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Electrical Characterization and Modeling of Reverse Leakage in Cubic and Hexagonal GaN Schottky Diodes

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Abstract

This work investigates reverse leakage current in Ni/Au Schottky diodes based on cubic GaN (c-GaN) and hexagonal GaN (h-GaN) using experimental characterization and technology computer-aided design (TCAD) simulations. Simulations were performed in Silvaco Victory Device using Shockley–Read–Hall recombination, Fermi–Dirac statistics, Schottky tunneling, and barrier-lowering effects to assess their ability to reproduce the measured reverse current–voltage (I–V) characteristics. The simulated results did not fully reproduce the experimental behavior, and variations in trap density and interface charge had a limited effect on the calculated leakage current within the investigated parameter ranges. The measured reverse current exhibited an approximately linear dependence on reverse voltage, which was not adequately described by the conventional transport models considered. An equivalent shunt resistance was therefore introduced to represent this non-ideal behavior, resulting in improved agreement between

simulation and experiment. These findings highlight the limitations of the investigated transport models and the potential utility of an equivalent shunt resistance representation for modeling reverse leakage in c-GaN and h-GaN Schottky diodes.

Keywords: c-GaN/h-GaN; Schottky barrier diodes; Reverse leakage current; TCAD simulation; Equivalent shunt resistance.

1 Introduction

Gallium nitride (GaN) Schottky diodes are attractive for high-power and high-frequency applications because of their wide bandgap, high critical electric field, and potential for fast switching operation [1, 2]. Among the two main crystal structures of GaN, cubic GaN (c-GaN), which adopts the zinc-blende structure, is of interest because it does not exhibit the spontaneous and piezoelectric polarization effects characteristic of the conventional polar orientation of hexagonal GaN (h-GaN) [3]. Nevertheless, the electrical performance of GaN Schottky diodes depends not only on the crystal structure but also on the semiconductor quality and the metal–semiconductor interface. In particular, reverse leakage current remains an important concern because it can limit device performance and increase power dissipation [4–6].

In an ideal Schottky diode, current transport is commonly described using thermionic emission theory [7]. However, experimental studies of GaN Schottky contacts have reported deviations from ideal thermionic-emission behavior, particularly under reverse bias [4–6, 8]. Depending on the device structure and operating conditions, possible contributions to reverse leakage include thermionic-field emission, tunneling, interface-state-assisted transport, and spatial variations in the Schottky barrier height [9–12]. These mechanisms may be influenced by surface conditions, structural defects, and dislocations. Consequently, the measured reverse current cannot always be described adequately by an ideal metal–semiconductor transport model alone.

The comparison between c-GaN and h-GaN Schottky diodes is therefore relevant for understanding how crystal structure, material properties, and interface conditions affect their electrical characteristics. Although the absence of the conventional spontaneous polarization along the c-axis in zinc-blende GaN distinguishes it from polar wurtzite GaN, this structural difference does not, by itself, guarantee lower reverse leakage. Indeed, Schottky diodes fabricated on c-GaN have also exhibited substantial deviations from ideal transport, including leakage associated with the metal–semiconductor interface [8, 13, 14]. The reverse-current behavior must therefore be evaluated experimentally rather than inferred solely from the crystal phase.

Technology computer-aided design (TCAD) simulations provide a framework for evaluating the contribution of semiconductor properties, junction electrostatics, and carrier-transport models to the current–voltage characteristics of Schottky diodes. Nevertheless, discrepancies may remain between simulated and measured currents when the implemented models do not fully represent the processes contributing to

leakage in a fabricated device. In such cases, an equivalent circuit containing a parallel conductance can provide a practical means of representing current contributions not captured by the primary diode model. Parallel conductance has previously been considered in the parameter extraction and analysis of non-ideal Schottky diodes [15]. In the present context, an equivalent shunt branch can be used phenomenologically to represent the residual current, without assuming that it corresponds uniquely to a specific microscopic conduction mechanism.

