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# Enhancement of optical property and crystal structure for GaN films on 2D MoS<sub>2</sub> buffer layer by nitridation treatment

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## ABSTRACT

The growth of GaN films on layered 2D-MoS<sub>2</sub>/c-sapphire substrate by plasma-assisted molecular beam epitaxy system was investigated. Pre-nitridation process and deposition time as growth parameters were employed to exploit the heteroepitaxial growth of GaN films at the temperature of 700 °C. The characterizations of surface condition, surface morphology, elemental composition, optical properties, crystal orientation and quality of GaN epitaxial films were conducted by reflection high energy electron diffraction (RHEED), scanning electron microscope (SEM), atomic force microscope (AFM), X-ray photoelectron Spectroscopy (XPS), Raman spectroscopy, photoluminescence spectroscopy (PL) and high-resolution X-ray diffraction (HR-XRD), respectively. The pre-nitridation process and growth duration can enhance the optical properties and crystal quality of GaN films on 2D-MoS<sub>2</sub>/c-plane sapphire. The pre-treatment of MoS<sub>2</sub> layer by nitrogen plasma before the growth, providing a wet layer of nitrogen for GaN growth, can eliminate the oxygen contamination and reduce the defects in the films. Band-to-band emission of Wurtzite GaN with the bandgap of 3.5 eV can be improved by pre-nitridation process, and yellow band emission can be suppressed due to the elimination of defect states in the films. Meanwhile, the crystal orientation and quality can be improved by the pre-nitridation process and longer duration of growth time. This study demonstrates a van der Waals epitaxial GaN films on 2D-MoS<sub>2</sub> layer with higher crystal quality by pre-nitridation process, and it provides a potential solution for the future applications of GaN-based devices.

## 1. Introduction

Gallium nitride (GaN), one of group III-nitride compound semiconductors, is an influential material for microelectronics and optoelectronic devices [1,2]. This is due to its excellent properties of wide and direct bandgap, high thermal stability, high breakdown field and good electron mobility. Currently, epitaxial growth of high quality GaN films makes it possible for many optoelectronic devices such as light emitting diodes (LEDs) [3], high-electron-mobility transistors (HEMTs) [4], solar cells [5,6], laser diodes (LDs) and photodetectors [7]. High crystal quality of GaN films can be obtained by the homoepitaxial growth [8]. However, the growth method still has suffering issues and challenges because of the high cost and scalability of bulk GaN [9]. Therefore, the employment of foreign substrate, that makes inexpensive process realize, should be a best way for getting high quality GaN films

[10,11]. Up to now, the deposition of GaN films on various substrates, exploited the heteroepitaxy growth technique by using buffer layers, surface pre-treatment and post-annealing process, is still a challenge as well [12–14].

The heteroepitaxy growth by molecular beam epitaxy (MBE) is the mainstream for the growth of high-quality GaN films on different substrate materials, especially for its higher growth temperature [15]. However, the existence of defects due to the lattice mismatch and thermal mismatch between GaN and the substrate was observed during the nucleation and growth process, deteriorating the crystal quality [16,17]. Reducing the microstructural defects is vitally significant step towards the high-efficiency GaN-based electronic and optoelectronic devices [18]. Usually, the complicated buffer layer techniques are used for the heteroepitaxial growth of high-crystal-quality GaN films. Recently, two-dimensional (2D) transition metal dichalcogenides (TMD)

