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Special Issue Reprint

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# Recent Advances in III-Nitride Semiconductors

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Edited by  
Peng Chen and Zhizhong Chen

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Editors

**Peng Chen**

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This is a reprint of articles from the Special Issue published online in the open access journal *Crystals* (ISSN 2073-4352) (available at: [https://www.mdpi.com/journal/crystals/special\\_issues/nitride\\_semiconductors\\_2](https://www.mdpi.com/journal/crystals/special_issues/nitride_semiconductors_2)).

For citation purposes, cite each article independently as indicated on the article page online and as indicated below:

Lastname, A.A.; Lastname, B.B. Article Title. <i>Journal Name</i> <b>Year</b> , <i>Volume Number</i> , Page Range.
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**ISBN 978-3-0365-8624-3 (Hbk)**

**ISBN 978-3-0365-8625-0 (PDF)**

**[doi.org/10.3390/books978-3-0365-8625-0](https://doi.org/10.3390/books978-3-0365-8625-0)**

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# About the Editors

## **Peng Chen**

Dr. Chen received his Ph.D. in Physics from Nanjing University in December 2000. From 2001 to 2007, he served as a Research Scientist and Principal Investigator at the Institute of Materials Research, Singapore S&T Research Agency, and a doctoral supervisor at the Department of Electrical and Computer Engineering, National University of Singapore. In 2007, he joined the Department of Physics at Nanjing University as a professor. He won the title of “Young and Middle-Aged Experts with Outstanding Contributions” in Jiangsu Province in 2010. In 2011, he won the “Outstanding Contribution Award” of “333 Talents Project” and the “Innovation Individual Award of China Industry-University Research”. He has been in charge of several international collaboration projects. As the Principal Investigator, he was in charge of the national “863” key project “Third Generation Semiconductor Devices and Evaluation Technology”, and also in charge of or participated in a number of National Basic Research Program, the National Natural Science Foundation of China and other major research projects. He has applied for more than 90 international and national patents. A total of more than 230 research papers have been published, of which more than 200 are cited in the SCI, including more than 40 high-level papers published by the first author or corresponding author in the fields of semiconductor optoelectronics, including in *Advanced Materials*, *Advanced Optical Materials*, *Small*, *IEEE Electron Device Letters*, *Applied Physics Letters* and *IEEE Photonics Journal*. He also participated in the compilation of four academic books.

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Dr. Zhizhong Chen received his Ph.D. in Physics from Nanjing University in 2000. From 2000 to 2002, he was a postdoctoral fellow at the postdoctoral flow station in condensed matter physics, Peking University, and as a Senior Engineer in LED Chip Department, Shanghai Blue Light Technology Co., Ltd. From 2002, he worked at the Institute of Condensed Matter Physics, School of Physics, Peking University and as an Associate Professor since 2004. In February 2005, he was a short-term visiting scholar at the Institute of High Energy Particles at the University of Leuven in Belgium. He also was a visiting scholar at the Institute of Optoelectronics, Strathclyde University, UK, from August 2009 to August 2010. He has been in charge of or participated in a number of national “973” and “863” projects, as well as the National Natural Science Foundation of China, the key research and development projects of Beijing and other major research projects. He has applied for more than 50 national patents. A total of more than 180 research papers have been published, including high-level papers published by the first author or corresponding author in the fields of semiconductor optoelectronics, including in *Applied Physics Letters*, *Optical Express*, *Scientific Reports* and *IEEE Photonics Journal*, which have been cited more than 2000 times.



# Preface

Dear colleagues,

Group-III nitrides, viz, GaN, InN, AlN and their compounds, are typical direct bandgap semiconductor materials. Interest in group-III nitrides stems from their irreplaceable and efficient blue UV luminescence capability. By adjusting the material composition of the alloy, the bandgap of the compound semiconductors formed by the group-III nitrides can be continuously changed from 0.7eV (InN) to 6.2eV (AlN), and its emission wavelength can cover from the near-infrared to the deep ultraviolet (UV) band wavelength range. Therefore, III-nitride semiconductors are considered the most suitable materials for green to deep ultraviolet (DUV) and white light sources. These solid-state light sources have spurred new developments in various fields including high-density optical storage, water treatment and biochemical detection. At present, many studies have been carried out on the development of light-emitting diodes and laser devices in the deep ultraviolet DUV spectral range below a 280 nm wavelength. Realizing laser emission at such a short wavelength requires high-quality materials with good internal quantum efficiency (IQE) and an appropriate cavity structure. Recent progress in GaN-based material quality and device design relies on well-mastered techniques of material growth and the formation of desired structures with other elements. This offers a significant possibility of creating high-quality materials and diverse functional devices.

