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Improved optical performance of GaN grown on pattered sapphire substrate*

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Abstract: An improved GaN film with low dislocation density was grown on a *C*-face patterned sapphire substrate (PSS) by metalorganic chemical vapor deposition (MOCVD). The vapor phase epitaxy starts from the regions with no etched pits and then spreads laterally to form a continuous GaN film. The properties of the GaN film have been investigated by double crystal X-ray diffraction (DCXRD), atomic force microscopy (AFM) and photoluminescence (PL), respectively. The full-width at half-maximum (FWHM) of the X-ray diffraction curves (XRCs) for the GaN film grown on PSS in the (0002) plane and the $(10\bar{1}2)$ plane are as low as 312.80 arcsec and 298.08 acrsec, respectively. The root mean square (RMS) of the GaN film grown on PSS is 0.233 nm and the intensity of the PL peak is comparatively strong.

Key words: double crystal X-ray diffraction; atomic force microscopy; photoluminescence; GaN; wet-etching
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1. Introduction

GaN-based wide bandgap semiconductors have attracted considerable interest, in terms of applications for optoelectronic devices, which operate in the blue, green and ultraviolet wavelength regions, as well as for electronic devices operating at high-temperature and high-power conditions, including traffic signals, full-color displays, automotive lighting and general room lighting[1−3]. However, owing to the large mismatch of lattice constant and thermal expansion between the epitaxial GaN film and sapphire substrate, high-density dislocations ranging from 10^8–10^{10} cm^{-2} lead to degradation in material quality. Threading dislocation (TD) in GaN degrade device performation through carrier scattering, nonradiative recombination and increased reverse-bias leakage current[4,5]. Many methods are adopted to decrease dislocation density. By epitaxial lateral overgrowth (ELOG) with SiN_x or SiO_2 mask patterned on as-grown GaN seed crystal, TD can be significantly reduced[6−8]. However, the two-step growth procedure is time consuming and the contamination is easily introduced. Recently, the maskless PSS technique has been widely proposed for its single-step growth process and high production yield[9]. Furthermore, the geometrical shape of the sapphire can reduce dislocation density and improve the quality of GaN film.

In this paper, GaN film is grown on a PSS fabricated by chemical wet etching, to avoid the surface damage normally induced by dry etching. A comparable optical improvement of GaN film is demonstrated.

2. Experiment

Figures 1 (a) and 1 (b) show top and cross-sectional images of the PSS. Fabrication of the PSS with inclined crystallography-etched facets is as follows: A 60 nm thick SiO_2 with hole-patterns was deposited on a *C*-plane sapphire substrate by plasma-enhanced chemical vapor deposition (PECVD) and defined by standard photolithography to serve as the wet etching mask[10]. The sapphire substrate was then wet etched using a mixture of H_2SO_4 and H_3PO_4 (H_2SO_4: H_3PO_4 = 3:1). The temperature was maintained at 280 °C. Finally, buffered oxide etch (BOE) solution was used to remove the SiO_2 mask. It was also found that the sapphire etching rate depends on the crystal orientation and decreases in the order *C*-plane > *R*-plane > *M*-plane > *A*-plane[10]. As a result , in Fig.1(a), the etch-pits of an (0001)-oriented sapphire substrate have a flat-surface of $\{0001\}$ *C*-plane with triangle-shape in the center.

Figure 1 (c) schematically depicts the cross-sectional image of the GaN sample on the PSS. The GaN epilayer was grown on PSS by MOCVD system with a Thomas Swan closely spaced showerhead reactor. Trimethylgallium, trimethylindium and ammonia were used as Ga, In and N sources, respectively. CP_2Mg and SiH_4 were used as the p-type and n-type doping sources, respectively. A mix gas of hydrogen and nitrogen was used as the carrier gas. The substrate was heated in the hydrogen ambient at 1100 °C for 10 min in order to remove contaminants. A thin buffer layer with a thickness of about 25 nm was deposited at 530 °C (LT-GaN) and crystallized at 1060 °C for 6 min. Undoped GaN (uGaN) was grown at 1030 °C at a pressure of 100 Torr. For a comparative analysis, GaN on plane sapphire was also fabricated under the same growth conditions.

