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Wing tilt investigations on GaN epilayer grown on maskless grooved sapphire by MOCVD

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Abstract GaN epilayer is grown on maskless periodically grooved sapphire by metal organic chemical vapor deposition (MOCVD) in this article. Wing tilt is detected by high resolution X-ray rocking curve. Inhomogeneous deformations between the wing and mesa regions are found by atomic force microscopy (AFM) characterization. The stress distribution is investigated using finite-element simulations. Inhomogeneous stress distribution in the mesa and wing regions is shown, which is also confirmed by micro-Raman spectroscopy. The results show that the wing tilt in GaN layers grown on maskless periodically grooved sapphire mainly originates from the different deformations for mesa and wing region caused by inhomogeneous stress distribution.

Introduction

Recently, GaN has been extensively studied because of its potential use in green blue and ultraviolet light emitting diodes [1, 2]. However, it is still difficult to obtain a high-quality GaN layer on the sapphire substrate both because of the large lattice mismatch and difference in the thermal expansion coefficients between the GaN film and sapphire substrate [3]. Conventional growth of GaN on sapphire often results in high threading dislocation densities (TD) (10^8–10^{10} cm^{-2}). It has been demonstrated that TDs affect both electrical and optical properties of the GaN material [4, 5]. Epitaxial lateral overgrowth (ELO) has been proven to be a powerful technique to reduce dislocation densities [6–9]. Recently, high-quality GaN film grown on maskless periodically grooved sapphire prepared by wet chemical etching has been reported [10, 11]. Compared with the usually used dry etching to get patterned substrates, wet etching have many advantages, such as avoiding the mechanical damages on the grooved sapphire surface, benefiting selective growth of GaN, and reducing threading dislocation, which had been confirmed to be a promising way to get high-quality GaN-based films.

Wing tilt is a general problem existed in GaN films grown by various ELO growth methods. It will result in the generation of extra dislocations and thus degrading the crystal quality. For the case of ELO growth method with mask, wing tilt has been attributed to grain boundary along the edge of mask, which is caused by threading dislocations [12]. For the maskless PE method, recent research results show that wing tilt is primarily thermally induced and which is different from the findings of ELO [13, 14]. Although the wing tilt was greatly suppressed or avoided under the optimized growth conditions for the method grown on maskless periodically grooved sapphire, the formation mechanism is also not clear. In this article, inhomogeneous deformations between the wing and mesa regions are found by atomic force microscopy (AFM) characterization. The stress distribution is investigated using finite-element (FE) simulations and micro-Raman measurement. Inhomogeneous stress distribution in the mesa and wing regions is shown. The results show that the wing tilt in GaN layers grown on maskless periodically grooved sapphire mainly originate from the different

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deformations for mesa and wing region caused by inhomogeneous stress distribution.

Experimental details

Standard two-step growth process was used to grow 1.5-µm GaN films in Axitron 2400G3HT MOCVD (metal organic chemical vapor deposition) with horizontal flow geometry. The GaN layer was grown on the 2-in. maskless grooved sapphire substrate. The trimethylgallium (TMGa) and NH_3 were used as precursors with H_2 as carrier gas. The growth was initiated by the deposition of a 25-nm thick GaN nucleation layer at 500 °C. After raising the temperature to 1,050 °C, 0.5-µm thick GaN buffer was grown and then lateral overgrowth is observed at 1,100 °C. The grooved sapphire substrate was prepared by wet chemical etching along $[11\bar{2}0]$ with 3-µm wide mesa and 3.5-µm wide groove. The detailed process for preparing grooved sapphire can be found in reference [11]. The wing tilt is characterized by X-ray diffraction (XRD) measurements using Bede D1 high resolution X-ray diffactometer (HRXRD). The surface morphology and deformations of the wings were characterized by AFM (NanoScope D3000 AFM) in a tapping mode. Micro-Raman measurement was performed with multichannel modular triple Raman systems (JY-T6400) to measure the stress of the GaN on mesa and in the wing regions, a 100× microscope objective lens was used to focus the laser beam and collect the scatter light. The spot diameter of the focused laser beam on the sample is about 1 µm, the solid-state diode laser (532 nm) was used as an excited source. FE analysis was carried based on a two-dimensional strain model and the code Abaqus.