In this work, the current–voltage characteristics of Ni/Au Schottky diodes fabricated on c-GaN and h-GaN are compared experimentally. The reverse leakage current of the c-GaN diode is then investigated using TCAD simulations implemented in Silvaco Victory Device [16]. The selected transport models are evaluated by comparing the simulated current with the experimental data over the measured reverse-bias range. Because the conventional TCAD calculation does not fully reproduce the measured reverse current, a voltage-dependent equivalent shunt resistance is introduced in parallel with the simulated Schottky-diode contribution. The resulting model is assessed in terms of its ability to represent the experimental current–voltage characteristics. The objective is to evaluate the limitations of the implemented TCAD description and the usefulness of an equivalent shunt-current model, rather than to assign the measured leakage to a unique microscopic mechanism.

2 Experimental details

The cubic GaN (c-GaN) films investigated in this study were grown by metalorganic chemical vapor deposition (MOCVD) on GaP (100) substrates, following the growth procedure described in our previous work [17, 18]. The films belong to the growth batch studied in [18], in which the crystalline phase, structural quality, and surface morphology were characterized. In addition, structural and spectroscopic characterization of c-GaN films grown on different substrates has shown that the substrate influences their structural quality, with improved characteristics reported for films grown on GaP compared with those grown on GaAs [17].

The donor concentration of the c-GaN sample used for device fabrication was determined by Hall-effect measurements. Measurements were performed on multiple samples from the same growth batch, including the sample used to fabricate the Schottky diodes. The measured donor concentration adopted in the TCAD simulations was $N_D = 5 \times 10^{17}\,\mathrm{cm}^{-3}$.

For comparison, hexagonal GaN (h-GaN) films were grown by MOCVD on sapphire using the growth system described in [17, 19]. Schottky diodes based on both GaN phases were fabricated using nominally identical contact geometries and metallization schemes to facilitate comparison of their current-voltage characteristics.

Before metallization, the samples were cleaned in an ultrasonic acetone bath and subsequently treated with a diluted hydrochloric acid solution for 10 s to remove surface oxides. The HCl-to-water volume ratio was 1:2. Ohmic contacts were deposited first and consisted of Ti (30 nm)/Al (150 nm)/Ti (30 nm)/Au (200 nm). The contacts were annealed at 500 °C for 2 min under a nitrogen atmosphere [10]. The Schottky

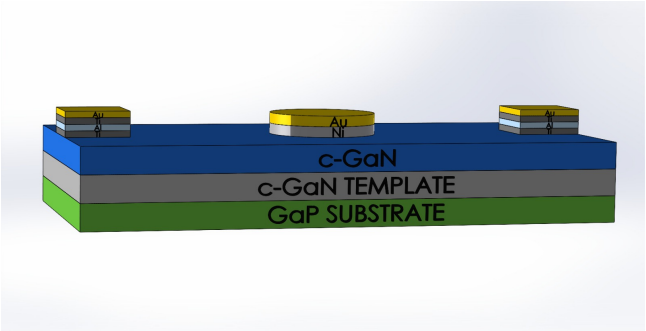


Fig. 1: Schematic cross-sectional representation of the layers of the c-GaN Schottky diode.

contacts were deposited after this annealing step to prevent the Ni/Au barrier metallization from being exposed to the high-temperature treatment. They consisted of Ni (40 nm)/Au (200 nm), with a circular contact diameter of 2 mm. The ohmic contacts had a nominal area of $2 \times 2\,\mathrm{mm}^2$, and the separation between the Schottky and ohmic contacts was 1.5 mm. All metal layers were deposited through shadow masks. Ti, Au, and Ni were deposited using a UNIVEX 300 Leybold evaporation system, whereas Al was deposited using an Edwards E306 system. The same fabrication sequence was used for the c-GaN- and h-GaN-based devices.

Figure 1 shows a schematic cross-sectional representation of the fabricated GaN Schottky diode, including the semiconductor layer and the corresponding metal-contact stacks.

The current–voltage (I–V) characteristics were measured at room temperature using a Keithley 4200-SCS semiconductor characterization system and a probe station housed in a dark enclosure to minimize the influence of ambient illumination. The applied voltage was swept from -1 to $+3$ V to characterize the reverse- and forward-bias behavior. The reverse-bias analysis was restricted to the experimentally measured range, from 0 to -1 V. The same measurement procedure was applied to the diodes fabricated on c-GaN and h-GaN.

