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Study on the Structure of GaN films deposited on MoS2/Sapphire via Plasma-Assisted Molecular Beam Epitaxy

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Abstract: The gallium nitride (GaN) films were grown on molybdenum disulfide (MoS2) layers via plasma-assisted molecular beam epitaxy (PA-MBE). The heterostructures of the GaN film were studied using reflection high-energy electron diffraction (RHEED) and HR-XRD. The heterostructures of GaN/MoS2/sapphire were revealed through cross-sectional transmission electron microscopy (TEM). The surface texture of the GaN films was analyzed using FE-SEM. Single-crystal heterostructure GaN films can be obtained on 2D MoS2/c-sapphire. The RHEED demonstrated spot patterns with high intensity showing the single crystal structure constructed in the GaN films. The GaN films on the surface exhibited a hexagonal structure. TEM images taken perpendicular to the surface revealed that, even after 60 minutes of epitaxial growth, the thickness of the GaN films remained consistent at approximately 4 nm. However, the 2D MoS2 layer was not observable in the images due to harm incurred during heteroepitaxial growth. Based on the surface structure, it was found that GaN films were successfully grown on the MoS2 layers using the PA-MBE system.

Keywords: Gallium Nitride; Molydenum Disulfide; Hetero-Epitaxial; Surfaca Hetero Structure; Molecular Beam Epitaxy

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1. Introduction

Gallium nitride (GaN), including as III-nitride, has excellent properties namely direct and wide band gap, high electron mobility, high breakdown voltage, and excellent thermal stability [1], [2]. All these characteristics make an adequate option for many applications, such as high-performance power devices, high bright light emitting diodes, high electron mobility transistors (HEMT), etc [3][4], [5]. However, the main challenge for this material is the difficulty to get the GaN bulk as substrate. Generally, GaN is grown on Si and Sapphire substrates that have enough of a big difference lattice [6], [7]. While great efforts have been made to improve material quality on these substrates. There is always an attempt to find a suitable substrate related to lattice-matched for growing quality GaN. For this aim, molybdenum disulfide (MoS2) is an ideal substrate for GaN because it possesses less in-plane lattice mismatch [8]–[11]. Additionally, the slight difference in coefficient of thermal expansion between the two materials allows the stability of lattice alignment during the cooling-down process [12], [13]. Nowadays, the researchers have been attacked in two-dimensional (2D) layered metal dichalcogenide (TMD) due to its intriguing properties of atom-scale thickness, direct bandgap, and particularly strong light-matter interactions [14], [15]. In corresponding devices, heterostructures composed of mono-MoS2 and ultrathin GaN demonstrated excellent optoelectronic and tunable electronic properties[16], [17].

Up to now, only a few studies of GaN film grown on MoS2 was reported. Gupta et. al. investigated the growth of GaN on several layers of MoS2 by metal-organic chemical vavor deposition (MOCVD) [15]. Tangi et al. studied the growth of GaN on monolayer MoS2 via MBE [14]. Among the growth techniques, plasma-assisted molecular beam epitaxy (PA-MBE) is a promising method for producing high-quality heteroepitaxial GaN layers that is both accurate and environmentally friendly [18]. The advantages of this system include an ultra-high vacuum (UHV) environment to avoid contaminants, in-situ monitoring that allows for precise control of layer-by-layer growth, and a low growth temperature. However, the reporting of surface morphology of GaN deposited on the 2D MoS2 layer via PA-MBE has not been widely exploited yet.

In this study, we reported the characteristic of the surface texture of GaN film grown on 2D MoS2 template over c-sapphire substrate to deepen understanding in this field. Various growth times were explored to distinguish the type of RHEED pattern mode before, during and after the growth GaN films. Further detailed investigations on the surfaces of both the MoS2 template and the GaN films have explained the structure formation and surface texture, as well as aided us in better understanding the growth GaN on 2D MoS2. This research demonstrates the viability of using PA-MBE in a hybrid GaN/MoS2 system and the initial high-quality surface GaN formation on 2D MoS2, which creates a new avenue for the deployment of related devices in the future.