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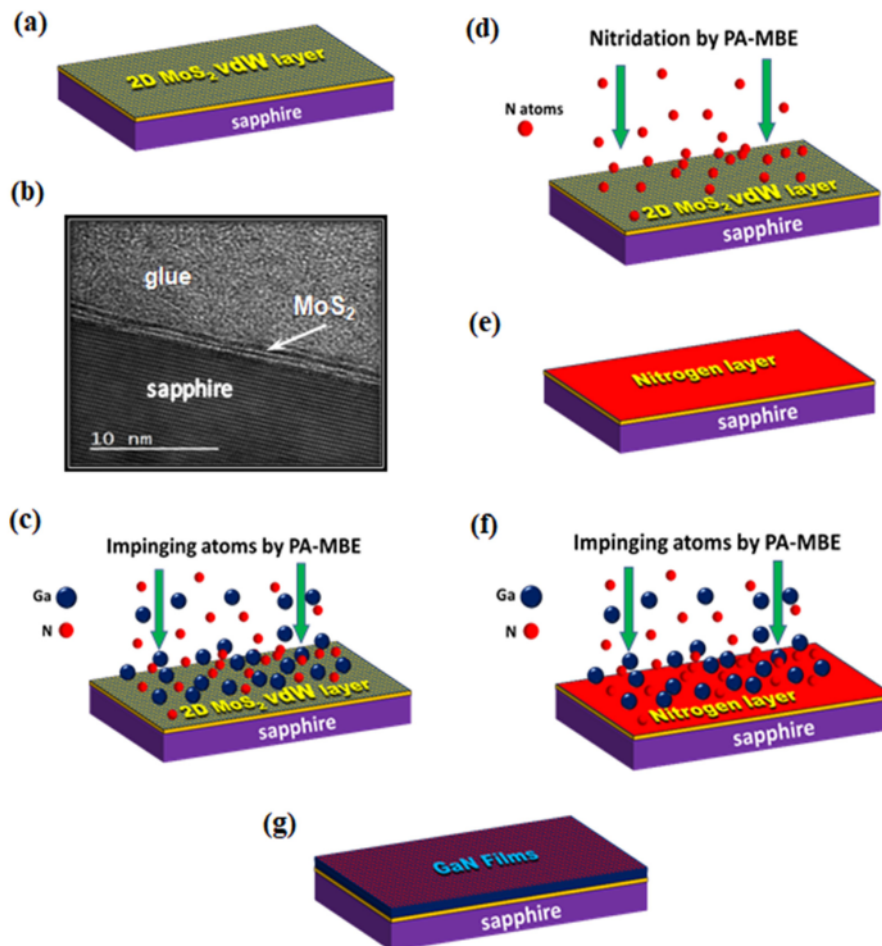
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38 was used as a buffer layer material for epitaxial growth, called van der Waals epitaxy (vdWE), which is employed to overcome the current issues [19,20]. Among TMD materials, 2D MoS<sub>2</sub> is the dominant epitaxial substrate for high crystal-quality GaN films [21,22]. To initiate bonding element over the MoS<sub>2</sub> layer should be essential step to improve 75 crystal quality of GaN films. However, the presence of several defects originated from the interface between the buffer layer and the grown film for heterostructure has constructed in the GaN film [23]. Therefore, pre-treatment process for the nucleation is believed that it could organize the epitaxial growth at the beginning of the films. So far, pre-treatment with nitridation has been utilized on the bulk surface and 2D graphene of heterostructure growth [24,25]. The influence of pre-treatment carried out on 2D MoS<sub>2</sub> buffer layer for creating the high-crystal quality of GaN is still unknown. Moreover, a thicker epitaxial film obtained by longer duration growth generally offered a better structure quality. The investigation on the pre-treatment process and duration of epitaxial growth should be an interesting topic for deeply understanding of heterostructure GaN films on 2D MoS<sub>2</sub> buffer layers. 33 In our previous report [26], GaN films on 2D MoS<sub>2</sub> layers/c-sapphire were fabricated by plasma-assisted molecular beam epitaxy (PA-MBE) 47 nm. The investigation of different MoS<sub>2</sub> buffer layers for the GaN growth was conducted at lower growth temperature of 600 °C and the

growth time of 20 min 54 this report, the pre-nitridation effect and growth time of 60 min at the temperature of 700 °C were studied in order to improve the crystal quality and optical property of GaN films on 2D MoS<sub>2</sub>. The growth parameters, both of pre-nitridation treatment and growth duration, could play an important role for the formation of high-quality GaN films. The *in-situ* reflection high energy electron diffraction (RHEED) can monitor the surface condition of GaN and MoS<sub>2</sub> buffer layer during the epitaxial growth. 71 *ex-situ* characterizations are conducted to exploit the physical properties of GaN films for the deposition process. The microstructure and optical properties for GaN films on 2D MoS<sub>2</sub> buffer layers can be enhanced by the pre-nitridation process and the increase of growth time.

## 2. Material and experimental method

67 Fig. 1 shows the growth schematic process of GaN films on 2D MoS<sub>2</sub> layers by PA-MBE system. Layered 2D MoS<sub>2</sub> was deposited on single crystal c-sapphire substrate in 2-in. diameter with 6 mm thickness. In the Fig. 1(a), the growth of MoS<sub>2</sub> layers was carried out by DCA pulse laser deposition (PLD) system at 800 °C with background pressure of  $8 \times 10^{-6}$  Torr equipped with KrF excimer laser and a commercial MoS<sub>2</sub> target (Gredmann Taiwan Ltd., 99.9% purity) [27]. Fig. 1(b) displays the



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Fig. 1. Schematic diagrams for the growth of GaN films: (a) Layered 2D MoS<sub>2</sub>/c-sapphire substrate as substrate, (b) Cross-sectional high resolution TEM image of MoS<sub>2</sub> on sapphire, (c) Epitaxial growth of GaN on 2D MoS<sub>2</sub>/c-sapphire, (d) Pre-nitridation treatment on MoS<sub>2</sub> buffer layer, (e) After nitridation process, the formation of nitrogen layer, (f) Epitaxial growth of GaN on 2D MoS<sub>2</sub>/c-sapphire with pre-nitridation process, and (g) Finished vdWE GaN films on 2D MoS<sub>2</sub>/c-sapphire.

cross-sectional transmission electron microscopy (TEM) image, and about 2–3 monolayers of MoS<sub>2</sub> present on c-sapphire substrate. This layered 2D MoS<sub>2</sub> plays as the buffer layer for the vdWE of GaN films. The growth of GaN films on 2D MoS<sub>2</sub>/c-sapphire employed the VAC PAMBE system [26]. Before the growth of all GaN films, thermal cleaning for the substrates was carried out at 600 °C for 40 min. In Fig. 1(c), GaN film was grown at the temperature of 700 °C for 60 min without nitridation treatment, named S1 in Table 1. On the other hand, two samples were grown at the same temperature with pre-nitridation treatment on MoS<sub>2</sub> at 700 °C for 5 min in Fig. 1(d) and (e), which can provide the nitrogen layer for the nucleation of GaN films. The GaN growth duration are 20 min for sample S2 and 60 min for sample S3, respectively. The growth procedure of GaN films is schematically shown in Fig. 1. Moreover, the summary of growth parameters is tabulated in detail in Table 1.

