

Article

Surface Morphology of GaN Films Grown on MoS₂/Sapphire

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Abstract: This study presents a comprehensive analysis of the epitaxial growth and surface characteristics of GaN films on 2D MoS₂/c-sapphire substrates. Reflection High Energy Electron Diffraction (RHEED) patterns demonstrate the evolution of the substrate and GaN film surfaces during growth. The subsequent growth of GaN films results in the emergence of hexagonal spots, indicative of a single crystal structure. The brightness intensifies with longer growth times, confirming the improvement in GaN crystalline quality. Atomic Force Microscopy (AFM) images provide further insights into the surface texture. The 2D MoS₂/c-sapphire substrate exhibits a textured surface, while GaN films display similar features with bright colors corresponding to GaN clusters. The Root Mean Square (RMS) surface roughness values of GaN films have a higher roughness compared to the substrate. Scanning Electron Microscopy (SEM) confirms the uniform coverage of GaN films, revealing smooth growth and organized hexagonal structures. These findings collectively demonstrate the successful epitaxial growth of GaN films on 2D MoS₂/c-sapphire substrates, providing valuable insights into their surface morphology and crystalline structure.

Keywords: Gallium Nitride; Molybdenum Disulfide; Surface Morphology, Heterostructure; Molecular Beam Epitaxy

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1. Introduction

Gallium nitride (GaN), also referred to as III-nitride, possesses remarkable attributes, including a direct and wide band gap, heightened electron mobility, high breakdown voltage, and exceptional thermal stability [1], [2]. These inherent characteristics position it as a compelling choice for any applications, such as high-performance power devices, high-brightness light-emitting diodes, and high electron mobility transistors (HEMT) [3][4], [5]. Despite its numerous benefits, the primary challenge faced by GaN lies in acquiring GaN bulk as a substrate. Typically, GaN is grown on Si and Sapphire substrates, which exhibit significant lattice differences [6], [7]. While substantial efforts have been dedicated to improving material quality on these substrates, the quest for an ideal, lattice-matched substrate for growing high-quality GaN remains ongoing. In this pursuit, molybdenum disulfide (MoS₂) emerges as a promising substrate for GaN, presenting minimal in-plane lattice mismatch [8]–[11]. Furthermore, the slight difference in the coefficient of thermal expansion between the two materials facilitates stable lattice alignment during the cooling-down process [12], [13]. Currently, researchers are directing their focus toward two-dimensional (2D) layered metal dichalcogenide (TMD), specifically MoS₂, due to its intriguing properties such as atom-scale thickness, a direct bandgap, and robust light-matter interactions [14], [15]. In devices designed with heterostructures comprising mono-MoS₂ and ultrathin GaN, exceptional optoelectronic and tunable electronic properties have been demonstrated [16], [17].

To date, limited investigations have been conducted on GaN film growth on MoS₂. Gupta et al. explored the growth of GaN on multiple layers of MoS₂ using metal-organic chemical vapor deposition (MOCVD) [15], while Tangi et al. examined the growth of GaN on monolayer MoS₂ via molecular beam epitaxy (MBE) [14]. Plasma-assisted molecular beam epitaxy (PA-MBE) stands out as a promising method for producing high-quality heteroepitaxial GaN layers due to its precision and environmentally friendly nature [18]. This technique offers several advantages, including an ultra-high vacuum (UHV) environment to prevent contaminants, in-situ monitoring enabling precise control of layer-by-layer growth, and a low growth temperature. Despite these benefits, there is a notable lack of extensive exploration into the surface morphology of GaN deposited on the 2D MoS₂ layer using PA-MBE.

In this investigation, we present an analysis of the surface morphology characteristics of GaN films grown on a 2D MoS₂ template on c-sapphire substrate, aiming to advance comprehension in this particular domain. Diverse growth times were scrutinized to discern the RHEED pattern mode types before, during, and after the growth of GaN films. In-depth examinations of both the MoS₂ template and the GaN films shed light on the surface morphology, enhancing our understanding of GaN growth on 2D MoS₂. The findings underscore the feasibility of employing PA-MBE in a hybrid GaN/MoS₂ system, showcasing the initial high-quality surface GaN formation on 2D MoS₂. This research opens up new possibilities for deploying related devices in the future.