2. Materials and Experiment Methods

GaN thin films are grown heterostructurally on the surface of 2D MoS2/c-sapphire substrate using the PA-MBE ULVAC system. Figure 1 show the experimental set-up for growth GaN film on the substrate (2D MoS2/c-sapphire). The base pressure of the MBE chamber is 6x10−10 Torr and the thermal cleaning process for the substrate is conducted at 600 °C for 30 minutes. Pre-nitridation treatment on the substrate is carried out at 700 ℃ for 5 min in which can provide the nitrogen layer for the nucleation of GaN films. Further, the epitaxial GaN film growth was carried out at 700 °C for 20, 40, and 60 minutes. The atomic flux of Ga is provided by the K-cell at 800 °C and the plasma nitrogen source is employed at 500-Watt RF power using 6N N2 flux at 0.8 sccm. Meanwhile, the growth of the MoS2 layer on 2-inch c-sapphire was generated using the PLD method equipped with an ArF excimer laser at 800 °C with a background pressure of 10−6 Torr [19]. During the growth process, the in-situ characterization using reflection high-energy electron diffraction (RHEED) operating at 20 kV monitored the structure of GaN films. After the growth process, the cross-section area was investigated in detail Transmission Electron Microscopy (TEM) with JEOL JEM-2100F at an accelerating voltage of 200 kV, and the field emission of scanning electron JEOL microscope (SEM) with an accelerating voltage of 15 kV conducted the morphology texture of GaN films. Finally, the crystallography was characterized using high-resolution X-ray Diffraction (HR-XRD).

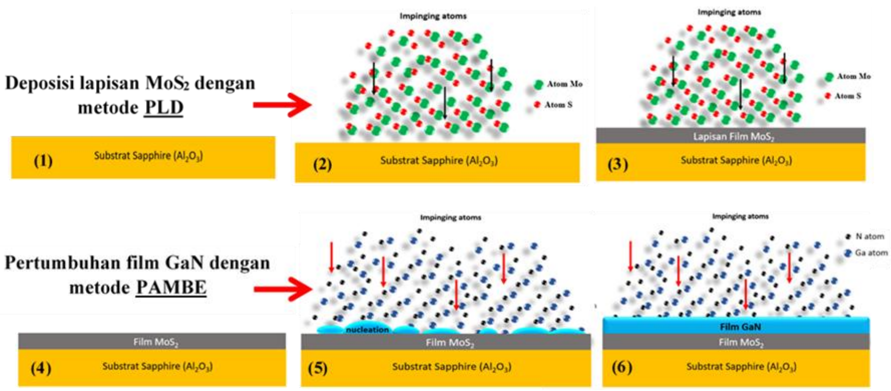

Figure 1. Growth GaN films on the substrate (2D MoS2/c-sapphire)

3. Results and Discussion

Fig 2 shows RHEED pattern of substrate and GaN films during epitaxially growth. The streaks pattern with high intensity are demonstrated by the surface structure of 2D MoS2/c-sapphire Fig 2.(a). Attending of this pattern related to 2D surface constructed on the MoS2 layer. Thus, the bright intensity associated with a single crystal structure formed in the layers. Based on the monitoring, MoS2 substrate was 2D surface with the crystalline structure. After growth GaN layers for 20 minutes, the spots pattern seems on the RHEED. The spots pattern associated with 3D GaN layers. The spots are arranged in a hexagonal pattern pointed to the single crystal of GaN. Following the growth to be 40 minutes, the spots show brighter patterns which indicate the increasing of crystalline quality on the GaN structure. At the growth end of 60 minutes in Fig 2(d), the spots pattern looks similar to the previous pattern Fig 2(c). It shows the epitaxial growth of GaN films obtained the same structure. According to the RHEED patterns, the single crystal with the hexagonal structure of GaN films have grown on 2D MoS2/c-sapphire. Futher, the observation of SEM will confirm on the morphology structure of the films.