MBE growth chamber's base pressure was set at  $6 \times 10^{-10}$  Torr. The oxygen plasma pressure was kept constant at  $9.7 \times 10^{-5}$  Torr, while the temperature of the Ga K-cell was maintained at 800 °C in a beam equivalent pressure of  $6 \times 10^{-8}$  Torr. The nitrogen plasma source was provided by the constant N<sub>2</sub> flow 0.8 sccm with 500 W of RF power [28]. RHEED operating at 20 kV was used to monitor the surface of both MoS<sub>2</sub> and GaN films during epitaxial growth. After the growing process, field emission scanning electron microscopy (FE-SEM, JSE-7000F, JEOL, Tokyo, Japan) and atomic force microscopy (AFM, C3000, Nanosurf, Liestal, Switzerland) were used to examine the surface morphology of the films. The surface chemistry of GaN was studied by X-ray photoelectron Spectroscopy (XPS, K-Alpha, Thermo Scientific, Waltham, MA, USA) with an Auger electron microprobe system. Raman spectroscopy was used to examine the vibration mode of molecules for GaN, MoS<sub>2</sub> and sapphire. The crystallography of GaN thin films was investigated by high-resolution X-ray diffraction (HR-XRD, D1, Bede Scientific Instruments, Durham, UK). Photoluminescence spectroscopy (PL) at room temperature with a UV laser of 266 nm was used to evaluate the optical properties of GaN thin films correlated to near band edge and yellow band emissions.

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### 3. Results and discussion

#### 3.1. RHEED

Fig. 2 illustrates the RHEED pattern recorded during GaN growth in MBE system. Before thermal cleaning, the streak pattern with low intensity related to crystalline structure of MoS<sub>2</sub> surface in Fig. 2(a). After thermal cleaning process, as shown in Fig. 1(b), the pattern was brighter, suggesting that MoS<sub>2</sub> surface became cleanliness. The streaky RHEED pattern corresponds to an atomically smooth surface that is free of oxide or contamination-borne undesirable layers. [29]. The thermal treatment at 600 °C for 40 min in vacuum could eliminate the oxide and adsorption of other molecular on the surface. Then, after the pre-nitridation process at 700 °C for 40 min, the streaky pattern was kept, but it became foggy shown in Fig. 2(c). This is because the nitrogen atoms were adsorbed on the surface of MoS<sub>2</sub> to form a nitrogen wetting layer. This layer of nitrogen on the surface could have influence on the growth of GaN films. After the growth of GaN films, Fig. 2(d) shows the RHEED pattern of sample S1, the streaky diffraction pattern became distinctly spotty. It denotes that single crystal of GaN with a rough surface was constructed on the films [30]. Two other samples with the pre-nitridation treatment

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(S2 and S3) are shown in Fig. 2(e) and (f), respectively. After the growth for 60 min, the intensity of spotty pattern was continuously stronger, manifesting that better crystalline structure constructed on the surface of GaN films. The *in-situ* observation by RHEED performs the surface condition of MoS<sub>2</sub> buffer layers and the growth of GaN films.

#### 3.2. FE-SEM

FE-SEM images as shown in Fig. 3 disclose surface morphology of GaN films (S1, S2 and S3) for the magnification of 15 K and 30 K. The morphology GaN films looks homogeny with small particles existing on the surface. It signifies that GaN was grown on the MoS<sub>2</sub> layers. The small particles related to Ga clusters spread on the surface associate with the incorporation of gallium atoms during cooling in the growth chamber. As the temperature drops, the low energy may impede the migration of Ga atoms that constructed the clusters on the surface. It was also similar trend for GaN films grown with pre-nitridation treatment (samples S2 and S3). As the growth time increases up to 60 min (S3), the hexagonal crystal of GaN structure was obviously observed in the films, shown in Fig. 3(e) and (f). It proved that pre-nitridation procedure with longer growth time was facilitated the improvement of surface morphology. According to FE-SEM observation, the surface texture of GaN film related to morphological formation is strongly influenced by both of pre-nitridation step and duration of the growth time.

#### 3.3. AFM

To comprehend the topology of the surface in detail, AFM has been used to examine the GaN films and MoS<sub>2</sub> layer as well. Fig. 4 shows the AFM images with a scan area of  $3 \mu\text{m} \times 3 \mu\text{m}$  and the Z-axis polynomial fit of 5 nm for each sample. Fig. 4(a) displays the surface of 2D MoS<sub>2</sub> layers/c-sapphire substrate noted as sample S, and Fig. 4(b), (c), (d) are AFM images of GaN films for S1, S2, and S3 samples, respectively. As shown in Fig. 4, the brighter white colour ascribes to the peak surface (Sp), and the darker black one is valley (Sv) generated on the surface. The brown colour associate to the average surface (Sa). The maximum high surface is noted as (Sy), accumulating between peak high and depth valley. The summarized surface roughness is tabulated in detail on Table 2. The root mean square (RMS) was obtained about 2.49, 2.51 nm, 5.43 nm, and 2.88 nm for S, S1, S2 and S3, and average surface roughness are 0.79 nm, 1.51 nm, 1.27 nm, and 1.32 nm, respectively.

