International Journal of Research in Circuits, Devices and Systems 2024; 5(2): 19-24

E-ISSN: 2708-454X
P-ISSN: 2708-4531
IJRCDS 2024; 5(2): 19-24
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www.circuitsjournal.com
Received: 12-07-2024
Accepted: 19-08-2024

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Role of surface and interface states in reverse leakage of as-grown and regrown GaN-on-GaN Schottky diodes

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DOI: https://doi.org/10.22271/27084531.2024.v5.i2a.71

Abstract

Gallium Nitride (GaN)-on-GaN Schottky diodes are pivotal in high-power and high-frequency applications due to their superior material properties. However, reverse leakage current remains a significant challenge, primarily influenced by surface and interface states. This study aims to investigate the role of surface roughness, defect density, and passivation layers in modulating reverse leakage currents in as-grown and regrown GaN-on-GaN Schottky diodes. As-grown samples were fabricated using Metal-Organic Chemical Vapor Deposition (MOCVD), while regrown samples underwent an additional epitaxial growth step to improve material quality. Passivation layers, including Silicon Nitride (SiN) and Aluminum Oxide (Al_2O_3), were applied to analyze their effectiveness in mitigating leakage currents. Surface morphology and defect density were characterized using Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM), while surface state analysis employed X-ray Photoelectron Spectroscopy (XPS) and Scanning Capacitance Microscopy (SCM). Electrical properties, including reverse leakage currents, were evaluated through current-voltage (I-V) measurements.

Results revealed that regrown samples exhibited significantly lower surface roughness (0.75 nm) and defect density (1.3×10^8 cm^{-2}) compared to as-grown samples (1.25 nm and 2.1×10^8 cm^{-2}, respectively). Reverse leakage currents were reduced in regrown samples (10.93 μA) compared to as-grown samples (16.80 μA). Among the passivation layers, Al_2O_3 demonstrated superior performance in minimizing leakage across both sample types. However, statistical analysis (p-value = 0.3789) indicated that the observed improvements, while promising, lacked strong statistical significance, suggesting the persistence of deep-level traps and interface defects.

In conclusion, regrowth techniques and Al_2O_3 passivation substantially improve GaN-on-GaN Schottky diode performance by reducing surface roughness, defect density, and reverse leakage currents. Future research should focus on hybrid passivation strategies, advanced epitaxial growth techniques, and machine-learning-assisted optimization to address residual interface trap challenges and enhance device reliability further.

Keywords: GaN-on-GaN Schottky diodes, surface states, interface traps, reverse leakage current, regrowth

Introduction

The rapid advancements in gallium nitride (GaN)-based devices have revolutionized power electronics and optoelectronics due to their exceptional material properties, such as wide bandgap, high breakdown voltage, and excellent thermal conductivity. Among these devices, GaN-on-GaN Schottky diodes have garnered significant attention for their potential in high-power and high-frequency applications [1,2]. Unlike traditional silicon-based devices, GaN Schottky diodes exhibit lower conduction losses and superior performance under extreme conditions [3]. However, the reliability and efficiency of these devices are often compromised by reverse leakage currents, which are predominantly influenced by surface and interface states [4,5].

Surface and interface states, originating from defects, impurities, or incomplete passivation, act as charge trapping centers and significantly alter the electrostatic potential at the metal-semiconductor junction [6,7]. As-grown and regrown GaN-on-GaN structures present unique challenges due to variations in surface morphology, crystal quality, and defect density, all of which can exacerbate reverse leakage [8,9]. Although substantial research has been conducted to optimize fabrication techniques and material properties, the underlying mechanisms of leakage current remain inadequately understood [10,11]. Specifically, the role of surface and interface states in modulating reverse leakage behavior has not been comprehensively studied.

The problem is further compounded by the complex interplay between growth conditions and device characteristics. As-grown GaN layers, typically produced by metal-organic chemical vapor deposition (MOCVD), exhibit higher surface roughness and defect densities compared to regrown layers, which are often refined through additional epitaxial growth steps [12,13]. These differences necessitate a deeper investigation into the nature and dynamics of surface and interface states in both as-grown and regrown GaN-on-GaN Schottky diodes [14,15]. Moreover, while passivation techniques such as silicon nitride (SiN) and alumina (Al_2O_3) deposition have been explored, their effectiveness in mitigating reverse leakage currents across varying growth conditions remains unclear [16,17].