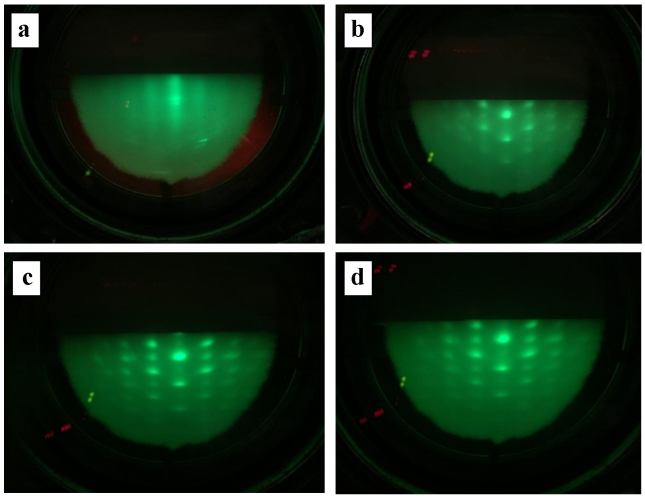

Figure 2. (a) RHEED pattern of 2D MoS2/c-sapphire, (b), (c) and (d) Grown GaN films for 20 min, 40 min, and 60 min

The arrangement of atoms in GaN microstructures and the heteroepitaxial interface between GaN and MoS2 layers were studied using high-resolution transmission electron microscopy (HR-TEM) to obtain information about the thickness and crystal structure of the GaN film and its interface with the substrate. Fig. 3 depicts the cross-sectional TEM images of the GaN film's heteroepitaxial structure and surface morphology, with Fig. 3(a) showing a cross-sectional image of GaN/2D MoS2/c-sapphire and Fig. 3(b) displaying the same location at a higher magnification. After 60 minutes of epitaxial growth, the thickness of the GaN films remained consistently around 4 nm, and according to the TEM image, they were grown on the substrate with a thin layer. However, the 2D MoS2 layer was not visible in the cross-section, suggesting that the layers were damaged during heteroepitaxial growth, which was confirmed by the nitridation process at a high temperature of the substrate (700 °C). Fig. 3(c) illustrates the surface morphology image of the GaN film, viewed at a magnification of 70,000x. The smooth growth of GaN films covering the substrate indicates that the coalescence epitaxy between Ga and N atoms for growing layers is comparable, and the structure of the GaN on the surface appears to be hexagonal. SEM results confirmed that the GaN films with a hexagonal structure covered the 2D MoS2/c-sapphire and that a single crystal of GaN film was generated on the substrate, consistent with the monitoring of RHEED.

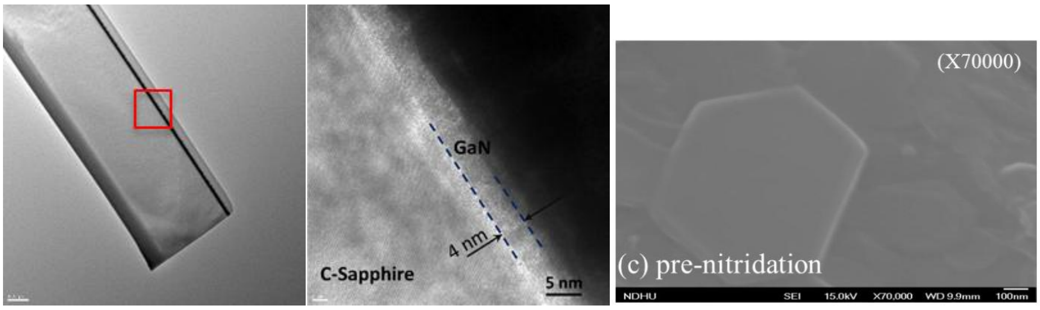

Figure 3. Cross-Section TEM images of (a) and (b) GaN/2D MoS2/c-sapphire substrate, (c) Surface FE-SEM of GaN films.