The RMS and Sa of 2D MoS<sub>2</sub> are lower than GaN films, which means a smoother surface of buffer layer was provided for GaN growth. After the epitaxial growth GaN films, the increase of peak high implies the enhancement of surface roughness. The result is consistent with the one of FE-SEM in Fig. 3. At the shorter duration growth of 20 min (S2), its RMS is higher than S1 and S3 samples grown for the duration of 60 min. The longer growing period simplifies the Ga and N atoms, allowing to desorption and reconstruction for proper film surface. Moreover, thermal annealing after epitaxial growth and sufficient thermal energy during epitaxial growth could lead to desorbing process for a smoother GaN film surface [31]. The surface morphology of GaN films grown on 2D MoS<sub>2</sub>/c-sapphire substrate is clearly influenced by growth time, which can be evidenced by AFM investigations.

**Table 1**  
Growth parameters for GaN films on layered 2D-MoS<sub>2</sub>/c-sapphire substrates.

GaN films	Buffer layers/substrate	Thermal cleaning		Pre-nitridation treatment		Growth temp. (°C)	Growth time (min)
		Temp (°C)	Time (min)	Temp (°C)	Time (min)		
S1	MoS <sub>2</sub> /c-sapphire	600	40	700	0	700	60
S2					5		20
S3					5		60

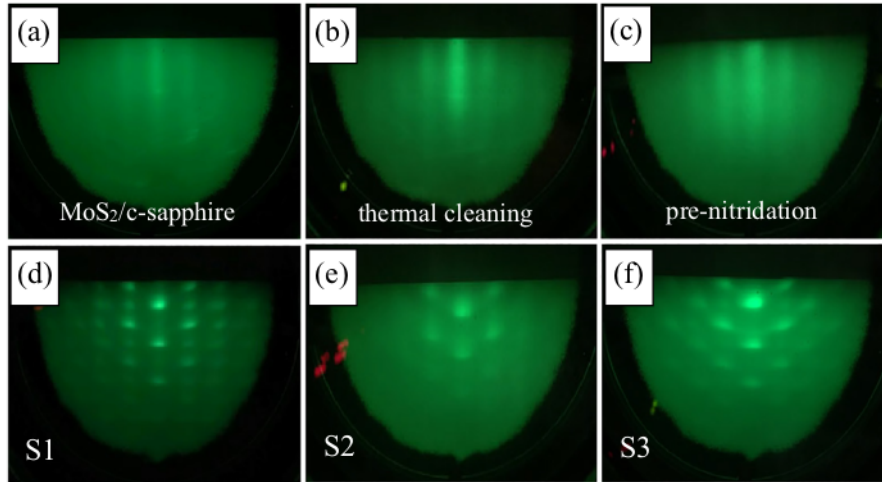


Fig. 2. (a) RHEED pattern of MoS<sub>2</sub>/c-sapphire, (b) After thermal cleaning at 600 °C for 20 min in vacuum, (c) After pre-nitridation for 5 min, (d) GaN films without pre-nitridation grown for 60 min (S1), (e) GaN films with pre-nitridation grown for 20 min (S2), and (f) GaN films with pre-nitridation grown for 60 min (S3).