TCAD simulation

The electrical characteristics of the c-GaN Schottky diode were simulated using Silvaco Victory Device. The simulated structure consisted of an n-type c-GaN layer with a Ni/Au Schottky contact and a Ti/Al/Ti/Au ohmic contact. The donor concentration was set to $N_D = 5 \times 10^{17}\,\mathrm{cm}^{-3}$, based on Hall-effect measurements performed on the sample used for device fabrication. The c-GaN bandgap energy was set to $E_g = 3.2\,\mathrm{eV}$, consistent with the value reported in [17].

The simulation geometry and contact configuration were defined to represent the experimentally fabricated device. The transport model included Shockley-Read–Hall (SRH) recombination and Fermi-Dirac statistics. Schottky-contact tunneling, including thermionic-field emission (TFE) and barrier-lowering effects, was also considered

where applicable to the selected model configuration. Trap density and fixed interface charge were investigated to assess their influence on the simulated current-voltage characteristics.

The simulated reverse current was compared with the experimental data over the measured bias range. This comparison was used to evaluate whether the conventional transport models and selected material and interface parameters could reproduce the measured reverse current. The limitations of the simulated results were then assessed before introducing an additional equivalent shunt-current contribution to the model.

3 Results and Discussion

Figure 2 compares the experimental current–voltage (I-V) characteristics of Schottky diodes fabricated on cubic GaN (c-GaN) and hexagonal GaN (h-GaN). Both devices exhibit rectifying behavior under forward bias, consistent with the formation of Schottky contacts on the two crystal structures. The forward current differs by approximately one order of magnitude between the devices. A more pronounced difference is observed under reverse bias, where the leakage current of the h-GaN diode is approximately three orders of magnitude higher than that of the c-GaN diode under comparable bias conditions. This behavior is consistent with previous reports on reverse leakage in c-GaN-based Schottky diodes [14, 20].

The experimental results establish a substantial difference in reverse conduction between the two devices. However, the measured current-voltage characteristics alone do not identify the physical origin of this difference. Variations in defect populations, interface properties, and local conduction paths may contribute to the observed behavior, but further analysis is required to assess their roles. Therefore, the subsequent investigation focuses on the c-GaN diode and evaluates whether conventional transport models can reproduce its measured reverse current using technology computer-aided design (TCAD) simulations.

Figure 3 shows the device structure implemented in Silvaco Victory Device for the TCAD simulation of the c-GaN Schottky diode. The simulated device consists of a uniformly doped n-type c-GaN layer with a donor concentration of $N_D = 5 \times 10^{17}\,\mathrm{cm}^{-3}$, a Ni/Au Schottky anode, and a Ti/Al/Ti/Au ohmic cathode. The geometry and contact configuration were defined to represent the experimentally fabricated device, and the material parameters were selected according to the experimental characterization and the assumptions described in the previous section. The simulations were used to evaluate the contribution of conventional transport models to the measured reverse-bias current before considering an additional equivalent leakage contribution.

The initial comparison between the simulated and experimental characteristics showed that the conventional transport model substantially underestimated the measured reverse leakage current. The simulated current was several orders of magnitude lower than the experimental value over the reverse-bias range considered. This discrepancy indicates that the transport processes and parameter values included in the baseline simulation were insufficient to reproduce the measured reverse conduction under the conditions investigated. Similar challenges in describing leakage currents

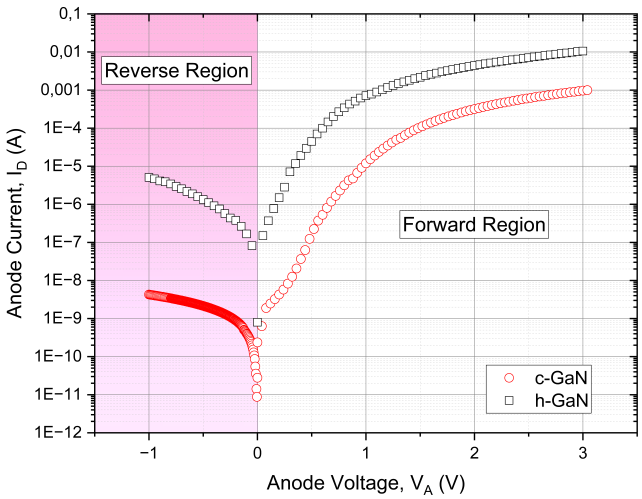


Fig. 2: Measured current-voltage (I-V) characteristics of Ni/Au c-GaN and h-GaN diodes.