HRXRD was utilized to examine the crystal orientation and quality of GaN films. The (0002) diffraction planes of the rocking curve in Fig. 4 confirmed that the films had a c-axis orientation and Wurtzite structure. The (0002) plane of the rocking curve also revealed the crystal quality of the GaN films. As shown in Fig. 4, the full width of half maximum (FWHM) of the (0002) GaN diffraction peak was 333.8 arcsec dan peak hight was 2494 cps. The smaller FWHM and the high intensity indicated a lower density of screw dislocation in the epitaxial GaN films. However, the FWHM was broad, indicating more defect structures related to screw dislocations. Due to the lattice mismatch between the buffer layer and GaN films, the defects could form more easily close to the interface. Conversely, the defect structure could be reduced in the layers away from the hetero-structural epitaxy interface. This result was demonstrated that the crystal quality of GaN films can be enhanced by the low temperature for pre-nitridation treatment and a longer growth duration of epitaxial Gan films.

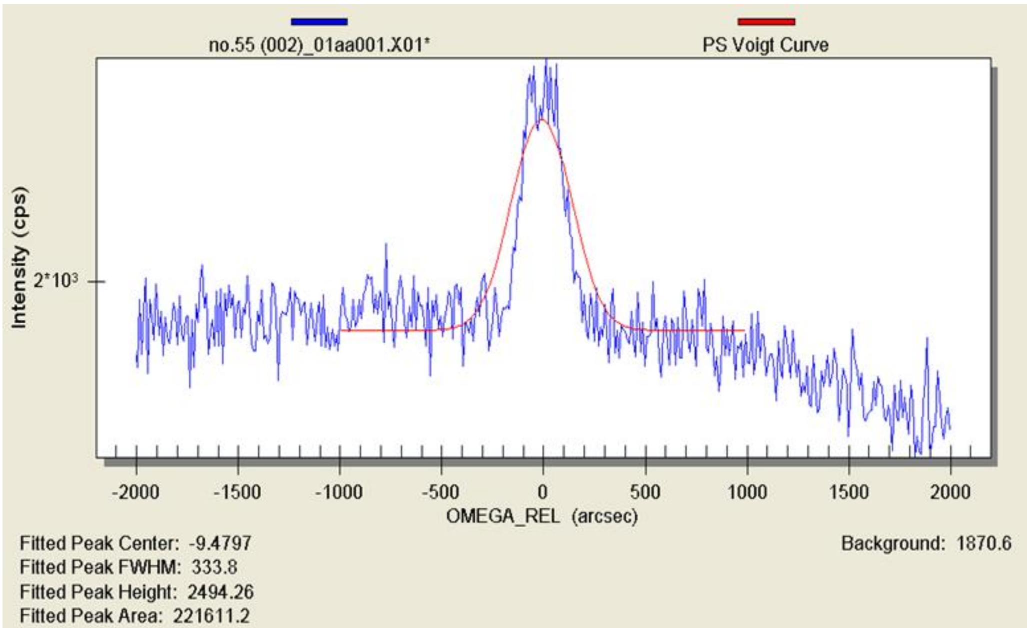

Figure 4. HR-XRD of GaN film

4. Conclusions

GaN films were successfully grown on a 2D MoS2/c-sapphire substrate using the PA-MBE system. During GaN epitaxial growth, the RHEED pattern demonstrated the presence of spots, indicating a single crystal structure of the 2D MoS2/c-sapphire substrate. The quality of the substrate's crystalline structure increased with the duration of growth. HR-TEM analysis was used to study the crystal structure and thickness of the GaN film and its interface with the substrate. Cross-sectional TEM images showed that the thickness of the GaN films remained around 4 nm after 60 minutes of epitaxial growth, while the 2D MoS2 layer was not visible due to damage during heteroepitaxial growth. The surface morphology of the GaN film exhibited smooth growth with a hexagonal structure. A smaller full width of half maximum and a higher peak intensity indicate good structure quality, related to low screw dislocation density in the films. The crystal quality of GaN films can be improved by using a low temperature for pre-nitridation treatment and increasing the duration of epitaxial growth.

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