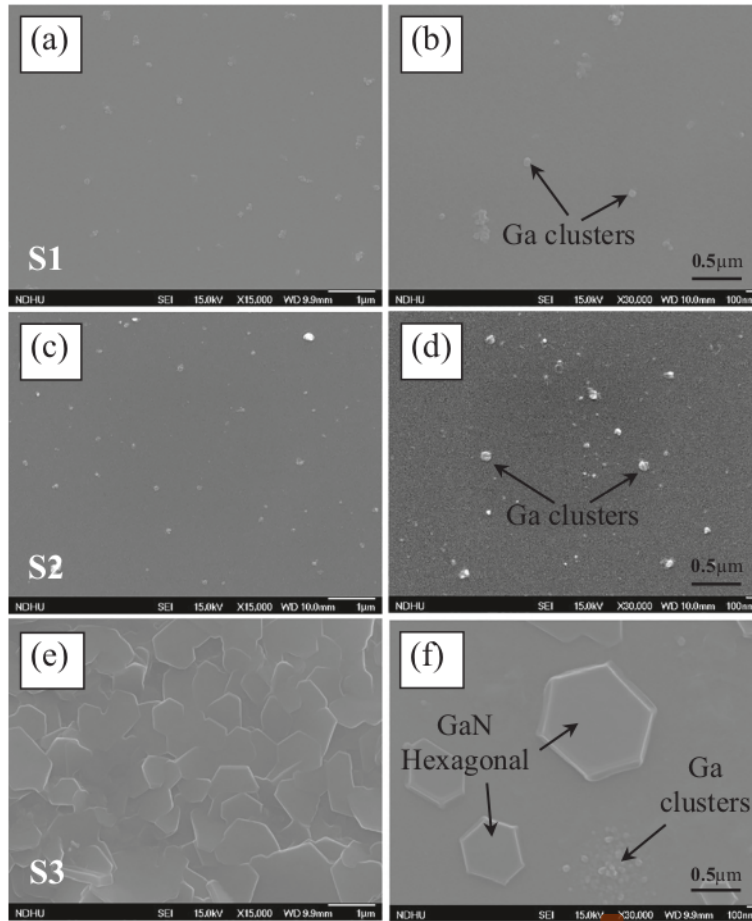


Fig. 3. FE-SEM images of GaN films for three samples in the magnification of 15,000× and 30,000×: S1 (a) and (b); S2 (c) and (d); S3 (e) and (f).

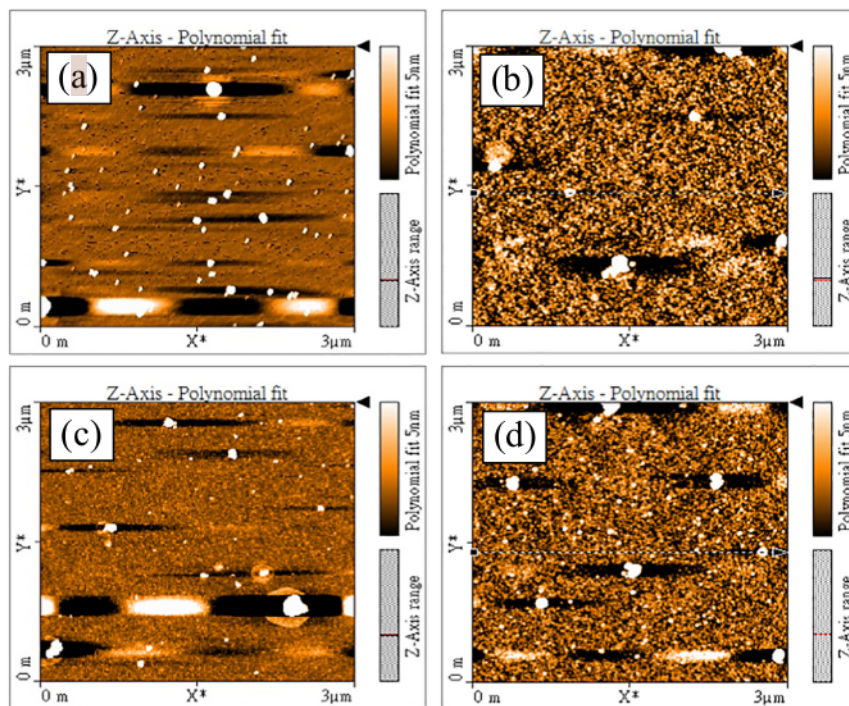


Fig. 4. AFM images: (a) buffer layers 2D MoS<sub>2</sub>/c-sapphire substrate, (b) S1, (c) S2, and (d) S3 samples of GaN films.

**Table 2**  
The surface roughness of GaN films and 2D-MoS<sub>2</sub>/c-sapphire substrate.

Samples	Area roughness (nm)				
	Sa	RMS	Sy	Sp	Sv
S	0.79	2.49	60.31	52.0	8.31
S1	1.51	2.51	52.92	38.08	14.84
S2	1.27	5.43	138.31	102.69	35.62
S3	1.32	2.88	106.64	67.07	39.57

### 3.4. XPS

The binding energies of Ga and N were measured by using X-ray photoemission spectroscopy (XPS) to evaluate the surface chemistry of GaN film. The calibration of XPS spectra was conducted by C 1s 284.8 eV. The Ga 3d and N 1s core level peak regions of GaN are revealed in Fig. 5. The fitted curve of Ga 3d by *Avantage* software shows three main peaks correlated to gallium metallic (Ga—Ga), gallium nitride (Ga—N) and gallium oxygen (Ga—O) bonding on the GaN films [32,33]. Their peaks are located around 18.3, 20.0, and 22.6 eV, respectively. The first peaks in blue line are attributed to Ga—Ga bonding generated on the surface, suggesting the present of Ga clusters on the surface as shown in SEM images of Fig. 3. The second and main peaks in red line are Ga—N bonding of GaN films, and the last one is related to Ga—O bonding. In addition, XPS is a semi quantitative measurement that can be used to clarify amount of the bonding element on the surface. Table 3 contains a detailed summary of the peak positions and percentages of bonding elements. Based on the fitting results of Ga 3d core level for samples S1, S2 and S3, the percentage of Ga—Ga bonding are 12.54, 3.56, and 9.29%. Thus, the Ga—N bonding are 85.30, 96.44, and 90.71%. The Ga—O bonding is about 2.16% in the sample S1, indicating small amount of surface oxidation for the sample. Ga—O component is observed at 2.6 eV higher BE side compared to main peak and it can be attributed to the

formation of Ga<sub>2</sub>O<sub>3</sub> at the surface due to atmospheric exposure [34]. The existence of Ga—O bonding on GaN films might degrade the electrical and optical characteristics [35].