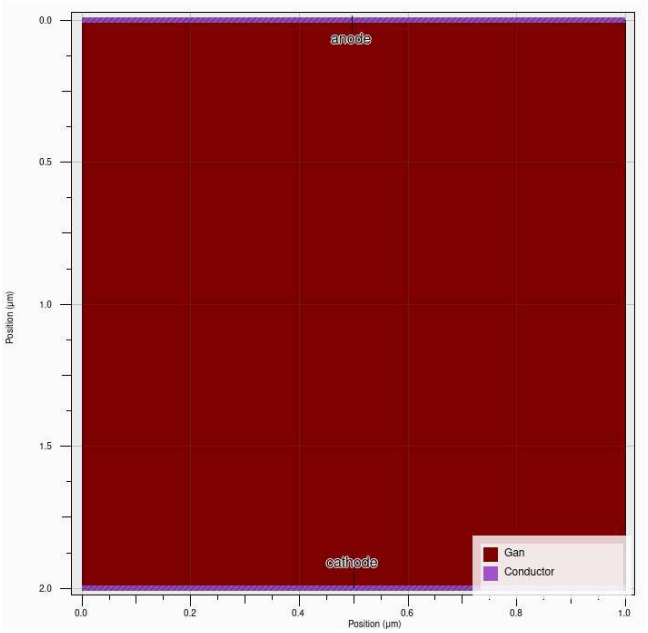


Fig. 3: TCAD structure implemented in Silvaco Victory Device for the simulation of the c-GaN Schottky diode. The simulated device consists of a uniformly doped n-type c-GaN layer with Ni/Au Schottky anode and Ti/Al/Ti/Au ohmic cathode contacts. The structure includes experimentally calibrated material parameters and physical models for reverse-bias transport analysis.

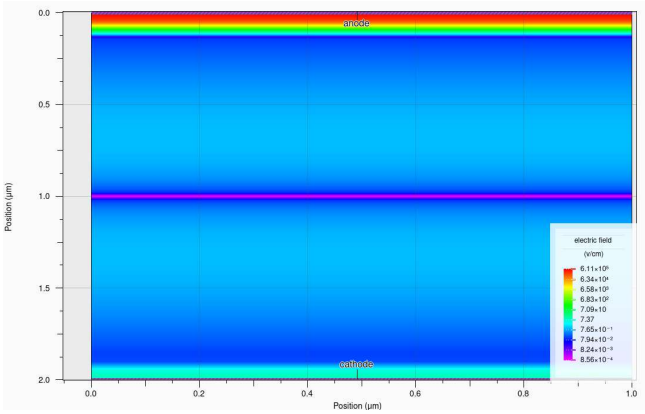


Fig. 4: Simulated conduction- and valence-band profiles of the c-GaN Schottky diode under equilibrium conditions (0 V) and reverse bias (-1 V). The band bending near the Schottky anode illustrates the formation of the depletion region and the modification of the interfacial potential under reverse bias.

in GaN-based Schottky structures have motivated the examination of additional transport contributions and non-ideal device behavior [11].

Rather than assigning this discrepancy to a specific microscopic mechanism, the following analysis examines whether an equivalent shunt-current contribution can represent the residual current not captured by the baseline TCAD model. This approach provides a phenomenological means of improving the agreement between simulation and experiment, while distinguishing the measured electrical behavior from the underlying physical mechanism, which cannot be established from the current-voltage data alone.