Results and discussion

Figure 1 shows X-ray rocking curves of the (0002) Omega scan with the direction of the incident X-ray beam were perpendicular to the stripe. Three diffraction peaks are observed. There are two satellite peaks and one peak at the center between the satellite peaks. The splitting of the XRD rocking curves indicated the crystallographic tilt existed. The two satellite peaks originated from the diffraction of the GaN in the wing regions are located 0.085°(±0.005°) from the center peak attributed to the diffraction of the GaN in the mesa region. To identify the mechanism of generating wing tilt, the morphology and stress analysis were performed.

Figure 2 displays the surface morphology of GaN grown on maskless grooved sapphire, and the periodically fluctuated structure can be clearly seen. The fluctuation period is same to that of the patterned substrate. Combining with the profile in line scan on the surface, the deformation in the surface fluctuation can be evaluated. The tilt angle Θ that is defined as arctan *h*/*d* as shown in Fig. 2 was estimated ranging from 0.102° to 0.112°. The value of the tilt angle of the surface morphology is similar to the value of the wing tilt measured by symmetry XRD as shown in Fig. 1. The results show the crystalline incline of GaN in the wing region relative to the GaN in the mesa leads to the fluctuated surface morphology.

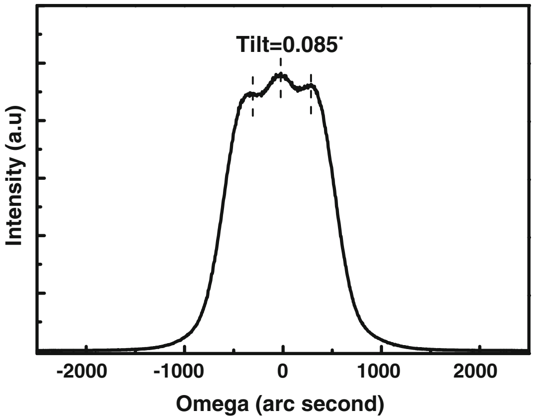

Fig. 1 X-ray rocking curves of the (0002) Omega scan with the direction of the incident X-ray beam is perpendicular to the stripe

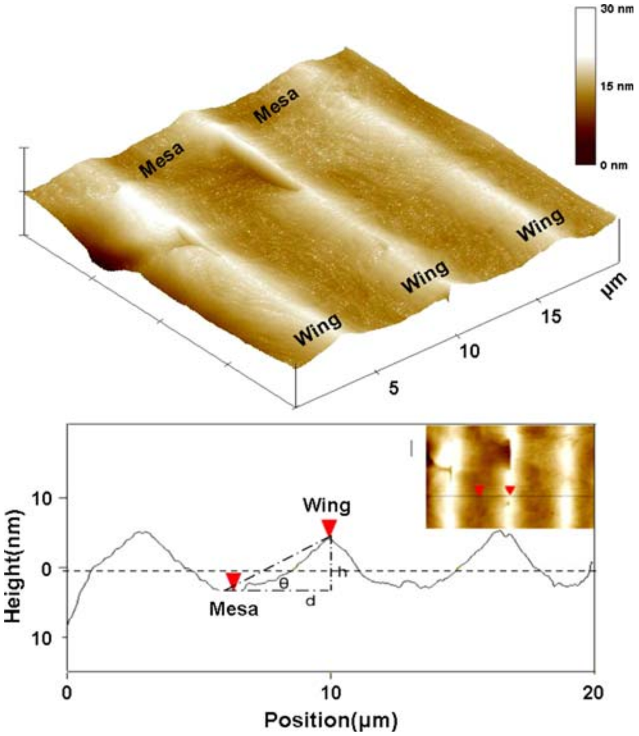

Fig. 2 Surface morphology of GaN grown on maskless grooved sapphire by AFM

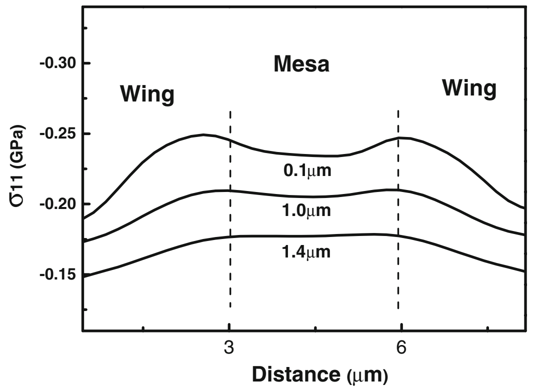

Fig. 3 Stress distribution of GaN grown on maskless grooved sapphire simulated by FE