GaN is also a promising candidate for next-generation power electronic applications because of its outstanding material properties, but its potential is far from being realized. Regarding whether GaN can be competent in the field of ultra-high voltage (UHV, >10 kV) applications, there is currently a huge controversy in the community, especially under the strong background of SiC in this field, although GaN has a farther limit than SiC based on the nature of the materials.

Therefore, this Special Issue includes 16 excellent works, covering a broad spectrum of topics from the study of materials, micro/nano structures and novel functional devices, to new applications in frontier fields. The topics include, but are not limited to:

- Growth of GaN-based materials and micro/nanostructures;
- Characterization of the materials and heterostructures;
- GaN-based novel devices, including emission, detection and power devices;
- Application and integration of other wide-bandgap materials and novel devices in novel electronics and photonics.

We believe that this Special Issue will contribute to the learning and communication of scientists, graduate students and engineers working in this field.

We deeply appreciate the outstanding research work of all authors. We are also very grateful to Mr. Mars Tan from the Editorial Office for his continuous assistance and support, which enabled our Special Issue to be successful.

**Peng Chen and Zhizhong Chen**  
*Editors*





Article

# Proposal for Deep-UV Emission from a Near-Infrared AlN/GaN-Based Quantum Cascade Device Using Multiple Photon Up-Conversion

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**Abstract:** We propose the use of an n-doped periodic AlN/GaN quantum cascade structure for the optical up-conversion of multiple near-infrared (near-IR) photons into deep-ultraviolet (deep-UV) radiation. Without applying an external bias voltage, the active region of such a device will (similar to an un-biased quantum cascade laser) resemble a sawtooth-shaped inter-subband structure. A carefully adjusted bias voltage then converts this sawtooth pattern into a ‘quantum-stair’. Illumination with  $\lambda = 1.55 \mu\text{m}$  radiation results in photon absorption thereby lifting electrons from the ground state of each main well into the first excited state. Three additional GaN quantum wells per period then provide by LO-phonon-assisted tunneling a diagonal transfer of these electrons towards the ground level of the neighboring period. From there, the next near-infrared (near-IR) photon absorption, electron excitation, and partial relaxation takes place. After 12 such absorption, transfer, and relaxation processes, the excited electrons have gained a sufficiently high amount of energy to undergo in the final AlN-based p-type contact layer an electron-hole band-to-band recombination. By employing this procedure, multiple near-IR photons will be up-converted to produce deep-UV radiation. Since for a wavelength of  $1.55 \mu\text{m}$  very powerful near-IR pump lasers are readily available, such an up-conversion device will (even at a moderate overall conversion efficiency) potentially result in an equal or even higher output power than the one of an AlN-based p-n-junction light-emitting diode. The proposed structures are therefore very interesting for applications such as ultra-high-resolution photolithography or printing, water purification, medical equipment disinfection, white light generation, or the automotive industry.

**Keywords:** nitride semiconductors; AlN/GaN superlattice; optical pumping; near-IR absorption; optically induced up-conversion; deep-UV emission

**Citation:** Hofstetter, D.; Bour, D.P.; Beck, H. Proposal for Deep-UV Emission from a Near-Infrared AlN/GaN-Based Quantum Cascade Device Using Multiple Photon Up-Conversion. *Crystals* **2023**, *13*, 494. <https://doi.org/10.3390/cryst13030494>