Figures 4 and 5 show the simulated band profiles of the c-GaN Schottky diode under equilibrium conditions and reverse bias. The band bending near the Schottky anode is consistent with the formation of a depletion region at the metal–semiconductor interface. Under reverse bias, the applied voltage modifies the band bending in the vicinity of the contact, while the conduction-band profile becomes comparatively flat farther from the interface, consistent with the quasi-neutral region of the n-type GaN layer. Figure 5 provides a magnified view of the interfacial region to facilitate examination of the Schottky barrier under the two bias conditions.

The simulated band profiles provide insight into the electrostatic conditions near the Schottky contact under reverse bias. The resulting band bending may influence field-assisted transport processes, including thermionic-field emission and tunneling, depending on the barrier properties and local electric field [11]. Nevertheless, the band profiles alone do not establish which mechanism dominates the measured reverse current. In particular, the baseline TCAD simulation substantially underestimates the experimental reverse current, even though it accounts for the electrostatic behavior of the Schottky junction.

The experimental current-voltage characteristics therefore suggest that the transport processes represented in the baseline simulation are insufficient to reproduce the

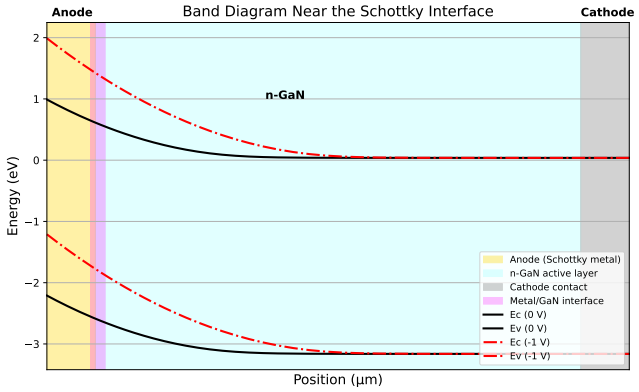


Fig. 5: Magnified simulated band diagram near the Schottky interface, showing the conduction- and valence-band profiles under equilibrium conditions (0 V) and reverse bias (-1 V). The figure highlights the metal/GaN interface and the Schottky barrier region, where reverse bias modifies the band bending and the conditions for carrier transport.

measured reverse conduction. An approximately linear dependence of reverse current on applied voltage can be consistent with an additional resistive leakage contribution; however, this behavior alone does not uniquely identify its microscopic origin. Accordingly, an equivalent shunt resistance is introduced in the following analysis as a phenomenological contribution to represent the current not captured by the baseline TCAD model [21]. This approach allows the measured current to be analyzed without assigning the residual leakage to a specific defect or transport mechanism that has not been independently established.

Figure 6 compares the experimental reverse current of the c-GaN Schottky diode with the TCAD-simulated Schottky contribution, the equivalent shunt current, and the total modeled current. Fig. 6 (top) shows the reverse I-Vcharacteristic in a linear scale, where the experimental current exhibits an approximately linear dependence on reverse voltage. The TCAD Schottky contribution alone underestimates the measured current over most of the reverse-bias range and does not reproduce the experimental slope. Therefore, an additional shunt leakage component was introduced to account for parasitic conduction paths.

The simulated band profiles indicate that reverse bias modifies the electrostatic potential and enhances the electric field near the Schottky contact. These conditions can facilitate field-assisted transport processes, including thermionic-field emission and tunneling, depending on the barrier properties and local electric field [11, 22]. However, an enhanced electric field does not, by itself, establish that these processes dominate the measured reverse current.

The Schottky tunneling models evaluated in Silvaco Victory Device increased the simulated reverse-current magnitude, but the resulting current–voltage characteristics remained strongly nonlinear compared with the approximately linear dependence

