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Materials Chemistry and Physics 80 (2003) 397–400

MATERIALS CHEMISTRY AND PHYSICS

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Short communication

The growth mechanism of micron-size V defects on the hydride vapor phase epitaxy grown undoped GaN films

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Received 1 October 2002; received in revised form 26 December 2002; accepted 3 January 2003

Abstract

Micron-size V defects were found on the hydride vapor phase epitaxy grown GaN films. When the film thickness increased, the diameter of V defects increased, but the density of the defects decreased. The defect has six $\{1\,\bar{1}\,0\,1\}$ facets, which encircle to form a concave hexagonal pyramid. Its shape is similar to that of epitaxial lateral overgrowth (ELO) GaN crystal grown on a dot-patterned GaN underlying layer. Through the analysis of the growth mechanism of ELO GaN, the growth mechanism of the V defects was investigated.

Keywords: GaN; Hydride vapor phase epitaxy; V defect; Epitaxial lateral overgrowth; Growth mechanism

1. Introduction

Nitride alloys have attracted considerable attention for light emitting diodes (LEDs) and laser diodes (LDs) application, due to their ability to cover a wide spectral range and their high-temperature stability. Most of these alloys are grown on sapphire substrates by using metalorganic vapor phase epitaxy (MOVPE) [1], molecular beam epitaxy (MBE) [2], and hydride vapor phase epitaxy (HVPE) [3]. However, a GaN layer usually contains several defects such as stacking faults, inversion domain boundaries, and threading dislocations (TDs), because of a large lattice mismatch and a thermal expansion coefficient difference between GaN and sapphire substrates [4,5]. It has been reported that TDs disrupt the InGaN/GaN MQW and initiate the V defects [6–12]. The V defects, however, do not always initiate from TDs. For instance, in highly strained InGaN/GaN MQWs, V defects were formed not only at the TDs, but also at the stacking mismatch boundaries and inversion domain boundaries [10,11].

The sizes of V defects were usually less than 100 nm [6–12]. Due to the small sizes of V defects, most of the previous studies only focused on the initiation (nucleation) mechanism of V defects but not on the growth mechanism. In this study, through the characterization of micron-size V defects on the HVPE grown GaN films, the growth mechanism was investigated.

2. Experiment

The samples studied were undoped GaN films grown by HVPE on a *c*-plane double polished sapphire substrate. They were from American Crystal Technology. The growth conditions for these films have been published elsewhere [13]. Generally, the growth temperature was around 1050 °C, the gas pressure was 100 Torr and the V/III ratio was between 10 and 100. The thickness of these GaN films ranged from 5.58 to 22.9 μm. Their surface morphology and optical properties have been reported previously [14]. In this study, the detail of V defect morphology was characterized by optical microscopy (OM), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). To obtain an exact three-dimensional copy of the V defect for analysis, the shape of V defect was transferred to a replica by RepliSet (Struers Germany).

3. Results and discussion

The SEM image of the V defects is shown in Fig. 1(a). The defects have six facets, which encircle to form a concave hexagonal pyramid, as illustrated in Fig. 1(b) TEM analysis revealed that V defects were connected with TDs at their bottom like reported in other papers [6–11]. The sizes and the density of V defects were found to change with the film thickness. As the thickness increased from 5.58 to 22.9 μm, the diameter of V defects increased from

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doi:10.1016/S0254-0584(03)00109-3

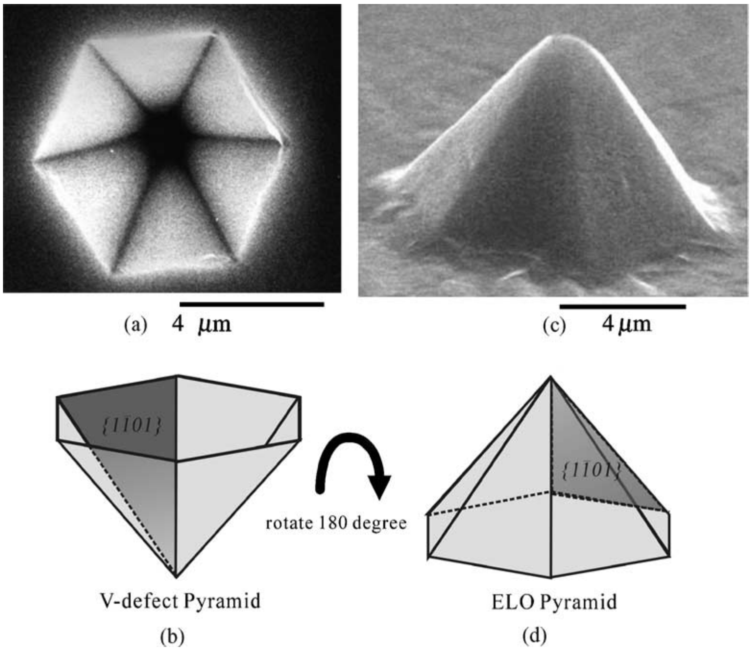

Fig. 1. (a) The SEM image of a V defect on the HVPE grown GaN film. The thickness of the film is 22.9 μm. The diameter of V defect is around 8 μm. (b) The schematic illustration of a V defect. It has six facets, which encircle to form a concave hexagonal pyramid. (c) The replica structure of V defect. Its shape is exactly the same as that of ELO GaN crystal grown on a dot-patterned GaN underlying layer, as shown in (d).