Academic Editors: Peng Chen and Zhizhong Chen

Received: 9 February 2023

Revised: 7 March 2023

Accepted: 8 March 2023

Published: 13 March 2023



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## 1. Introduction

Deep ultraviolet (deep-UV) light (also called UV-C radiation) is of crucial importance for many applications in environmental and life sciences. Up to now, different approaches to generate such short-wavelength radiation have been reported. Among them are frequency-doubling of blue InGaN-based laser diodes [1], cathodoluminescence on  $\text{Y}_2\text{O}_3$  [2], or an electric discharge through [Ar]-gas striking a graphene/hexagonal BN/graphene heterostructure [3]. Since the direct generation of spectrally narrow deep-UV radiation using semiconductor-based light-emitting diodes (LEDs) still suffers from issues such as low doping, high contact resistance, or poor efficiency, alternative methods such as up-conversion of multiple near-IR photons for the subsequent emission of a single deep-UV photon are being actively investigated [4–6]. Such up-conversion processes have already enabled a variety of interesting applications ranging from bio-imaging [7] or solar energy conversion [8] to high-density optical storage [9].

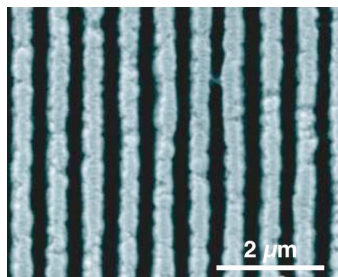
Very promising semiconductor materials for such deep-UV applications are AlN and GaN. This is not only because of the 2014 Physics Nobel Prize in this area [10,11] or the III-nitrides' great radiation hardness, chemical inertness, and mechanical stability. Rather, it is also due to their potential as opto-electronic materials of choice for the entire visible wavelength range [12]. By using inter-subband (ISB) transitions in AlN/GaN-based multi-quantum well structures, it is even possible to access the near-IR wavelength range [13,14]. For these reasons, III-nitride semiconductors have become very interesting for ultrafast detector applications in both the mid- and the near-IR or in free-space optical telecommunications.

In the present publication, however, we will discuss a completely new device idea—taking advantage of optically up-converting near-IR light into deep-UV light. The resulting short-wavelength radiation can—for instance—be used for the sterilization of medical equipment [15], water purification [16], deep-UV lithography [17], or high-density optical data storage [18].

## 2. Experimental Setup

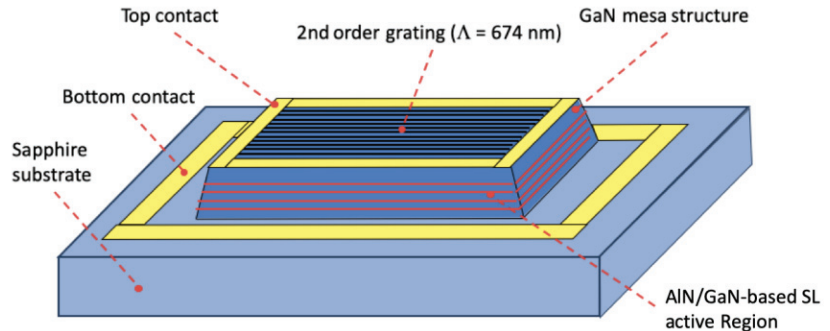
For the fabrication of the envisaged devices, the following layer structure is proposed. On top of a high-quality AlN/sapphire template [19], a fully relaxed 2  $\mu\text{m}$ -thick n-doped AlN:Si layer ( $N_D = 5 \times 10^{17} \text{ cm}^{-3}$ ) will be grown. The latter serves both as a quasi-substrate and a lower contact material. It will be overgrown by the active region which consists of a 12-period superlattice containing relaxed AlN barriers and strained GaN quantum wells (QWs). The layer structure of one period—starting with a barrier layer—corresponds to the following sequence: **15/15/15/15/15/15/20/15** Å. Boldface numbers denote AlN barriers, roman numbers stand for GaN QWs; and n-type modulation-doped layers ([Si],  $N_D = 2 \times 10^{18} \text{ cm}^{-3}$ ,  $E_A = 25 \text{ meV}$ ) are marked by underlining. The final top contact layer consists of 200 nm fully relaxed, p-doped AlN:Be ( $N_A = 3 \times 10^{17} \text{ cm}^{-3}$ ,  $E_A = 37 \text{ meV}$ ), and it will be prepared by metal modulated epitaxy (MME) [20]. The entire SL will thus essentially have the lattice constant of relaxed AlN.