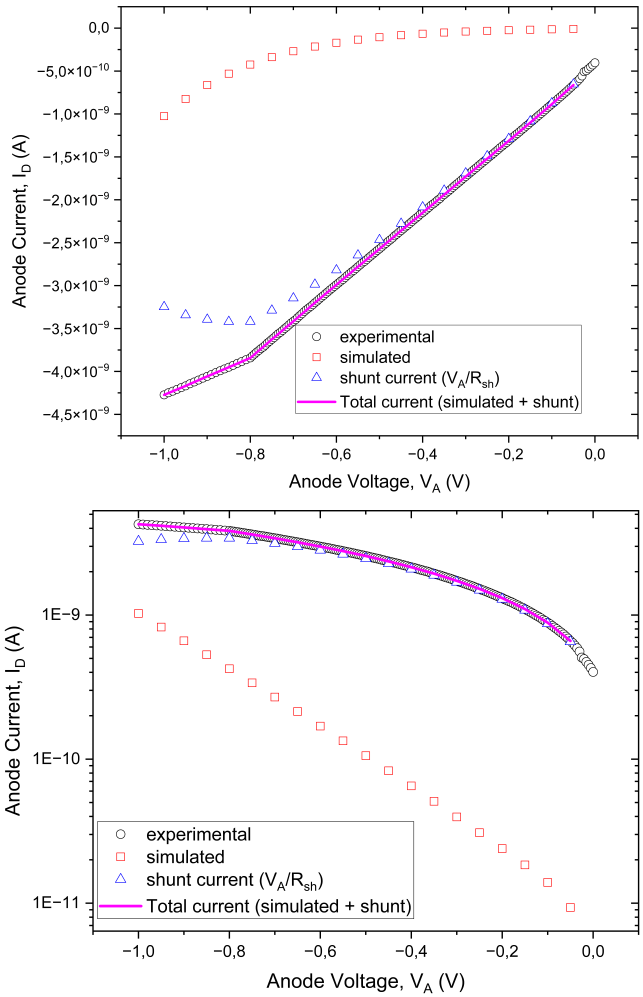


Fig. 6: Reverse current analysis of the c-GaN Schottky diode: (top) linear-scale comparison between experimental data, TCAD Schottky simulation, equivalent shunt current, and total modeled current; (bottom) semilogarithmic representation of the same data. The total current, obtained as in Eq. (2), reproduces the experimental reverse leakage behavior, indicating the presence of parasitic shunt leakage paths in addition to the Schottky contribution.

observed experimentally over the investigated reverse-bias range. Furthermore, variations in bulk trap density and fixed interface charge produced limited changes in the simulated current within the parameter ranges investigated. These results indicate that the transport descriptions and parameter variations considered here were insufficient to reproduce the measured reverse-current characteristics. They do not exclude contributions from defect- or interface-related processes.

To improve the representation of the measured current, an equivalent shunt branch was introduced in parallel with the Schottky-junction branch. Parallel conductance has previously been considered in Schottky diode analysis and parameter extraction [15]. In the present study, the shunt branch is treated as a phenomenological circuit contribution that accounts for the residual current not reproduced by the TCAD model.

A voltage-dependent shunt resistance was considered because a constant resistance did not adequately reproduce the measured current variation over the investigated bias range. The effective resistance was represented by

$$R_{\mathrm{sh}}(V_A) = R_0 \exp(-\alpha |V_A|) \tag{1}$$

where (R_0) is the extrapolated shunt resistance at zero applied voltage and (α) is an empirical parameter describing its voltage dependence. This expression is intended to represent the observed bias dependence of the residual current; it is not a microscopic transport law. The sign and fitted parameters must be consistent with the experimental data and the implemented current model.

The total modeled current was calculated as

$$I_{\mathrm{total}}(V_A) = I_{\mathrm{TCAD}}(V_A) + I_{\mathrm{sh}}(V_A) \tag{2}$$

where

$$I_{\mathrm{sh}}(V_A) = \frac{V_A}{R_{\mathrm{sh}}(V_A)} \tag{3}$$

The voltage and current signs follow the convention used for the experimental and simulated data.

Figure 6 compares the measured reverse current with the TCAD contribution, the equivalent shunt current, and the resulting total current. The linear-scale plot illustrates the difference between the experimental current and the TCAD-only result, whereas the semilogarithmic plot facilitates comparison across the measured current range. Incorporating the shunt contribution improves the agreement between the total modeled current and the experimental trend over the investigated reverse-bias range, down to -1 V, although some discrepancies remain.

The extracted shunt resistance is on the order of 10^8 Ω. For a constant resistance of this magnitude, a voltage drop of approximately 1 V would correspond to a current of about 10 nA. In the present model, however, the shunt resistance decreases with increasing reverse-bias magnitude, and therefore the actual shunt current depends on the applied voltage. The extracted resistance should consequently be interpreted as an effective circuit parameter representing the additional leakage contribution required to reproduce the experimental characteristics, rather than as a direct measurement of defect density or evidence of a specific microscopic conduction path.