2. Materials and Experiment Method

The experimental configuration for the growth of GaN films on the substrate (2D MoS₂/c-sapphire) is illustrated in Figure 1. 2D-MoS₂ is deposited onto the sapphire substrate using the pulsed laser deposition (PLD) technique by impinging Mo and S atoms. The layers of GaN films are synthetically cultivated on the surface composed of a 2D MoS₂/c-sapphire substrate through the utilization of the MBE ULVAC system [19-20]. The MBE chamber maintains a base pressure of 6×10^{-10} Torr, and the thermal cleaning process for the substrate occurs at 600 °C for a duration of 30 minutes. A pre-nitridation treatment on the substrate is executed at 700 °C for 5 minutes, providing a nitrogen layer conducive to the nucleation of GaN films. Subsequently, the epitaxial GaN film growth develops at 700 °C for 30 and 60 minutes. The K-cell at 800 °C supplies the atomic flux of Ga atoms, while a plasma nitrogen as N atoms source, operating at 500-Watt RF power with a 6N N₂ flux at 0.8 sccm, is employed.

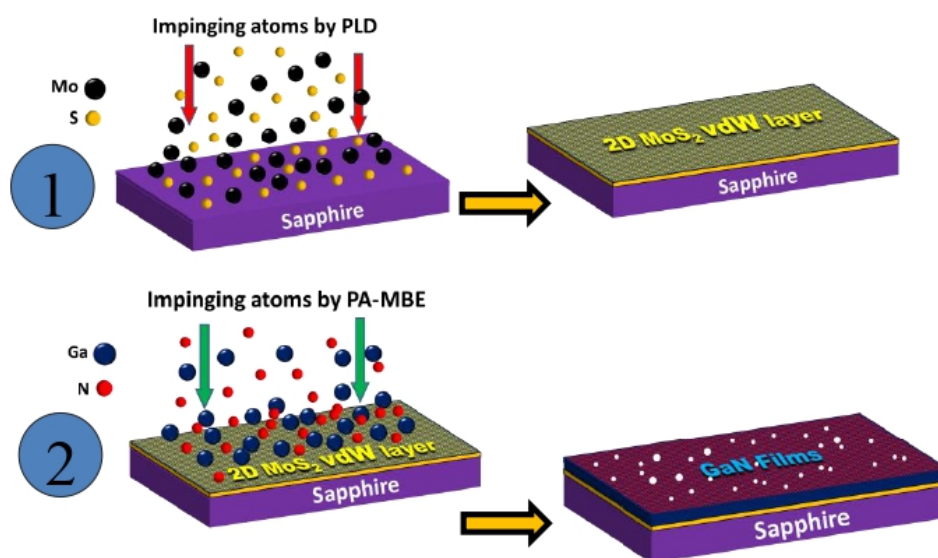


Figure 1. Growth GaN films on the substrate (2D MoS₂/c-sapphire)

Concurrently, the MoS₂ layer on a 2-inch c-sapphire substrate is generated through the Pulsed Laser Deposition (PLD) method, employing an ArF excimer laser at 800 °C

under a background pressure of 10^{-6} Torr. Throughout the growth process, in-situ characterization utilizing Reflection High-Energy Electron Diffraction (RHEED) at 20 kV monitors the structure of GaN films. Post-growth, a detailed investigation of the morphology texture of GaN films is examined using a field emission scanning electron microscope (SEM) with a 15 kV accelerating voltage. In addition, atomic force microscopy (AFM) with Nano Surf C3000 AFM was applied to observe the surface roughness.