Using an ultraviolet HeCd-laser ( $P = 100 \text{ mW}$ ,  $\lambda_{\text{HeCd}} = 325 \text{ nm}$ ), a second-order diffraction grating with a period of  $\Lambda = (1.55 \mu\text{m}/2.3) = 674 \text{ nm}$  is holographically defined by two-beam interference. After photoresist exposure and development, the resulting pattern is metalized (Pt/Pd/Au 10/10/200 nm)—followed by metal lift-off. Using the grating's metal stripes as an etch mask, the semiconductor surface is then dry-etched using  $\text{Cl}_2/\text{H}_2$ -based reactive ion etching with an inductively coupled plasma (ICP-RIE) [21]. The etch depth will be 100 nm—i.e., about halfway through the p-type contact layer. A small portion of such a grating looks typically like the example in the SEM image shown in Figure 1. In order to achieve a very strong diffraction, an enhanced coupling strength grating with a low-index liner and a high-index cover layer may be used [22].



**Figure 1.** Scanning electron microscopy (SEM) image of a second-order diffraction grating for vertical coupling. The period of this grating is  $\Lambda = 674 \text{ nm}$ , as shown by the scale bar. The metal layers are identical to the p-type metallization used for the contacts.

In a next step, square-shaped mesa structures with a side length of 200  $\mu\text{m}$  and a height of 1.2  $\mu\text{m}$  are defined using, again, ICP-RIE. Such a mesa is schematically presented in Figure 2.

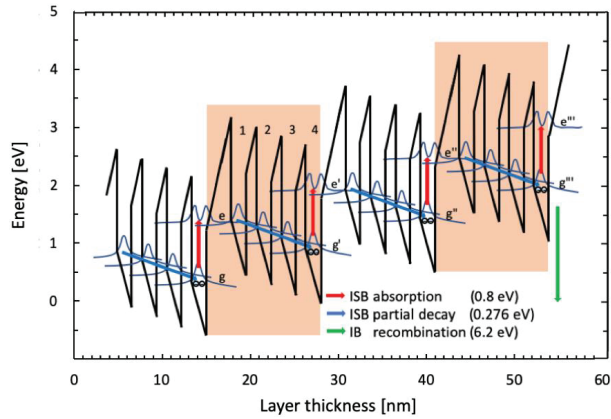


**Figure 2.** Schematic drawing of the square-shaped AlN/GaN-based inter-subband mesa with a diffraction grating on top. Metallization allows electrical contact at the top and the bottom of the mesa.

P-type contact metals (Pt/Pd/Au 10/10/200 nm) will then be lift-off deposited on the shoulders of the square mesas. The resulting ‘contact contour’ provides a common electrical connection to all grating lines of a given mesa structure and assures a sufficiently large top contact area. The relatively high p-type doping of the upper contact layer guarantees a good Ohmic contact. The n-type lower contact metal layers—to be deposited on the dry-etched areas outside the mesas—consist of Ti/Al/Ni/Au (10/10/10/200 nm). These contacts will then be annealed at 825  $^{\circ}\text{C}$  for 1 min.

### 3. Proposed Operation of the Device

When applying zero bias voltage, the conduction band structure schematically appears sawtooth-shaped. There, the label ‘g’ denotes the first main well’s ground state while ‘e’ is its first excited state. Labels with primes (such as  $g'$ ,  $g''$ , ...) indicate levels in the second, third, ... main QW. In order to operate this device, a total voltage of 6.2 V (corresponding to an electric field of 413 kV/cm) will be applied between the top and the bottom contact layers of the mesa. This results in a stair-like conduction band structure; as shown in Figure 3. The above voltage will be carefully adjusted in order to result in a sufficiently small forward current (<1 mA)—indicating a slightly incomplete level alignment and a missing anti-crossing of the relevant energy levels ‘e’ and ‘1’ (see Figure 3). In order to provide the small amount of remaining electric field, the mesa under investigation will be illuminated vertically from above using light with a wavelength of 1.55  $\mu\text{m}$ . The second-order grating diffracts this vertically incoming radiation into the directions parallel to the mesa surface. Due to subsequent light propagation in the horizontal direction, strong inter-subband absorption will take place in the 1.5 nm wide, n-doped GaN ([Si],  $N_D = 2 \times 10^{18} \text{ cm}^{-3}$ ) QW layers.