Possible physical origins of non-ideal leakage in Schottky devices include spatial variations in barrier height, as described by the Schottky barrier patch model [12], surface-related conduction, and defect-associated transport. Recent experimental studies of GaN Schottky barrier diodes have identified trap-assisted tunneling (TAT) and variable-range hopping (VRH) as possible reverse-leakage mechanisms under different

temperature conditions [23]. Threading dislocations and associated defects have also been investigated as potential contributors to leakage in GaN-based devices [24, 25]. These mechanisms provide a plausible physical context for the non-ideal current observed in the present study. However, because the measurements and modeling performed here do not independently resolve the microscopic transport mechanisms, no specific mechanism can be identified as the dominant source of leakage in the c-GaN diodes investigated.

The structural properties of the c-GaN films used in this study provide additional context for interpreting the measured leakage current. As reported in our previous work [18], the same film batch was subjected to structural and morphological characterization, including an evaluation of its crystalline quality and dislocation density. The films exhibited good crystalline quality, although the presence of structural defects cannot be ruled out. Nevertheless, the structural characterization reported in [18] does not, by itself, establish a direct relationship between the measured dislocation density and the reverse leakage current of the Schottky diodes investigated here.

Overall, the results show that the conventional transport models evaluated in this study do not fully reproduce the measured reverse current of the c-GaN Schottky diode. Introducing a voltage-dependent equivalent shunt branch improves the representation of the experimental characteristics within the investigated bias range. The main contribution of this approach is to demonstrate how an equivalent parallel leakage component can account for the residual current not captured by the implemented TCAD transport description, without requiring an unsupported assignment to a unique microscopic leakage mechanism.

4 Conclusions

The TCAD analysis showed that the conventional transport models evaluated in this study did not fully reproduce the measured reverse leakage current of the fabricated c-GaN Schottky diode. Although the inclusion of Universal Schottky Tunneling (UST) and barrier-lowering effects increased the simulated reverse current, the resulting current–voltage characteristics exhibited a nonlinear dependence that did not adequately reproduce the experimentally observed behavior.

To address this discrepancy, a phenomenological parallel shunt branch with a voltage-dependent resistance was introduced. Combining this contribution with the TCAD-simulated current improved the agreement with the experimental reverse current–voltage characteristics over the investigated bias range, down to -1 V. These results demonstrate that an equivalent shunt component can provide a practical circuit-level representation of the residual leakage current not captured by the implemented transport models.

Defect-assisted transport, surface-related conduction, and spatial variations in Schottky-barrier height are possible origins of non-ideal reverse leakage. However, the present current–voltage analysis does not identify the dominant microscopic mechanism. The extracted shunt resistance should therefore be interpreted as an effective circuit parameter rather than direct evidence of a specific conduction process. Overall, this work highlights the limitations of the evaluated TCAD transport models in

describing reverse-bias conduction and demonstrates the usefulness of an equivalent-circuit approach for representing the residual leakage current in c-GaN Schottky diodes.

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CRediT

Y. Hernandez Barrios: Conceptualization, methodology, Formal analysis, Writing & Original Draft, Writing - Review & Editing. **J.A.Santis Espinosa:** Conceptualization, Validation, Formal analysis, Supervision, Project administration,Writing review & editing. **J.G. Sánchez López:** Data Curation, review and editing, Visualization. **Samuel Cruz:** Data Curation, Supervision, review & editing,Visualization. **S. Garduño Vértiz:** Data Curation, Supervision, review & editing,Visualization.

All authors reviewed and approved the final version of the manuscript.

data

The data that support the findings of this study are available from the corresponding author upon reasonable request.

supplementary data

No supplementary data are available for this article.

Declarations

This article does not contain any studies with human participants or animals performed by any of the authors. Therefore, ethical approval and consent are not applicable. Ethics, consent to participate, and consent to publish declarations Not applicable.

Competing interests

The authors declare no competing interests

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