20 nm to 8 μm, while the density decreased from 2.5×10^9 to $5.7 \times 10^4\,\mathrm{cm}^{-2}$ [15].

Similar V defects have been reported by several research groups [6–12]. However, most of their V defects were obtained from the InGaN/GaN MQWs instead of undoped GaN films. The size of their V defects was less than 100 nm, which was too small to study the growth mechanism.

To examine the micron-size V defects in detail, the shapes of defects were transferred to a replica. As shown in Fig. 1(c), the replica structure has a simple three-dimensional facet structure, which is composed of a hexagonal pyramid covered with six facets. The shape of this pyramid is exactly the same as that of epitaxial lateral overgrowth (ELO) GaN crystal grown on a dot-patterned GaN underlying layer, as shown in Fig. 1(d) [16–20]. Therefore, analyzing ELO GaN films can contribute to the development of fundamental understanding of the growth mechanism of V defects.

The ELO technique based on the selective area growth (SAG) has recently been demonstrated to be effective in reducing the density of TDs in GaN. ELO consists of partially covering a conventional GaN layer with a mask and performing subsequent regrowth. Therefore, GaN is overgrown over the masked areas by using the GaN grown in the mask opening as a seed. Two kinds of patterns were usually used in ELO GaN: (1) dot pattern; (2) stripe pattern. Through the analysis of the growth mechanism of these ELO GaN films, the growth mechanism of the V defects is discussed in the following section.

When dot pattern was used, the shape of ELO GaN crystal was a pyramid structure bounded by six stable $\{1\,\bar{1}\,0\,1\}$ side facets [17–22]. It is important to note that the observed shapes of most crystallites are the results of surface energy anisotropy [23]. From this observation, it appears that the surface energies of the $\{1\,\bar{1}\,0\,1\}$ facets are lower than that of other planes, meaning $\{1\,\bar{1}\,0\,1\}$ facets have stable surfaces

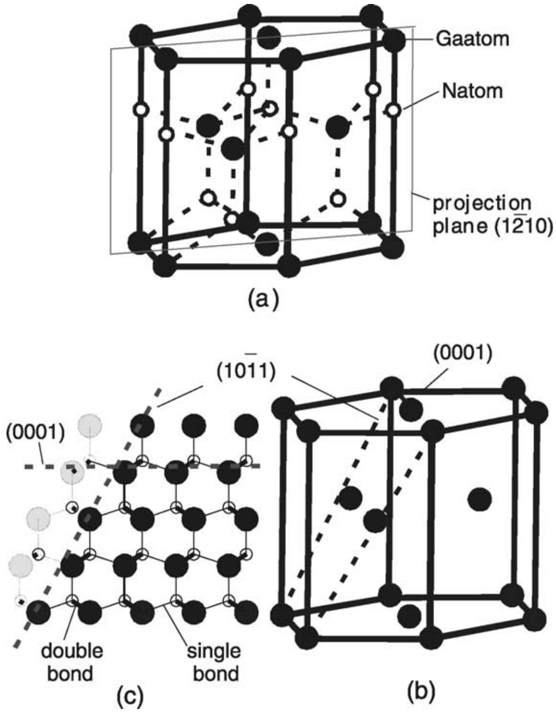

Fig. 2. (a) Atomic model of a GaN crystal. (b) The $(1\,\bar{1}\,0\,1)$ and $(0\,0\,0\,1)$ facets of V defect in a GaN crystal structure. (c) Atomic model of a GaN crystal in $[1\,\bar{2}\,1\,0]$ projection.

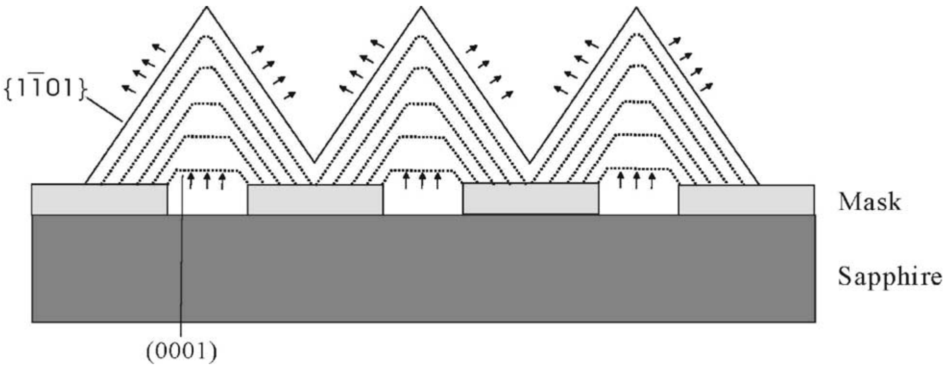

Fig. 3. Schematic illustration of the growth model of V defect.

and their growth rates are slow [21,22]. The growth mechanism of $\{1\bar{1}01\}$ pyramid structures can be applied to that of V defects.