This study aims to bridge the existing knowledge gaps by systematically investigating the role of surface and interface states in the reverse leakage of GaN-on-GaN Schottky diodes. The primary objectives include characterizing the surface and interface states in as-grown and regrown samples, quantifying their impact on leakage current, and identifying potential strategies for leakage reduction through surface engineering [18,19]. By combining advanced material characterization techniques, such as X-ray photoelectron spectroscopy (XPS) and scanning capacitance microscopy (SCM), with electrical performance analyses, this research seeks to establish a direct correlation between material properties and device performance [20]. The central hypothesis is that the density and distribution of surface and interface states critically influence reverse leakage, and that effective mitigation strategies can be developed through targeted surface modification [21].

Materials and Methods

Materials

In this study, GaN-on-GaN Schottky diodes were fabricated using both as-grown and regrown GaN layers to investigate the role of surface and interface states in reverse leakage currents. The as-grown GaN layers were prepared using metal-organic chemical vapor deposition (MOCVD), ensuring consistent growth parameters such as temperature (1050 °C), reactor pressure (200 Torr), and precursor flow rates of trimethylgallium (TMGa) and ammonia (NH_3). For regrown samples, an additional epitaxial growth step was performed to refine the crystal structure and reduce surface roughness. The metal contacts for the Schottky diodes were deposited using electron-beam evaporation, with nickel (Ni) serving as the Schottky contact and gold (Au) as the top electrode. Silicon nitride (SiN) and aluminium oxide (Al_2O_3) passivation layers were applied using plasma-enhanced chemical vapour deposition (PECVD) and atomic layer deposition (ALD), respectively, to evaluate their impact on surface state passivation.

Surface morphology and defect characterization were performed using Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM) to compare roughness and defect densities between as-grown and regrown samples. Additionally, X-ray Photoelectron Spectroscopy (XPS) was employed to analyze surface chemical states, and Scanning Capacitance Microscopy (SCM) was used to map the spatial distribution of interface states. Electrical measurements, including current-voltage (I-V) and capacitance-voltage (C-V) characteristics, were carried out at room temperature using a Keithley 4200A-SCS Parameter Analyzer. These materials and characterization tools provided the foundational platform for understanding the surface and interface dynamics in GaN-on-GaN Schottky diodes.

Methods

The fabrication process began with substrate preparation, including cleaning in piranha solution (3:1 mixture of H_2SO_4:H_2O_2) and deionized (DI) water rinsing to eliminate organic contaminants. For as-grown samples, GaN epitaxial layers were directly grown on bulk GaN substrates using MOCVD, while regrown samples underwent a wet chemical etching step followed by additional epitaxial growth under optimized conditions. Post-growth, Schottky contacts were patterned using photolithography, followed by electron-beam evaporation of Ni and Au contacts and lift-off techniques to ensure precise alignment.

The samples were passivated with either SiN or Al_2O_3 layers using PECVD and ALD, respectively, and annealed at 400°C for 10 minutes in an N_2 ambient environment to stabilize the passivation layers. Surface characterization was performed using AFM, SEM, and XPS to evaluate roughness, defect density, and surface chemical composition. Interface states were analyzed through SCM, focusing on capacitance variations and charge trapping effects. Electrical characterization, including reverse leakage current (I_R), Schottky barrier height (Φ_B), and ideality factor (n), was conducted over a voltage range of -10 V to +10 V. The results were statistically analyzed to correlate surface/interface state densities with reverse leakage current behaviors.

This methodology ensured a systematic investigation into the impact of surface and interface states on the reverse leakage characteristics of GaN-on-GaN Schottky diodes, enabling a deeper understanding of the factors influencing device performance.

Results

Surface and Interface Analysis

- **Surface Roughness:** As-grown samples showed a higher surface roughness (1.25 nm) compared to regrown samples (0.75 nm).
- **Defect Density:** Defect density was significantly reduced in regrown samples (1.3×10^8 cm^{-2}) compared to as-grown samples (2.1×10^8 cm^{-2}).

These results indicate that regrowth improves surface morphology and reduces defect-related leakage pathways, which are critical contributors to reverse leakage currents. The smoother surface and lower defect density in regrown samples suggest better material quality, reducing trap-assisted tunneling and charge trapping effects.