By the pre-nitridation treatment, it could facilitate the nitrogen atom to initiate the nucleation site in the interface since nitrogen has both higher energy migration (1 eV) and higher adsorption (4.6 eV) compared to Ga [36]. It could also inhibit the attendance of Ga vacancies in the interface. The presence of Ga vacancies in the structure layers can absorb oxygen atoms as atmospheric exposure to samples and it could lead to form Ga—O bonds with other Ga atoms. Based on Ga 3d XPS results, S2 and S3 samples with pre-nitridation treatment have greater Ga—N bonding than S1 samples.

N 1s core level spectra have been also fitted by using 3 components (N—Ga, Ga LMM Auger features and N—Ox) as shown in Fig. 5(d), (e) and (f). N—Ga peak appears at  $397.03 \pm 0.14$  eV. Ga related Auger features appear at 2.4 eV lower BE side compared to main peak (N—Ga). For the samples with pre-nitridation treatment, the peak presented at  $399.53 \pm 0.05$  eV in the N 1s spectrum as shown in Fig. 5(e) and (f) could be related to N—Ox bonding created on the surface due to the N-face polarity of GaN [37]. Detail peak positions and relative percentages are summarized in Table 3.

### 3.5. Raman

The specific molecular bond vibration of 2D MoS<sub>2</sub>/c-sapphire substrate and GaN films were identified by Raman spectroscopy. Fig. 6 displays the Raman spectroscopy at room temperature observed at the range of 300 to 800 cm<sup>-1</sup>. There are four main peaks (418.4, 449.4, 575 and 750 cm<sup>-1</sup>) presented from sapphire substrate [38], while MoS<sub>2</sub> has a Raman shift of roughly 382 cm<sup>-1</sup> for E<sub>2g</sub> and 408 cm<sup>-1</sup> for A<sub>1g</sub> [39]. The E<sub>2g</sub> mode is associated with molybdenum and sulphur atomic displacement in the basal plane, whereas the sulphur atomic vibration upright to the basal plane corresponds to the A<sub>1g</sub> phonon. The Raman peak

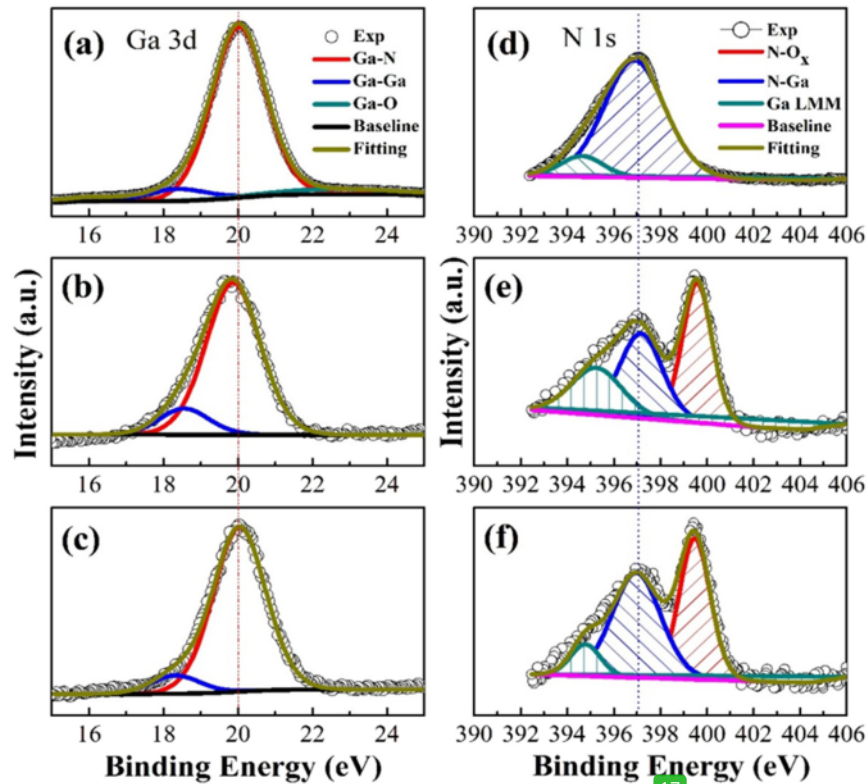


Fig. 5. XPS spectra of Ga 3d and N 1s core level spectra for GaN films grown on 2D MoS<sub>2</sub>/c-sapphire: S1 (a) and (d); S2 (b) and (e); S3 (c) and (f).

Table 3  
Summary of fitting results for the Ga 3d and N 1s core level spectra.