3. Results and Discussion

Figure 2 illustrates the RHEED pattern observed during the epitaxial growth of both the substrate and GaN films. In Fig 2(a), a foggy image is indicated by a RHEED pattern evaluating the surface of substrate with low crystalline structure. After thermal cleaning process in Fig 2(b), the high-intensity streaks pattern is evident on the surface structure of 2D MoS₂/c-sapphire. This pattern is attributed to the presence of a 2D surface constructed on the MoS₂ layer, with the bright intensity corresponding to the formation of a single crystal structure within the layers. It supports that thermal treatment led to clean out the oxide deposited on the surface. The monitoring process reveals that the MoS₂ substrate possesses a 2D surface with a crystalline structure. After 30 minutes of GaN layer growth, a spots pattern emerges in the RHEED in Fig 2(c), indicating the presence of 3D GaN layers. These spots are arranged in a hexagonal pattern, pointing to the formation of a single crystal of GaN. Continuing the growth for 60 minutes, the spots exhibit brighter patterns, signifying an improvement in the crystalline quality of the GaN structure shown in Fig 2(d). The spots pattern resembles that of the previous pattern in Fig 2(c), affirming the epitaxial growth of GaN films with a consistent structure. RHEED patterns confirm the growth of single crystals with a hexagonal structure in GaN films on 2D MoS₂/c-sapphire. Further validation of the films' morphology structure will be obtained both of AFM and SEM observations.

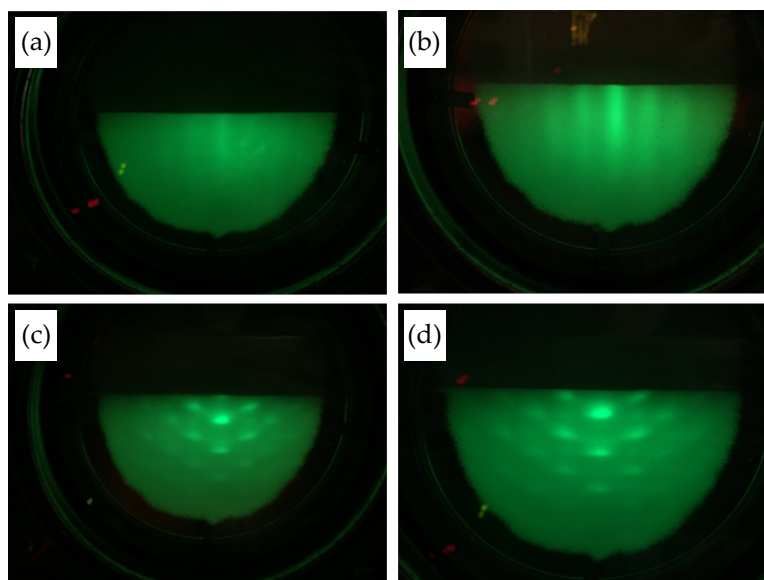


Figure 2. RHEED pattern of 2D MoS₂/c-sapphire (a), after thermal cleaning (b), grown GaN films for 30 min(c), and 60 min (d)

Fig. 3 displays Atomic Force Microscopy (AFM) images capturing the surfaces of 2D MoS₂/c-sapphire and Fig. 4 shows for GaN films. The surface scanned of 2D MoS₂ including to scan area $3 \times 3 \mu\text{m}$ in Fig 3(a), scan amplitude peak Fig 3(b), and scan mean line peak in Fig 3(c), sequentially. AFM allows for a detailed analysis of surface texture. Bright colors represent high points, indicating protrusions or elevations, while dark colors may denote depressions or lower areas. In the AFM image of 2D MoS₂/c-sapphire, brown areas, representing the average surface, provide insights into the overall texture and smoothness of the material. Line scans, as shown in Fig. 3(c), involve taking measurements along a

straight path to analyze variations in surface height or roughness. Furthermore, GaN AFM images show in Fig 4, demonstrating the similar feature to 2D MoS₂/c-sapphire. Bright colors relate to GaN clusters attending on the surface in Fig 4(a). The evidence of its presence on the surface confirmed by the higher peak shown in line scans in Fig 4(c).