**Figure 3.** Conduction band structure under an applied bias voltage of 6.2 V on 12 periods—corresponding to an electric field of 413 kV/cm. QWs/barriers 1, 2, 3, 4 correspond to one SL period. Excitation through photon absorption (vertical red arrows) and partial relaxation (oblique blue arrows) are schematically shown. The vertical transition energy in the main QW measures 800 meV ( $\lambda = 1.55 \mu\text{m}$ ). The green arrow marks the interband transition in the deep-UV.

As shown schematically in Figure 3, the absorbed near-IR radiation efficiently lifts electrons from the ground level (labelled level ‘g’) into the excited QW state (labelled level ‘e’). From there, the electrons have two possibilities to proceed. They will either drop back vertically into level ‘g’ or transfer—in a second step—towards the neighboring QW (labelled level ‘1’). Due to the specifically designed multiple LO-phonon resonances of the quantum stair, this process is extremely efficient and assumed to have a higher probability than the vertical one back to level ‘g’.

Therefore, those electrons which perform the above two-step process with absorption in the main QW and LO-phonon-induced transfer into well ‘1’ are very likely to further transit through the adjacent ‘quantum stair’. In this case, they will finally end up at the ground level of the next active region period (g’), from where they will be excited again. This way, they travel through the entire structure and they gain a certain amount of energy for each traversed period. At this point, the probability of such a multiple excitation process will be estimated.

After each optical excitation of 800 meV, the electrons will lose some of their acquired energy by undergoing three subsequent relaxations. This energy loss corresponds to three GaN-based LO-phonon energies ( $3 \times 92 \text{ meV} = 276 \text{ meV}$ ), thus roughly one-third of the initial energy of 800 meV. Since these optical pumping and decaying processes take place simultaneously in each of the 12 active region periods, a successive climbing across the entire quantum stair—at least of a certain fraction of the entire electron population—will occur. Obviously, we note that  $12 \times (0.8 - 0.276) \text{ eV} = 6.288 \text{ eV}$  is just slightly above the AlN bandgap of 6.2 eV. As this climbing constitutes the exact opposite of the ‘normal’ quantum cascade current flow, we will—as a net effect—see a slight reduction in the injection current.

How are we going to prevent the electrons from making a ‘too early’ recombination—i.e., already after two or three instead of 12 periods? Simply by growing only one single p-doped layer: namely the final layer of the structure. Therefore, the electrons have to reach the last (thin) QW layer of the structure. From there, the 12<sup>th</sup> optical absorption lifts the electrons onto a sufficiently high level to undergo afterward the desired inter-band recombination in AlN.

Concerning the efficiency of such a device, the following reasoning applies: an optical input power of 1 W will first be diffracted and lead to an ideal diffraction efficiency of 50% (i.e., 500 mW). This amount of power will be available for inter-subband excitation and carrier transport. By further admitting that—by a specific design exploiting a LO-phonon resonance as presented in reference [23]—a ‘two-step excitation/transfer’ towards level ‘1’

