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Stress at the coalesced boundary of GaN grown on maskless periodically grooved sapphire

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Rectangular voids were found at the coalescence boundary in GaN laterally grown on maskless periodically grooved sapphire by metal organic chemical vapor deposition (MOCVD) in this paper. Stress distribution investigations were performed by micro-Raman spectroscopy. An increased compressive stress was found at the coalescence boundary in the wing regions. Using finite element analysis method, we found the rectangular voids present at the wing regions are the major source of stress concentration.

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1. Introduction

GaN and related materials have unique electrical and optical properties, which have been attracted much attention due to their promises in blue and ultraviolet light emitting device applications [1-2]. Conventional growth of GaN on sapphire often results in high threading dislocation (TD) densities due to the large lattice mismatch between two materials. The threading dislocations are electrically active and degrade transport, emission, and detection, which limit the achievement of devices with improved performance [3]. Epitaxial lateral overgrowth (ELO) has been proven to be a powerful technique to reduce dislocation densities [4,5]. Many groups have developed several effective modified form of ELO Such as PE (pendeo-epitaxy) [6,7], CE (Canti-Bridge epitaxy) [8,9], etc. GaN epilayers grown on maskless grooved sapphire substrates has been reported in recent years [10-11], which has been proved that it can effectively reduce the threading dislocation [12]. It will be a promising way to get higher quality GaN-based materials films using this method.

In this paper, rectangular voids were found at the coalescence boundary in GaN laterally grown by maskless grooved sapphire substrate. Stress distribution investigations were performed on GaN laterally grown on maskless groove sapphire by micro-Raman spectroscopy. An increased compressive stress was detected at the coalescence boundary. By finite element analysis method (FEA), we conclude that the void in the coalescence boundary is likely the source of stress concentration.

2. Experimental section

The sample was 4.5 μm unintentional doped GaN grown on maskless grooved (0001) sapphire substrate by MOCVD. The grooved sapphire substrate was prepared by standard photolithography and wet chemical etching. Then the patterned substrate was loaded into the MOCVD reactor after cleaning by deionized water. And GaN films were deposited on them following by the standard two-step growth process in the Axitron 2400G3HT MOCVD with horizontal flow geometry, trimethylgallium (TMGa) and NH_3 were used as precursors and with H_2 carrier gas. Typical growth temperature is 1100 ^{o}C. More details about this method were described elsewhere [12].

The cross-section of GaN was characterized using Hitachi S-4200 scanning electron microscopy (SEM). Micro-Raman scatting experiments were carried out in backscatting geometry at room temperature, which were performed with multichannel modular triple Raman systems (JY-T6400), a 100X microscope objective lens was used for focusing the laser beam and collection of the scatter light. Under such conditions, the spatial resolution of instrument is about 1μm, the solid-state diode laser (532 nm) was used as an excited source. Finite element analysis was performed with two-dimensional model, using the code ABAQUS [13].

Fig. 1 showed the schematic procedure of fabricating maskless periodically grooved sapphire, which was prepared by standard photolithography and wet chemical etching. First, sapphire substrate was periodically patterned along [11-20] with 3-μm-wide SiO_2 strip and

3.5-μm-wide opening. Then, the patterned sapphire was etched in the solution of $H_2SO4:H_3PO_4=3:1$ followed by dipping in the solution of $HF:H_2O$ =1:10 for removal of SiO_2.

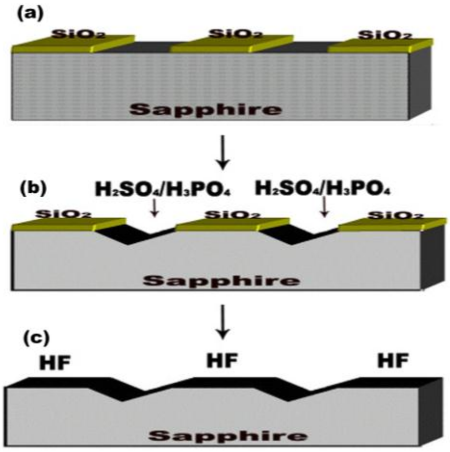

Fig. 1. A schematic of the procedure to prepare grooved sapphire by wet chemical etching. (a) Sapphire substrates were periodically patterned along [11-20] with 3-μm-wide SiO_2 *strip and 3.5-μm-wide opening. (b) Subsequently, the patterned sapphire was etched in the solution of* $H_2SO4:H_3PO_4=3:1$ *at 400 °C for 2h (c) Removal of* SiO_2 *in the solution of* $HF:H_2O$ *=1:10 at room temperature.*

Fig. 2 was the plan-view scanning electron microscopic (SEM) picture of GaN grown on maskless grooved sapphire. GaN layers were initially formed on the mesa, as the growth proceeded, GaN layers laterally extend then forming wing region. The inset was the magnified picture of the coalescence boundary in the wing region, and the rectangular void can be clearly seen.

