, the 13-pair MQW cross-sectional TEM micrograph shows that the V-defects include some distinct stripes, and these stripes are parallel to the side-walls $\{10\bar{1}1\}$ and $\{\bar{1}011\}$. The V-defect clearly connects to threading dislocations (TDs). The stripes parallel to the sidewalls $\{10\bar{1}1\}$ and $\{\bar{1}011\}$ of the V-defects accord with the models of X. H. Wu and K. Watanabe. In Figure 2, there is no obvious concomitant TDs stopping at the apex of V-defects. From TEM, the angle between the two $\{10\bar{1}1\}$ facets is approximately 55.6°, which is basically consistent with the theoretical value of 56.1°. Although strain (mainly related to TD) may play a central role in the nucleation of V-defects, the strain (and comparable strain energy) in InGaN MWQ on the pyramid planes should be the same as that on the (0001) plane (the mismatch of GaN and InN in a- and c-directions is about 12 %). Therefore, strain relief should not be the reason for the growth of V-defects. On the contrary, the decrease of GaN incorporation (and growth rate) in the pyramid plane compared with the (0001) plane is the main reason for the growth of V-defects. The direction of the inclined plane terminating quantum well is determined by the relative growth rate of the material in the V-defect compared to the growth in the adjacent (0001) plane. In the normal growth of InGaN/GaN MQW, the growth temperature of GaN barrier is about 290 °C lower than that of high temperature GaN to restrain the re-evaporation of In. Under the condition of nominally used for MQW growth, the more refractory component (GaN in this case) has limited surface diffusion, so the defect morphology is controlled by dynamics. At high temperature, when the surface diffusion rate is high, the V-defects are flattened rapidly by GaN.

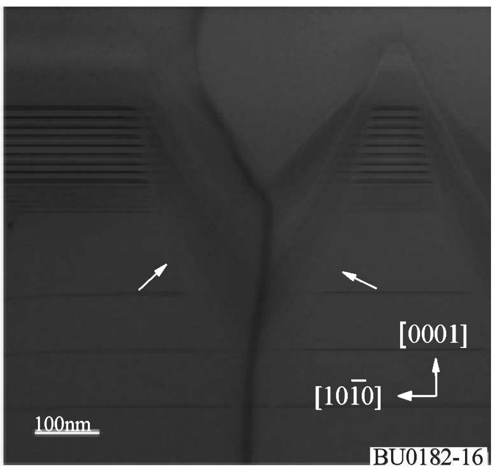

Fig. 2. TEM images of V-defects in the InGaN/InGaN MQW. The white arrowheads indicate the thin MQWs on the $(10\bar{1}1)$ and $(\bar{1}011)$

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