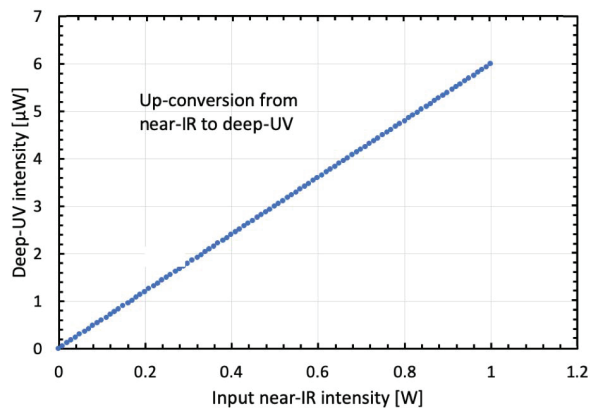
is (due to its shorter lifetime of  $\tau_{e1} = 0.3$  ps) about three times as probable as a vertical transition back to level 'g' with  $\tau_{eg} = 0.8$  ps [24], we estimate a power of 375 mW going towards the 'forward direction' while only 125 mW will go towards the 'backward direction'. This situation is equivalent to the one of a quantum cascade detector: While both the ('inefficient') vertical and the ('desired') diagonal excitation will be designed to have roughly the same probability of 50%, the diagonally excited electrons will be rapidly transferred by LO-phonon-assisted tunneling into the next well of the quantum stair. The carriers then swiftly reach the ground state of the following period, where they will be excited again. After 12 such excitations, we therefore obtain  $1 \text{ W} \times (0.375 \text{ W}/1 \text{ W})^{12} = 7.7 \text{ }\mu\text{W}$  reaching the p-contact layer of the structure. With a roughly 80% conversion efficiency towards the deep-UV wavelength range, we estimate that a total power of  $6 \text{ }\mu\text{W}$  of deep-UV radiation at a wavelength as short as 200 nm will be generated in such a device. This value needs to be compared for instance with an AlN LED at  $\lambda = 210$  nm emitting 0.02 mW (Taniyasu et al. [25]), an AlGaIn LED at  $\lambda = 231$  nm emitting 3.5 mW (Knauer et al. [26]), or an AlGaIn LED at  $\lambda = 304$  nm emitting 40 mW (Khan et al. [27]). From this short list, it becomes clear that going to an even shorter wavelength results in a rapidly decreasing output power.

Finally, as is quite generally the case for light-emitting diodes, the output will at first follow the torus-shaped radiation pattern typically seen in AlN (mainly horizontal radiation). However, it will then be efficiently diffracted towards a roughly vertical direction by the diffraction grating already used for the optical input.

#### 4. Prospective Results

In order to measure this power with a sufficiently high signal-to-noise ratio, the incoming infrared radiation will be chopped at a frequency of 10 kHz. Although this could be done mechanically by a rotating chopper wheel, it is more efficient to perform this task electrically by directly applying a pulsed input signal between the top and the bottom contacts of the mesa. Between two electrical pulses, the conduction band structure is thus unbiased. During the electrical pulses, however, it looks biased like in Figure 3. Therefore, this structure changes periodically between its flat and its stair-like configuration. The resulting small difference in the injection current can be detected best using a sensitive lock-in technique. The latter typically allows the measurement of 1% of the mean measurement values. In this case, this would be on the order of  $1\% \times 6 \text{ }\mu\text{W} = 60 \text{ nW}$ .

Given the previously calculated  $6 \text{ }\mu\text{W}$  of deep-UV power for a near-IR input power of 1 W, a linear efficiency curve can be assumed in a first approximation. Figure 4 therefore presents the deep-UV output intensity as a function of near-IR optical input power.



**Figure 4.** Calculated output intensity at an energy corresponding to the AlN bandgap of 6.2 eV ( $\lambda = 200$  nm) as a function of optical illumination at  $\lambda = 1.55 \text{ }\mu\text{m}$ . For the available range of input intensities, no pronounced saturation effects are to be expected.

Although the achievable output power of the proposed device with 6  $\mu\text{W}$  seems to be relatively modest, one sees easily that this up-conversion has the potential for more interesting power levels. In addition, despite the fact that with AlN-based p-n-junction devices output powers approaching the 1 mW range have been achieved at a wavelength of 230 nm, going to an even shorter wavelength range will be fundamentally difficult. It is clear, however, that many interesting applications crucially rely on the additionally available photon energy corresponding to a wavelength of 200 nm instead of 230 nm. In any case, the device proposed here constitutes a useful intermediate approach until p-n-junctions in AlN are up to the point. Already at a modest device performance, more than 6  $\mu\text{W}$  of deep-UV optical output power can be generated. In addition, the presented up-conversion approach is particularly interesting due to the fact that very powerful  $\lambda = 1.55 \mu\text{m}$  pump lasers are easily available. Finally, the optical excitation and relaxation scheme shown here is relatively simple and straightforward to implement.