Crystallographic properties were evaluated by (0002) and $(10\bar{1}2)$ DCXRD measurement using the PhiliP DCXRD system. Photoluminescence spectra were characterized using an

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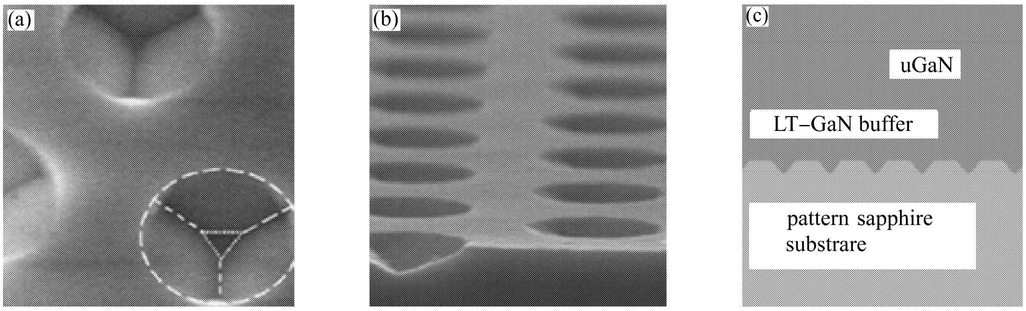

Fig.1. (a) Top image of a PSS; (b) Cross-sectional image of the same PSS; (c) Schematic drawing of the sample structure.

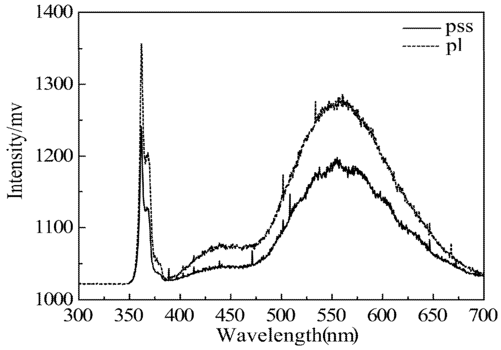

Fig.2. PL spectra of samples pss and pl.

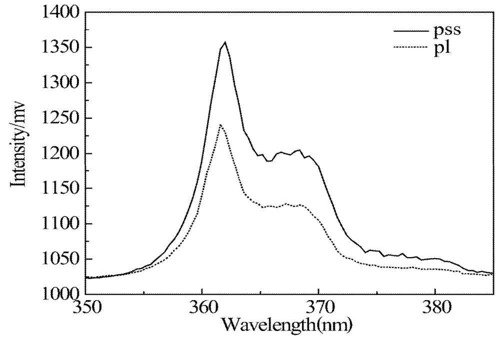

Fig.3. Near band emission of samples pss and pl.

excitation source of 325 nm from a He-Cd laser. The surface morphology was characterized by AFM.

3. Results and discussion

For convenience, the GaN grown on the PSS is denoted pss, and the GaN grown on plane sapphire is denoted pl. Figure 2 shows the PL spectra of samples pss and pl. Sharp band edge emission is observed, and the blue band and yellow band also appear. The band edge emission corresponds to free excitons (FE) and shallow donor bound excitons (DBE), and DBE associates with the defects such as nitrogen vacancy (V_N). A blue band has been reported in Refs.[11,12], attributed to donor-valence band transition. As for the yellow band, this might be observed for a number of reasons; a systematic and detailed analysis is necessary, which is out of the scope of this study. However, it has been reported that the origin of enhanced yellow emission inside the defects is deep gap states formed by Ga-impurity complexes, which are trapped at the side faces[13].

Figure 3 shows that the PL intensity of sample pss is stronger than that of sample pl. The intensity of the near-band-edge PL emission of GaN is indicative of its optical quality, so