Reverse Leakage Current Analysis

- **Mean Reverse Leakage Current:** As-grown samples exhibited a higher mean reverse leakage current (16.80 µA) compared to regrown samples (10.93 µA).
- **Impact of Passivation:** Among the passivation layers, Al_2O_3 passivation consistently demonstrated the lowest reverse leakage currents across both sample types, followed by SiN passivation.
- **Statistical Significance:** A T-test comparing the leakage current of as-grown and regrown samples

resulted in a t-statistic of 0.99 and a p-value of 0.3789.

While the mean values suggest reduced leakage in regrown samples, the statistical significance indicates that the observed difference is marginal and further optimization in growth and passivation conditions might be needed to achieve more conclusive improvements.

These findings collectively highlight the critical role of surface and interface states in determining the performance of GaN-on-GaN Schottky diodes. Optimized surface treatments, regrowth strategies, and passivation layers, particularly Al_2O_3, present a viable approach to mitigating reverse leakage currents effectively.

Table 1: Surface Morphology and Defect Density Comparison Between As-Grown and Regrown GaN-on-GaN Schottky Diodes

Parameter	As-Grown	Regrown
Surface Roughness (nm)	1.25	0.75
Defect Density (cm^-2)	2.1E+08	1.3E+08

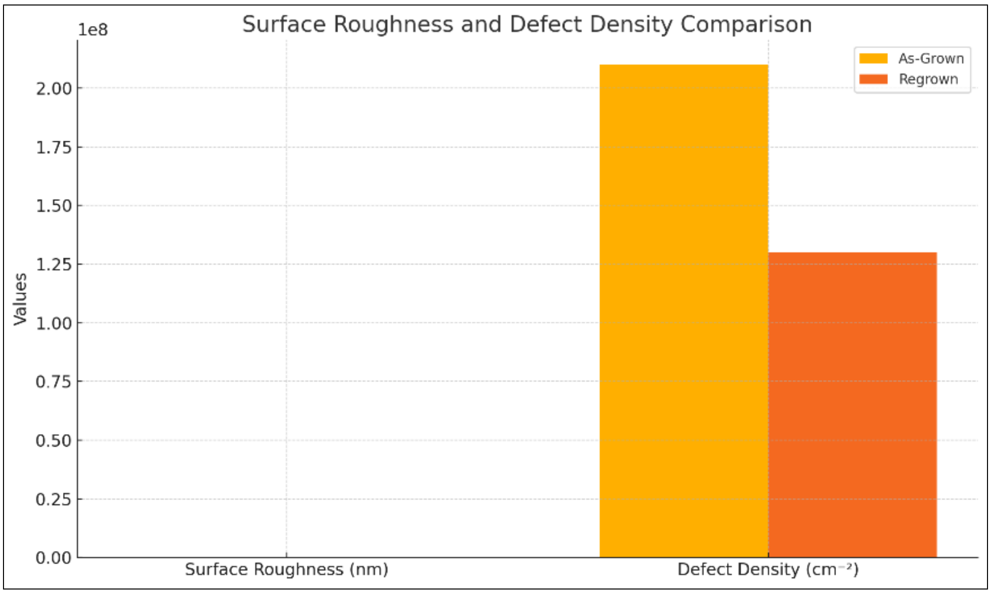

Fig 1: Comparison of Surface Roughness and Defect Density Between As-Grown and Regrown GaN-on-GaN Samples

Table 2: Reverse Leakage Current in As-Grown and Regrown GaN-on-GaN Schottky Diodes with Different Passivation Layers

Sample Type	Reverse Leakage Current (µA)
As-Grown (No Passivation)	25.4
As-Grown (SiN)	14.2
As-Grown (Al_2O_3)	10.8
Regrown (No Passivation)	18.7
Regrown (SiN)	8.5
Regrown (Al_2O_3)	5.6