The stress distribution from the FE analysis is shown in Fig. 3. FE analysis was based on the two-dimensional orthotropic linear elastic theory, in-plane strain conditions, and using the code Abaqus. Elastic constants, Poisson's ratio, coefficients of thermal expansion from the references [13, 14], and the temperatures of the initial and final state were used as input parameters. The temperature was changed from 1,100 to 25 °C during the cooling process. The thermal stress is due to the mismatch of thermal expansion coefficient between GaN and the sapphire substrate during the cooling process after epitaxial growth. According to the FE analysis results, both the mesa and wing regions are under compressive stress, and inhomogeneous stress distribution can clearly be seen in the mesa and wing regions. And the highest in-plane compressive stress E_{xx} is shown around the GaN/sapphire interface ($z = 0.1$ μm), the strains in the mesa and wing regions are inhomogeneous along the *c*-axis normal, the mesa region shows a larger stress than the wing region. As the method grown on the patterned sapphire excluded the interactions between the mask and the GaN films in the wing region as a result of differences in the coefficients of thermal expansion, there was lower compressive stress in the GaN wing regions.

Figure 4 shows the micro-Raman spectra performed at room temperature for the wing and mesa region with backscatting geometry. The weak peak at 417.95 cm^{-1} on both regions corresponds to the phonon scattering from sapphire substrate. The principle peaks are labeled as the E_2 (high) at 570.3 and 569.8 cm^{-1} for the mesa and wing region, respectively. It is well known that the E_2 (high) mode has been proven to be sensitive to stress in GaN [15]. The stress can be characterized by the frequency shift of the E_2^H mode in the micro-Raman spectroscopy. In the wing region, the A_1 (TO) and E_1 (TO) peaks are also observed, which is forbidden in backscattering geometry along *c*-axis. The emergence of such peaks suggested the pyramidal growth of the GaN before coalescence [16]. The stress in the GaN film is mainly caused by the result of the mismatch in the thermal expansion coefficient and crystal lattice between GaN and substrate. Thus, both the mesa and wing regions are under compressive stress compared with strain free GaN crystal, which shows E_2 (high) in the location at 567.2 cm^{-1} [17]. Increased compressive stress is found at the mesa region. Micro-Raman spectroscopy shows higher degree of stress, therefore, present in the mesa region, which is in agreement with the FE results.

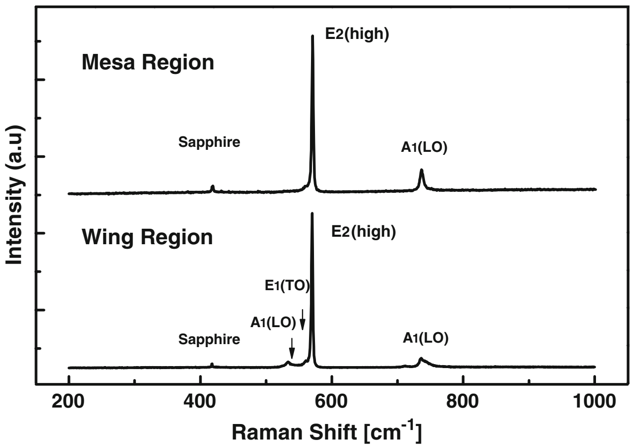

Fig. 4 Micro-Raman spectra of mesa and wing region of GaN grown on maskless periodically grooved sapphire

Conclusion

In conclusion, two-dimensional deformations and stress distributions in GaN films grown on maskless periodically grooved sapphire substrates were investigated by AFM, two-dimensional FE analysis and micro-Raman spectroscopy. The stress distribution was investigated using FE simulations. Inhomogeneous stress distribution in the mesa and wing regions was shown, which was also confirmed by micro-Raman spectroscopy. The results show that the wing tilt in GaN layers grown on maskless periodically grooved sapphire mainly originate from the different deformations for mesa and wing region caused by inhomogeneous stress distribution.

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