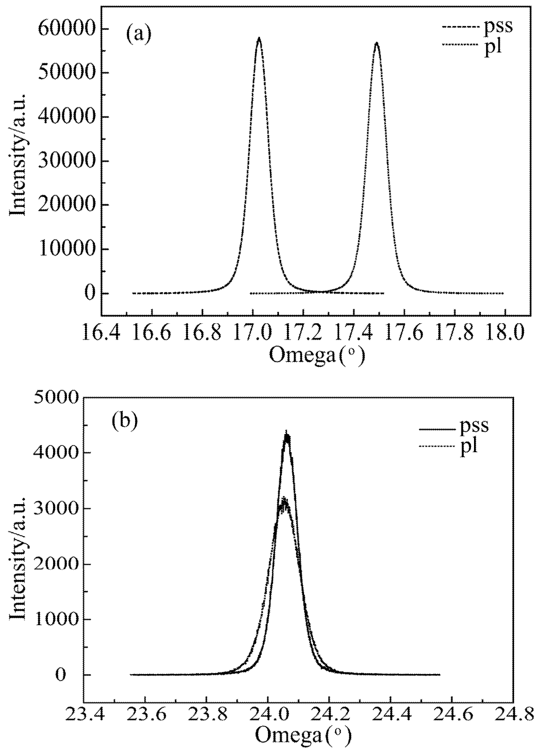

Fig.4. (a) (0002) DCXRD spectra of samples pss and pl; (b) $(10\bar{1}2)$ DCXRD spectra of samples pss and pl.

sample pss has a higher optical quality. The ratio of intensity of band-edge emission to yellow emission is an important parameter related to crystal quality. The ratio of samples pss and pl are 1.38 and 1.25 respectively. This also indicates that the sample pss possesses a better quality. Besides, the near band-edge peak of unstrained GaN is 363.4 nm, sample pss has smaller shift of peak than sample pl, so strain is also smaller.

Figure 4 shows the (0002) and $(10\bar{1}2)$ XRCs of samples pss and pl. The FWHM of the X-ray diffraction curves for sample pss in the (0002) plane and the $(10\bar{1}2)$ plane are as low as 312.80 arcsec and 298.08 arcsec, respectively. The FWHM of the X-ray diffraction curves for sample pss in the (0002) plane and the $(10\bar{1}2)$ plane are 323.64 arcsec and 426.60 arcsec, respectively. Symmetric (0002) curves show information about the screw dislocation density that is mainly generated from the different step heights of the substrate. Asymmetric $(10\bar{1}2)$ curves show information about the mixed and pure edge dislocation densities that are mainly generated from the coalescence process among the misoriented individual islands. The wider curve indicates that the dislocation density in the

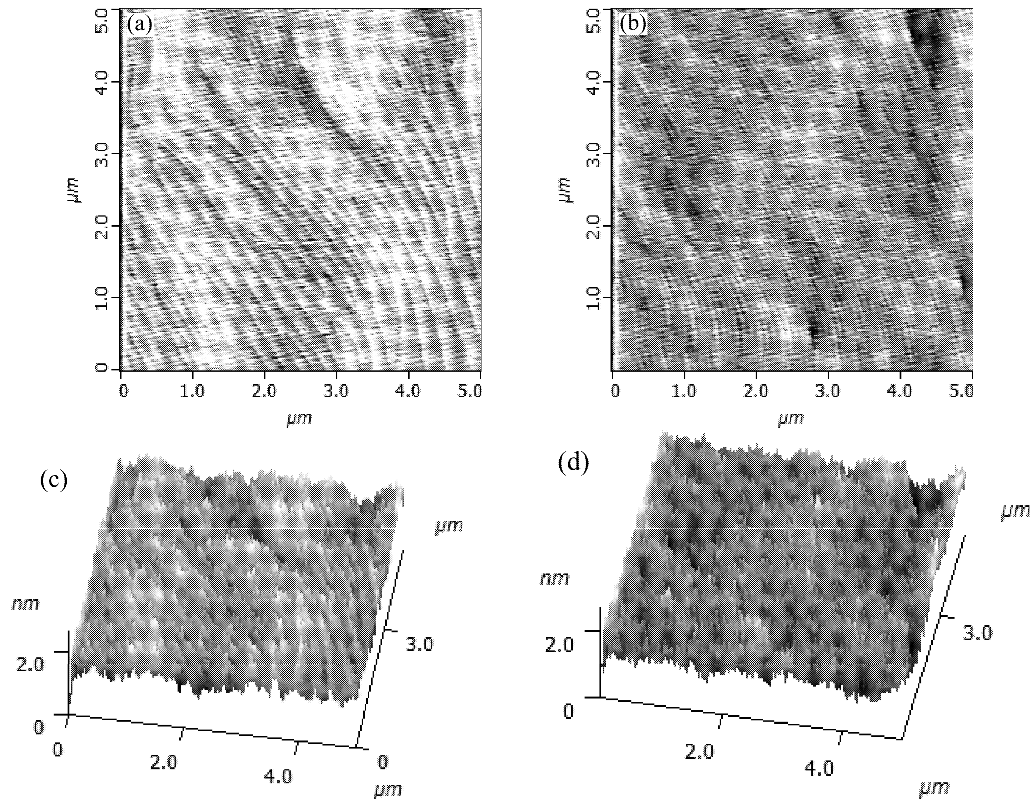

Fig.5. (a) AFM 2D image of sample pl; (b) AFM 2D image of sample pss; (c) AFM 3D image of sample pl; (d) AFM 3D image of sample pss.