Sample	Peak	Relative (%)	N-1s	Peak	Relative (%)
S1	Ga-Ga	18.38	Ga-LMM	394.63	10.8
	Ga-N	20.02	N-Ga	396.89	89.2
	Ga-O	22.68	N-Ox	-	-
S2	Ga-Ga	18.38	Ga-LMM	395.26	23.5
	Ga-N	19.89	N-Ga	397.17	35.6
	Ga-O	-	N-Ox	399.58	40.8
S3	Ga-Ga	18.33	Ga-LMM	394.68	5.5
	Ga-N	20.04	N-Ga	396.93	51.4
	Ga-O	-	N-Ox	399.48	43.1

intensity ratio ( $E_{2g}/A_{1g}$ ) can also be used to determine the quality of a 2D-MoS<sub>2</sub> layer [40]. The peak intensity ratio of the PLD MoS<sub>2</sub> is 0.71, indicating a better quality of layer constructed for GaN growth in comparison with the one by CVD [26]. The  $E_{2g}$  and  $A_{1g}$  peaks vanished after the development of GaN films because they were covered by GaN thin films.  $E_2$  transverse optical (TO) and  $A_1$  longitudinal optical (LO) modes may be found at 567 and 730 cm<sup>-1</sup>, respectively, for the typical Raman modes of wurtzite GaN [41]. In Fig. 6, the  $A_1$  mode of GaN thin films could be observed at 730 cm<sup>-1</sup> near the c-sapphire shoulder peak (750 cm<sup>-1</sup>), especially for the sample S3. However, the peak of  $E_2$  mode, was difficult to observe in the report, which could be because of the insufficient thickness of GaN films.

### 3.6. PL

PL spectra of GaN films with and without nitridation treatment, as well as different growth times, are shown in Fig. 7. The PL experiment

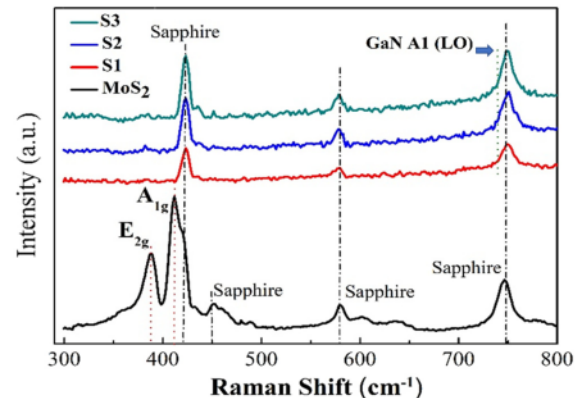
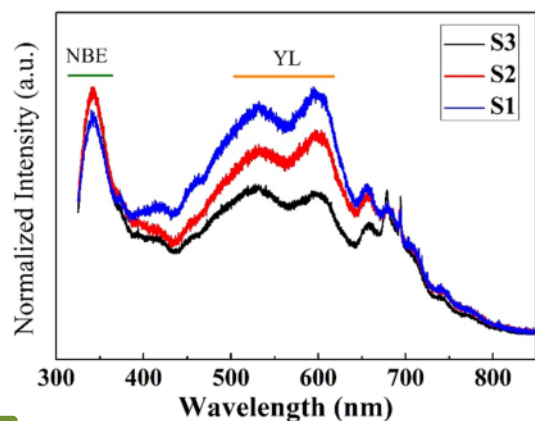


Fig. 6. Raman spectra of 2D MoS<sub>2</sub>/c-sapphire substrate and three GaN films: S1 (without pre-nitridation), S2 (with pre-nitridation and 20-min growth), and S3 (with pre-nitridation and 20-min growth).

was conducted at room temperature to explore the optical properties of GaN films. Near band edge (NBE) emission at 3.4 eV and yellow band (YB) emission from 2.0 to 2.8 eV are the typical primary peaks in GaN films [42]. The transition of excited electrons from the conduction band to the valence band was linked to NBE emission [43], while the defect state in the GaN was the source of YB emission [44]. As shown in Fig. 7, the first main peak of 352 nm was clearly observed, which is related to the NBE emission. The second wide peak was seen between 443 and 688



10 Fig. 7. The room-temperature photoluminescence spectra of GaN films: S1 (without nitridation), S2 (with pre-nitridation and 20-min growth), and S3 (with pre-nitridation and 60-min growth).

nm as a YB emission related with the defect structure. In the NBE emission, the normalized intensity of the peaks for the GaN films grown without pre-nitridation (S1) is lower than the samples with pre-nitridation treatment. Moreover, S1 sample has a broader and higher YB emission peak, suggesting more defects formed in GaN films. On the contrary, the two samples with pre-nitridation treatment (S2 and S3), the peaks of YB emission are lower than the one without pre-nitridation. It represents that the nitrogen plasma pre-treatment can modify the growth mechanism of GaN and decrease the defects in GaN, especially reduce the presence of Ga vacancies in the structure. Therefore, the yellow bend emission of GaN films can be suppressed. The pre-nitridation might facilitate initial bonding and structure greater in the interface between MoS<sub>2</sub> and GaN films. A good interface structure in a heterostructure promotes the quality of epitaxial growth. In addition, a longer duration of growth films was effective for reducing the defect structure in the GaN films as shown in YB emission for S3 sample, which indicates the superior crystal quality. According to the analysis of optical properties for GaN films, pre-nitridation and growth duration can enhance the physical properties of GaN films.