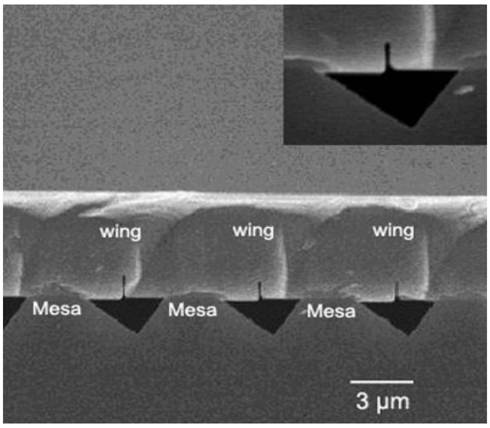

Fig. 2. Cross-section SEM image of a 4.5μm thick GaN film grown on maskless grooved sapphire. The inset shows the rectangular shape voids at the coalescence boundary.

Fig. 3 showed the line scan of E_2 frequency obtained by Raman mapping. The Raman spectra were performed from near the top surface. Increased stress is visible at the coalescence boundary. It is well known that the E_2(high) mode has been proven particularly sensitive to stress in GaN epitaxial films [14]. Stresses are generated as a result of the mismatch in the thermal expansion coefficient of substrate. It can be clearly seen both the mesa and wing regions are under compressive stress compared with strain free GaN crystal sample, which shows E_2(high) in the location at 567.2 cm^{-1} [15]. Meanwhile, increased compressive stress was found at the coalescence boundary of two adjacent in the wing region. So a higher compressive is shown in the wing region above the rectangular-shaped void. We assume the rectangular voids in our sample are likely to the sourced of compressive stress concentration.

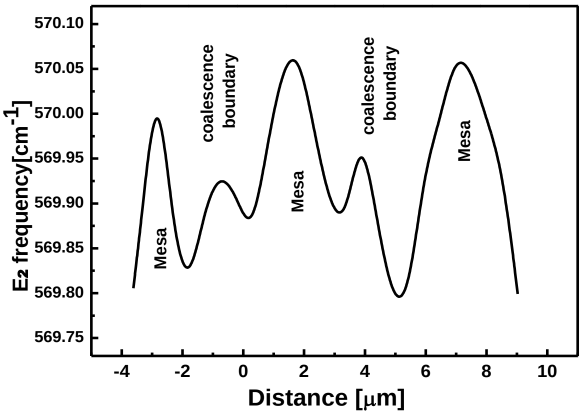

Fig. 3. Micro-Raman line scan of E_2 *frequency recorded from near the top surface.*

Fig. 4 shows linescan of stress distribution along the rectangular void in horizontal direction in the vicinity of a rectangular-shaped void of GaN obtained using finite element analysis using the code ABAQUS. Elastic constants, Poisson's ratio, and thermal expansion coefficients were used as input parameters [16,17]. The FEA results illustrated stress concentration in the vicinity of rectangular void. According to FEA analysis, stress componentσ_{xx} increases with the distance approaching the void. Stress concentration was showed in of in the vicinity of the tip of the void at the coalescence boundary, which was determined about 0.54 GPa. FEA analysis results confirmed that increased stress at the coalescence boundary originates from rectangular voids.

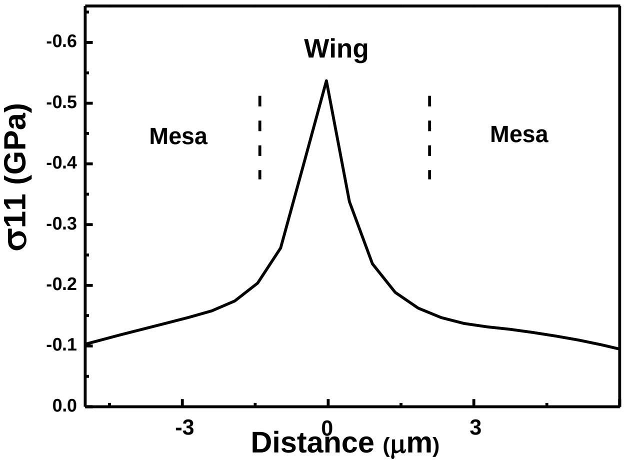

Fig. 4. Stress componentσ_{xx} *in the vicinity of voids of GaN laterally grown on maskless periodically grooved sapphire.*

3. Conclusions

In conclusion, rectangular voids were found at the coalescence boundary in GaN grown by masklesss periodically grooved sapphire. Micro-Raman scattering results show an increased stress in the wing regions. By the FEA analysis, we conclude that rectangular voids present at the coalescence boundary are the source for increased stress at the coalescence boundary.

Acknowledgments

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