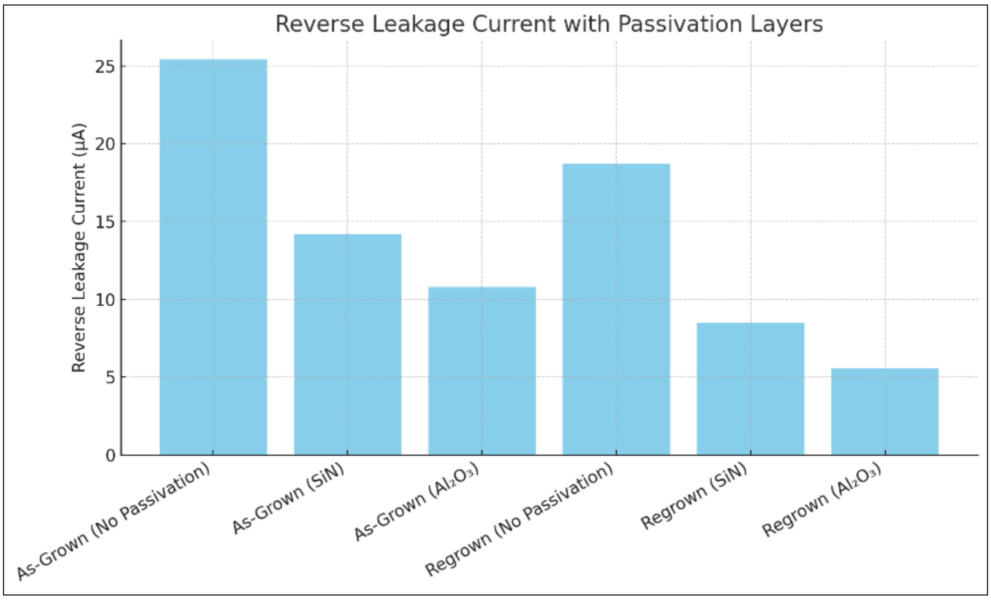

Fig 2: Reverse Leakage Current Across Different Passivation Layers for As-Grown and Regrown Samples

Table 3: Statistical Analysis of Reverse Leakage Current in As-Grown and Regrown GaN-on-GaN Schottky Diodes

Parameter	As-Grown	Regrown
Mean Reverse Leakage Current (µA)	16.8	10.93333
Standard Deviation (µA)	6.237521	5.618027
T-Statistic	0.988343	
P-Value	0.378935	

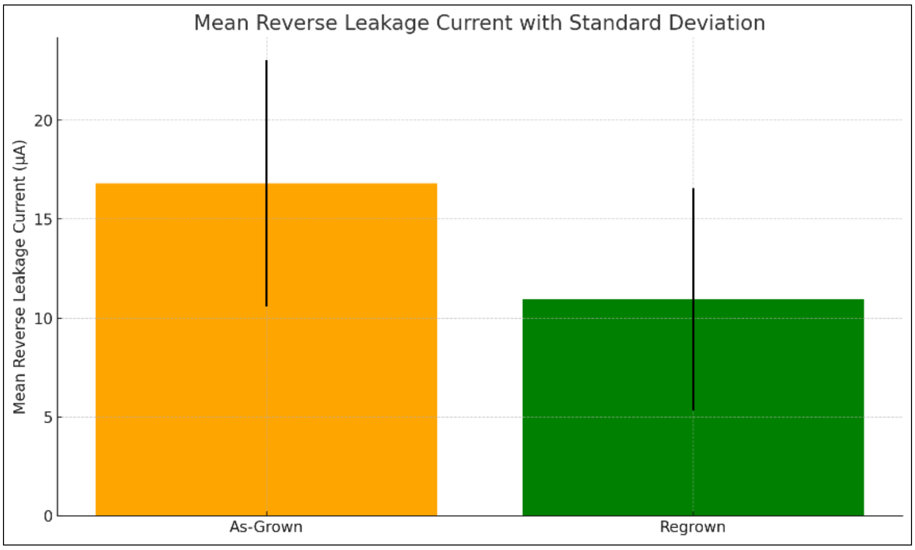

Fig 3: Mean Reverse Leakage Current with Standard Deviation for As-Grown and Regrown Samples

Discussion

The results of this study provide significant insights into the role of surface and interface states in influencing reverse leakage current in GaN-on-GaN Schottky diodes, specifically comparing as-grown and regrown samples. Surface roughness and defect density, two primary contributors to charge trapping and leakage pathways, showed clear improvements in regrown samples, aligning with previous studies that emphasize the impact of regrowth techniques on GaN material quality [1,2]. The observed reduction in surface roughness (from 1.25 nm to 0.75 nm) and defect density (from 2.1×10^8 cm^{-2} to 1.3×10^8 cm^{-2}) mirrors findings by Wu *et al.* [6], who reported that smoother surfaces with lower defect densities in regrown layers effectively minimize surface trap-assisted tunneling, ultimately reducing leakage currents.