Table 1. Diffraction peak locations and strain of samples pss and pl.

GaN film	(0002) location (°)	(0004) location (°)	$(10\bar{1}2)$ location (°)	$(20\bar{2}4)$ location (°)	$e^{\perp}$(%)	$e^{\parallel}$(%)
Sample pss	17.0055	36.2251	24.0606	54.6307	0.1929	0.0941
Sample pl	17.5157	36.5995	24.0539	54.6100	0.3664	0.5958

GaN film is higher[14]. Thus, the DCXRD results indicate that the dislocation density in sample pss is much lower than that of sample pl.

The strain can be calculated by

$$d_{0001} = \frac{2\lambda}{2\sin(\theta_{0002} + \Delta\theta_1)} = \frac{4\lambda}{2\sin(\theta_{0004} + \Delta\theta_1)} \tag{1}$$

$$c = d_{0001} \tag{2}$$

$$d_{10\bar{1}2} = \frac{\lambda}{2\sin(\theta_{10\bar{1}2} + \Delta\theta_2)} = \frac{2\lambda}{2\sin(\theta_{20\bar{2}4+\Delta\theta_2})} \tag{3}$$

$$d_{hkl} = \frac{1}{\sqrt{\frac{4}{3}(\frac{h^2 + hk + k^2}{a^2})\frac{l^2}{c^2}}} \tag{4}$$

$$e^{\perp} = (c - c_o)/c_o \tag{5}$$

$$e^{\parallel} = (a - a_o)/a_o \tag{6}$$

The space between the (0001) planes, namely d_{0001}, and between the $(10\bar{1}2)$ planes, namely $d_{10\bar{1}2}$, θ_{0002}, θ_{0004}, $\theta_{10\bar{1}2}$ and $\theta_{20\bar{2}4}$ are the locations of reflection peaks in the (0002) plane, the (0004) plane, the $(10\bar{1}2)$ plane and the $(20\bar{2}4)$ plane, respectively. $\Delta\theta_1$ and $\Delta\theta_2$ are the system errors. a and c are the strained lattice parameters. a_0 and c_0 are the unstrained lattice parameters, which are 0.3189 and 0.5185 nm, respectively. $e^{\perp}$ and $e^{\parallel}$ are the out-of-plane strain and in-plane strain, respectively.

Table 1 shows the DCXRD results of samples pss and pl calculated using the equations above. Compared with sample pl, the $e^{\perp}$ and $e^{\parallel}$ of sample pss are lower, so the crystal quality of sample pss is better than sample pl.

Figure 5 shows the AFM images with a 5 × 5 μm^2 scan area of the samples pss and pl. There are smooth terrace steps and dark spots on the GaN surface. Nano pipes and GaN droplets are not observed. If the atomic step-flow growth mode allows for fast adatom diffusion to the intrinsic steps, the parallel and straight terraces, as seen in Fig.5, suggest a typical step-flow morphology or growth mode. RMS roughness is an important parameter to value surface roughness. The RMS roughness of sample pl and sample pss are 0.256 and 0.233 nm, respectively. On the other hand , the dislocation density of sample pl and sample pss are found to be 8.4×10^7 and 2.8×10^7 cm^{-2} respectively by simply counting the dark spots at the edge of steps. Sample pss has improved quality. The results obtained from AFM and DCXRD are in agreement.

4. Conclusion

In this paper, GaN film grown on a PSS is investigated by different characterization methods (DCXRD, PL and AFM) in detail. From PL measurement we find sample pss has a stronger peak than sample pl. From the DCXRD measurements, the FWHM of the X-ray diffraction curves for the GaN film grown on the PSS in the (0002) plane and the $(10\bar{1}2)$ plane are as low as 312.80 arcsec and 298.08 arcsec, respectively. According to related equations, the strain parameters are calculated, which are low. AFM measurement suggests a step-flow morphology for the GaN surface and the dislocation density is found to be in the order of 10^7 cm^{-2}. Consequently, the results show that GaN film on a PSS is of better quality.

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