Fig. 2 shows the $(1\bar{1}01)$ and (0001) facets of V defect in a GaN crystal structure. The surface of GaN was Ga-polarity because the films were grown on sapphire substrates [11,13]. As shown in Fig. 2(c), Ga atom on the $(10\bar{1}1)$ facet of V defect has one (or two) broken bond, while that on the (0001) has three broken bonds. In other words, $\{1\bar{1}01\}$ facets are more stable than (0001). Therefore, the initiation of the growth on the $\{1\bar{1}01\}$ facets is more difficult than that on the (0001). Since the growth rates of $\{1\bar{1}01\}$ facets are slow, the V defect is composed of six stable $\{1\bar{1}01\}$ side facets. As illustrated in Fig. 3, the diameter of V defect will increase with the deposition time (the thickness of film). When the thickness of GaN film reached 22.9 μm, the diameter was as large as 8 μm. It was much larger than the diameters of the V defects of the MOCVD grown InGaN/GaN MQWs. Their diameters were less than 100 nm [6–12].

As for the stripe pattern, the growth of the ELO GaN was found to depend on two factors: (1) the deposition method; (2) the direction of the stripe [19–21,24,25]. Since this paper is on the growth mechanism of V defects on the HVPE GaN films, the following discussion will only focus on the ELO GaN by using HVPE method. In the study of Hiramatsu et al. [21], they found the surface of HVPE grown ELO GaN was not uniform when $\langle 11\bar{2}0\rangle$ line-patterned windows were used. Initially, GaN with $\{1\bar{1}01\}$ equivalent facets grew selectively on the SiO_2 window area. Then this growth was followed by lateral overgrowth of the GaN onto the SiO_2 mask. Since the lateral overgrowth rates of $\{1\bar{1}01\}$ facets were small, the uniform surface of (0001) was not obtained. As illustrated in Fig. 4, the surface was covered with $\{1\bar{1}01\}$ facets due to their slow growth rate [21]. However, in the study of Usui and co-workers [24], the laterally grown GaN regions coalesced to form a flat smooth (0001) surface. Consequently, no $\{1\bar{1}01\}$ facets were found on the surfaces. The development of these $\{1\bar{1}01\}$ facets on $\langle 11\bar{2}0\rangle$ stripe windows can be used to explain the changes in the diameter and the density of the V defects. When the thickness of GaN film increased from 5.58 to 22.9 μm, most of the V defects vanished due to the coalesced of the $\{1\bar{1}01\}$ facets. Therefore, the density of the V defects decreased significantly from 2.5×10^9 to $5.7 \times 10^4\ \mathrm{cm}^{-2}$. However, for those remaining V defects, they grew from 20 nm to 8 μm due to the slow growth rates of $\{1\bar{1}01\}$ facets.

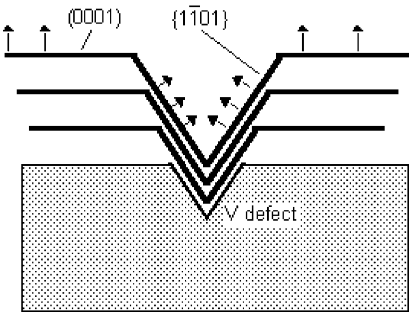

Fig. 4. Schematic illustration of the formation of $\{1\bar{1}01\}$ facets on the HVPE grown ELO GaN on the $\langle 11\bar{2}0\rangle$ stripe windows.

4. Summary

In this study, through the analysis of growth mechanism of ELO GaN crystal, the growth mechanism of V defects on the HVPE undoped GaN films has been investigated. When the thickness of GaN film increased from 5.58 to 22.9 μm, most of the V defects vanished due to the coalesced of the $\{1\bar{1}01\}$ facets. For those remaining V defects, they grew from 20 nm to 8 μm due to the slow growth rate of stable $\{1\bar{1}01\}$ side facets.

Acknowledgements

This project was funded by National Science Council (NSC) of the Republic of China under grant NSC90-2216-E009-037, and has benefited from the facilities and equipment of Semiconductor Research Center at Chiao Tung

University. The authors would like to thank S.C. Wang for valuable discussions.

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