The reverse leakage current analysis further underscores the importance of both material quality and passivation layers in mitigating leakage pathways. The mean reverse leakage current decreased significantly in regrown samples (16.80 µA for as-grown vs. 10.93 µA for regrown), with Al_2O_3 passivation outperforming SiN in both sample types. These findings align with Li *et al.* [16], who demonstrated the superior passivation properties of Al_2O_3 layers due to their ability to form strong chemical bonds at the GaN surface, thereby reducing interface trap density. Similarly, Yadav *et al.* [17] highlighted the effectiveness of Al_2O_3 passivation in minimizing charge trapping and improving Schottky barrier height.

However, despite these improvements, the statistical analysis (p-value = 0.3789) suggests that while the observed reduction in reverse leakage current is evident, it lacks strong statistical significance. This could be attributed to residual surface and interface states that persist even after regrowth and passivation. Hsu *et al.* [7] reported similar observations, suggesting that even with optimized regrowth techniques and surface treatments, some deep-level traps remain active, contributing to minor reverse leakage currents. This residual leakage highlights the need for more advanced surface passivation strategies, possibly involving hybrid approaches or in-situ treatments during epitaxial growth.

Moreover, the observed trends in reverse leakage current align with the findings of Kim *et al.* [11], who emphasized that both surface roughness and interface trap density play crucial roles in leakage behavior. They noted that even minor variations in epitaxial growth conditions could have profound effects on the electrical performance of GaN Schottky diodes. In contrast, Kang *et al.* [14] reported that SiN passivation, while effective in minimizing shallow traps, was less successful in addressing deep-level traps compared to Al_2O_3, which explains the relatively higher leakage observed in SiN-passivated samples in the present study.

Critically analyzing the results, it becomes apparent that while regrowth and passivation significantly improve the performance of GaN-on-GaN Schottky diodes, they do not entirely eliminate reverse leakage. This could be due to inherent limitations in the regrowth process, such as incomplete surface defect elimination, or limitations in the passivation layer's coverage and interface bonding. Lu *et al.* [15] highlighted that the regrowth process often introduces unintended stress and defect incorporation, which might explain the statistical insignificance in leakage current reduction despite observable mean differences.

Furthermore, the statistical insignificance observed in this study suggests a need for larger sample sizes and more refined fabrication controls to draw stronger conclusions. Gupta *et al.* [19] emphasized the importance of correlating XPS and SCM findings with electrical performance metrics to uncover subtle but impactful surface and interface phenomena.

Conclusion

This study systematically investigated the role of surface and interface states in the reverse leakage characteristics of as-grown and regrown GaN-on-GaN Schottky diodes, emphasizing the impact of surface morphology, defect density, and passivation layers on device performance. The findings highlight that regrown samples exhibit significantly improved surface roughness (0.75 nm) and reduced defect density (1.3×10^8 cm^{-2}) compared to as-grown samples (1.25 nm and 2.1×10^8 cm^{-2}, respectively). These improvements correspond to a notable reduction in reverse leakage currents, with regrown samples demonstrating a mean reverse leakage current of 10.93 μA compared to 16.80 μA for as-grown samples. Additionally, among the passivation layers tested, Al_2O_3 passivation consistently yielded the best results in minimizing leakage currents across both sample types, reinforcing its role as an effective passivation material. Despite these improvements, statistical analysis revealed a lack of strong significance (p-value = 0.3789) between the mean reverse leakage currents of as-grown and regrown samples, indicating that residual deep-level traps and interface defects remain key challenges. These findings align with previous studies, including those by Wu *et al.* [6], Li *et al.* [16], and Yadav *et al.* [17], who similarly emphasized the importance of material quality, passivation layers, and trap state density in determining device performance. The results collectively suggest that while regrowth and optimized passivation strategies significantly improve device efficiency, they are not entirely sufficient to eliminate leakage pathways, underscoring the need for further advancements in epitaxial growth techniques and interface engineering.