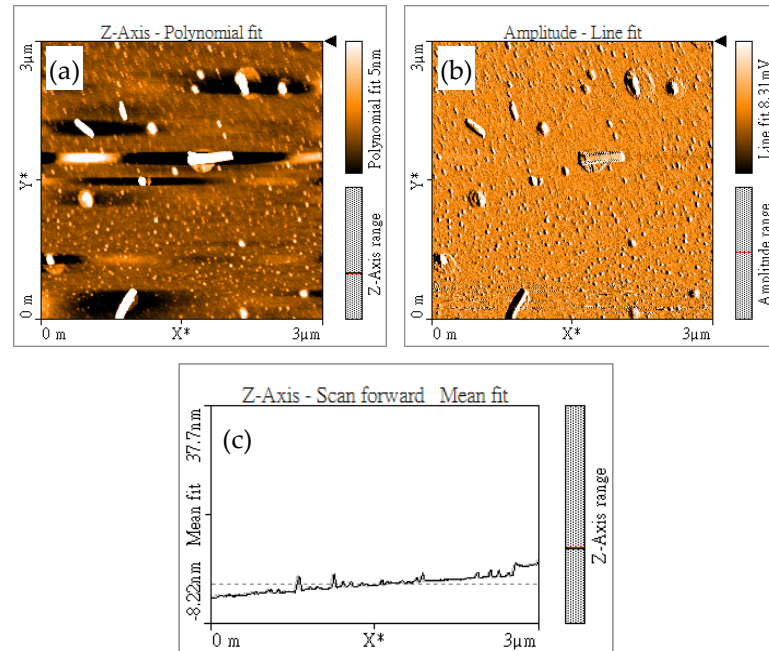


Figure 3. AFM images 2D-MoS₂/c-sapphire substrate (a). Scan area 3 × 3 μm, (b). Scan amplitude peak, (c). Scan mean line peak.

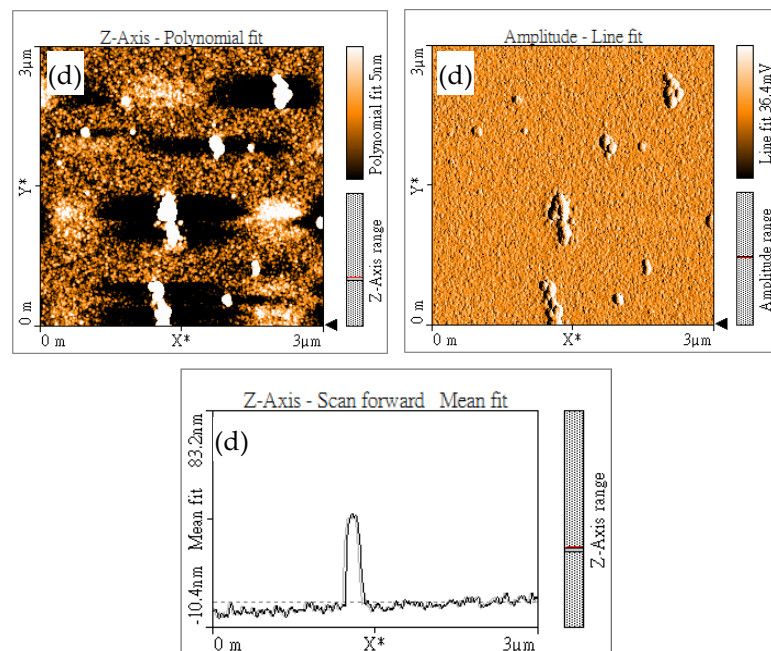


Figure 4. AFM images GaN/2D MoS₂/c-sapphire substrate (a). Scan area 3 × 3 μm, (b). Scan amplitude peak, (c). Scan mean line peak.