### 3.7. HR-XRD

To obtain the information of crystal structure, HRXRD was employed to analyze both the crystal orientation and crystal quality of GaN films. Fig. 8 denotes the  $\omega$  scanning of GaN films. The (0002) diffraction planes of rocking curve manifested that the films were all of c-axis oriented and Wurtzite structure. The plane (0002) of rocking curve can also be used to indicate the crystal quality of GaN films. As shown in Fig. 8, the full width of half maximum (FWHM) of (0002) GaN diffraction peak are 234.0, 247.9 and 220.3 arcsec, for sample S1, S2 and S3, respectively. The smaller FWHM evidenced the lower-density of screw dislocation in the epitaxial GaN films [45]. However, in shorter growth time in Fig. 8 (b) of sample S2, the FWHM is higher than others, representing more defect structure related to screw dislocations. The defects could construct easier close to the interface due to lattice mismatch between buffer layer and GaN films [46]. On the contrary, the defect structure can be decreased in the layers away from the interface of heterostructural epitaxy. The result was demonstrated by sample S3 displayed in Fig. 8(c), which has smaller FWHM value. The crystal quality of GaN films can be improved by the pre-nitridation treatment and a longer growth duration.

### 4. Conclusions

43 In this work, van der Waals epitaxial growth of GaN films on 2D MoS<sub>2</sub>/c-plane sapphire by PA-MBE system is demonstrated. During the MBE growth, the effects of pre-nitridation and deposition duration on the GaN films are investigated. The *in-situ* RHEED patterns monitored the sequential growth process, from 2D MoS<sub>2</sub> buffer layer of streaky pattern to GaN films of spotty pattern. It denotes that single crystal of GaN was constructed on the MoS<sub>2</sub>. By the longer duration growth time, the spotty pattern was continuously longer, manifesting a better crystalline structure of GaN films. After the growth, the surface morphology of GaN films was observed by SEM and AFM images. The hexagonal GaN structure was also formed on the surface films as pre-nitridation treatment and the increase of growth time was employed. While the smoother surface can be achieved by the longer duration of growth time. The chemical composition of GaN films was confirmed by XPS spectra. The pre-nitridation process, providing an initial wetting layer of nitrogen, can get rid of the contamination of oxygen on the GaN films. In the measurement of optical properties, including PL and Raman spectra, NBE emission of Wurtzite GaN with the bandgap of 3.5 eV is greatly enhanced by pre-nitridation treatment, and yellow band

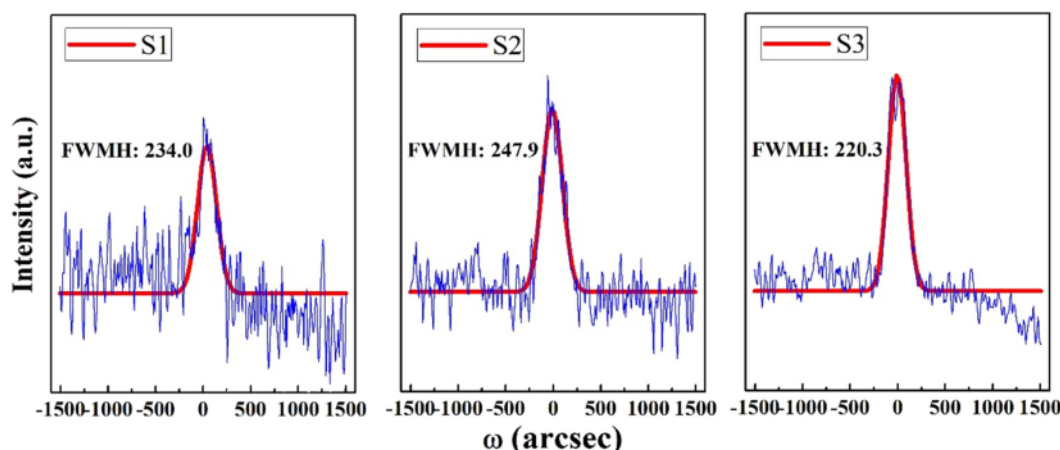


Fig. 8. HR-XRD of GaN (0002) rocking curve profiles and their fitting for three samples: S1 (without nitridation), S2 (with pre-nitridation and 20-min growth), and S3 (with pre-nitridation and 60-min growth).



emission can be suppressed due to the elimination of defect states. The Raman  $A_1$  peak, associated with longitudinal optical vibration mode of GaN, can be identified for the sample with pre-nitridation treatment for one-hour growth. The physical properties of GaN films are related to 46r microstructures. Therefore, the plane (0002) of rocking curve of HR-XRD was used to observe the crystal quality of GaN films. The smallest FWHM value was observed for the sample with pre-nitridation treatment for one-hour growth indicating the best crystal quality of GaN films. In summary, the pre-nitridation process and 37r growth duration can enhance the optical properties and crystal quality for the growth of GaN films on 2D MoS<sub>2</sub>/c-plane sapphire by PA-MBE, which is important for further applications in electronics and optoelectronics.

#### 22 CRediT authorship contribution statement

**Iwan Susanto:** Visualization, Formal analysis, Writing – original draft. **Chi-Yu Tsai:** Investigation, Formal analysis, Data curation. **Yen-Teng Ho:** Resources, Methodology. **Pi-Yu Tsai:** Resources, Validation. **Ing-Song Yu:** Conceptualization, Writing – review & editing, Supervision, Project administration.

#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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