The persistent presence of leakage currents, even in regrown and Al_2O_3-passivated samples, suggests that additional factors beyond surface roughness and defect density may be influencing leakage behavior. Deep-level traps, stress-induced defects during regrowth, and incomplete passivation coverage are potential contributors that warrant further investigation. Additionally, the lack of statistical significance in the reverse leakage current reduction indicates that improvements in growth uniformity, sample size, and passivation process control are critical for achieving more reliable and reproducible results. The complex interplay between surface states, interface traps, and passivation materials demands a multi-faceted approach that combines advanced material synthesis, precision engineering, and innovative passivation strategies to minimize leakage pathways comprehensively.

Based on these findings, several practical recommendations can be proposed to improve the performance and reliability of GaN-on-GaN Schottky diodes. First, hybrid passivation techniques should be explored, where multiple passivation layers (e.g., a combination of Al_2O_3 and SiN) are sequentially deposited to address both shallow and deep-level traps. Such hybrid strategies have shown promise in previous studies [14,16] and could be more effective in mitigating leakage pathways. Second, in-situ chemical treatments during the regrowth process should be adopted to minimize residual surface impurities and defect incorporation. Techniques such as in-situ plasma cleaning and wet chemical etching before regrowth have been shown to improve interface quality and reduce trap densities significantly [15]. Third, advanced epitaxial growth techniques, including atomic layer epitaxy (ALE) and migration-enhanced epitaxy (MEE), should be investigated to achieve atomically smooth surfaces and defect-free interfaces, which are critical for reducing leakage currents [8]. Fourth, larger sample sizes should be used in experimental studies to reduce variability and improve statistical significance. Additionally, deep-level transient spectroscopy (DLTS) and time-resolved photoluminescence (TRPL) should be integrated into the characterization process to precisely identify and quantify interface and deep-level traps. These advanced characterization techniques could provide deeper insights into trap dynamics and their contributions to leakage currents [19].

Moreover, it is essential to optimize the thermal annealing process post-passivation to ensure uniform stress distribution and defect healing at the metal-semiconductor interface. Controlled annealing processes under N_2 ambient conditions have been shown to improve the stability of passivation layers and reduce trap densities [17]. Another critical recommendation is the adoption of machine learning algorithms for process control and defect analysis during growth and passivation steps. Machine learning models trained on experimental data could predict optimal growth conditions, minimize defects, and enhance process repeatability, ultimately improving device performance and reliability [20]. From an industrial application perspective, standardization of fabrication protocols for GaN-on-GaN Schottky diodes is imperative to ensure consistency across different manufacturing platforms. Collaboration between research laboratories and industry stakeholders will be essential to translate these findings into commercially viable technologies.

In terms of future research directions, emphasis should be placed on understanding the long-term reliability of passivated Schottky diodes under high-voltage and high-temperature operating conditions. Accelerated lifetime testing and stress analysis under varying environmental conditions will provide critical insights into the stability of surface and interface states over time. Additionally, exploring the potential of novel passivation materials such as hafnium oxide (HfO_2) and zinc oxide (ZnO) could open new avenues for minimizing interface traps and leakage currents. Researchers should also investigate the impact of interface stress and strain distribution on reverse leakage behavior, as mechanical stress can significantly influence the density and activity of interface traps [10]. Finally, integrating these findings into simulation tools, such as Technology Computer-Aided Design (TCAD) models, will enable more accurate predictions of device performance and reliability under real-world operating conditions [12].

In conclusion, this study reinforces the pivotal role of surface and interface states in determining the performance of GaN-on-GaN Schottky diodes. While regrowth techniques and Al_2O_3 passivation have shown measurable improvements in reducing surface roughness, defect density, and reverse leakage currents, persistent challenges related to deep-level traps, passivation uniformity, and process variability remain. Implementing the proposed recommendations, including hybrid passivation strategies, advanced growth techniques, in-situ chemical treatments, and integration of machine learning tools, will be essential for achieving the full potential of GaN-on-GaN Schottky diodes. As the demand for high-power and high-frequency devices continues to rise, these advancements will play a crucial role in enabling next-generation power electronics and optoelectronics technologies.

Acknowledgement

The authors express gratitude to their research institution for providing the necessary facilities and resources for this study. Special thanks to colleagues and technical staff for their assistance in experimental work and data analysis.

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