The Root Mean Square (RMS) surface roughness both of 2D MoS₂/c-sapphire substrate and GaN surface, calculated over scan areas of 3 μm × 3 μm. The Root Mean Square (RMS) value is a key parameter used to quantify surface roughness. In the described paragraph, the RMS value of GaN is calculated, providing a numerical measure of the surface roughness over a specific scan area. Details of surface roughness, including maximum surface

roughness (Sa), RMS, totally height (Sy), peak height (Sp) and valley depth (Sv), are provided in Table 1. AFM results are often used to compare different materials or assess the impact of specific growth processes. In the given context, a comparison between 2D MoS₂/c-sapphire and GaN films suggests that the growth of GaN films influences to an improved surface structure.

Table 1. Surface texture of substrate (2D-MoS₂/sapphire) and GaN films

No	Materials	Sa (nm)	RMS (nm)	Sy (nm)	Sp (nm)	Sv (nm)
1	Substrate 2D-MoS ₂	0.79	2.26	53.53	37.68	-15.85
2	GaN Films	2.47	5.51	90.84	72.80	-18.04

The surface morphology of the GaN film is depicted in Fig. 5 through Scanning Electron Microscopy (SEM) images at a magnification of 15,000x. The SEM observations reveal a smooth and uniform coverage of GaN films on the substrate. This smooth growth indicates comparable epitaxial coalescence between gallium (Ga) and nitrogen (N) atoms during the layer's growth process. In addition to the continuous GaN layer, hexagonal structures of GaN with sizes ranging from 0.2 to 1 micrometer are also observed on the surface. These hexagonal features suggest a well-defined and organized arrangement of GaN structures. The SEM results affirm the presence of a hexagonal structure in the GaN films, covering the 2D MoS₂/c-sapphire substrate. This observation aligns with the RHEED monitoring, indicating the generation of a single crystal with hexagonal structure of GaN films are grown on the substrate. The SEM analysis provides valuable insights into the surface characteristics and crystal structure of the GaN films, highlighting their uniformity and well-defined hexagonal features.

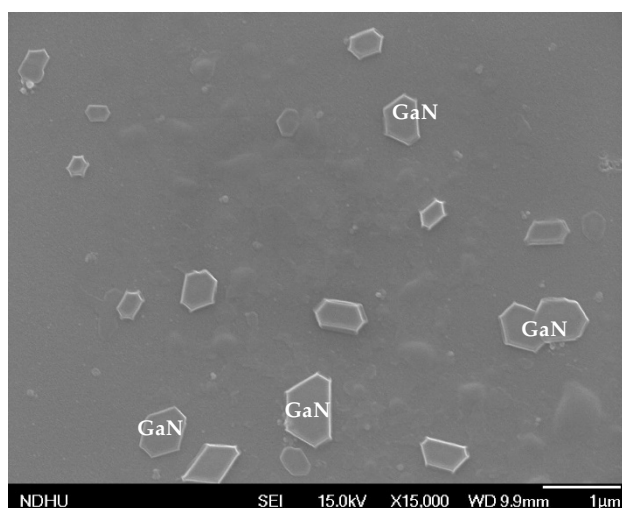


Figure 5. FE-SEM images of surface morphology of GaN films with 15.000x magnification

4. Conclusions

In conclusion, the RHEED patterns provide a comprehensive view of the epitaxial growth process. The initial foggy pattern on the substrate transforms into high-intensity streaks after thermal cleaning, indicating the emergence of a well-defined 2D MoS₂ surface. The subsequent growth of GaN films results in hexagonal spots, evolving into brighter patterns over 60 minutes, confirming the formation of single-crystal GaN structures. AFM analysis details the surface textures of 2D MoS₂/c-sapphire and GaN films. Notably, GaN exhibits bright clusters on the surface, as confirmed by line scans. The RMS surface rough-

ness values quantify the differences between 2D MoS₂/c-sapphire and GaN films, indicating that GaN films contribute to an improved surface structure. SEM images reinforce these findings, showcasing the uniform coverage of GaN films with well-defined hexagonal structures. Overall, the combined results from RHEED, AFM, and SEM analyses provide a comprehensive understanding of the growth and morphology of GaN films on the 2D MoS₂/c-sapphire substrate, highlighting their single-crystal nature and improved surface structure.

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