## 5. Conclusions

In the present publication, we have outlined, conceived, and analyzed a new type of optical up-conversion device for the generation of deep-UV radiation. The proposed III-nitride semiconductor structure is based on carefully designed inter-subband transitions in a regular, chirped AlN/GaN-based superlattice. Using this structure, it will be possible to up-convert near-IR radiation into the deep-UV wavelength range. Although such multi-stage up-conversion processes are in general limited in their efficiency, the generated output power will in this case take advantage of the specific design. It uses LO-phonon-induced, mainly diagonal transfer of the excited charge carriers toward the ground state of the next period, thereby prolonging their lifetime quite considerably. In addition, the generated output power will obviously profit from readily available, watt-level optical input intensities in this important telecom wavelength range. Finally, thanks to better crystal growth, fabrication, and processing techniques—along with a higher level of characterization technology—considerable improvements are to be expected in the very near future.

**Author Contributions:** Conceptualization, D.H. and H.B.; methodology, D.H.; software, D.H. and H.B.; validation, D.P.B. and D.H.; formal analysis, D.H.; writing—original draft preparation, D.H.; writing—review and editing, D.H., H.B. and D.P.B. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research received no external funding.

**Data Availability Statement:** The original data can be obtained from the first author of this article.

**Acknowledgments:** The authors would like to thank all of the involved colleagues and institutions—in particular, Lutz Kirste from the Institute of Applied Solid State Physics of the German Fraunhofer Gesellschaft and Cynthia Aku-Leh from ISCIENCES LLC. in Ann Arbor, MI, USA for their precious contributions to this work. We also greatly acknowledge scientific advice from John E. Epler from Lumileds, Inc., San Jose, CA, USA.

**Conflicts of Interest:** The authors declare no conflict of interest.

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Article

# MOCVD of InGaN on ScAlMgO<sub>4</sub> on Al<sub>2</sub>O<sub>3</sub> Substrates with Improved Surface Morphology and Crystallinity

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**Abstract:** ScAlMgO<sub>4</sub> (SAM) is a promising substrate material for group III-nitride semiconductors. SAM has a lower lattice mismatch with III-nitride materials compared to conventionally used sapphire (Al<sub>2</sub>O<sub>3</sub>) and silicon substrates. Bulk SAM substrate has the issues of high cost and lack of large area substrates. Utilizing solid-phase epitaxy to transform an amorphous SAM on a sapphire substrate into a crystalline form is a cost-efficient and scalable approach. Amorphous SAM layers were deposited on 0001-oriented Al<sub>2</sub>O<sub>3</sub> by sputtering and crystallized by annealing at a temperature greater than 850 °C. Annealing under suboptimal annealing conditions results in a larger volume fraction of a competing spinel phase (MgAl<sub>2</sub>O<sub>4</sub>) exhibiting themselves as crystal facets on the subsequently grown InGaN layers during MOCVD growth. InGaN on SAM layers demonstrated both a higher intensity and emission redshift compared to the co-loaded InGaN on GaN on sapphire samples, providing a promising prospect for achieving efficient longer-wavelength emitters.

**Keywords:** MOCVD; epitaxy; III-nitrides; crystallization; InGaN

**Citation:** Wang, G.; Li, Y.; Kirch, J.; Han, Y.; Chen, J.; Marks, S.; Mukhopadhyay, S.; Liu, R.; Liu, C.; Evans, P.G.; et al. MOCVD of InGaN on ScAlMgO<sub>4</sub> on Al<sub>2</sub>O<sub>3</sub> Substrates with Improved Surface Morphology and Crystallinity. *Crystals* **2023**, *13*, 446. <https://doi.org/10.3390/cryst13030446>

Academic Editors: Peng Chen and Zhizhong Chen

Received: 11 February 2023

Revised: 24 February 2023

Accepted: 2 March 2023

Published: 4 March 2023



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## 1. Introduction

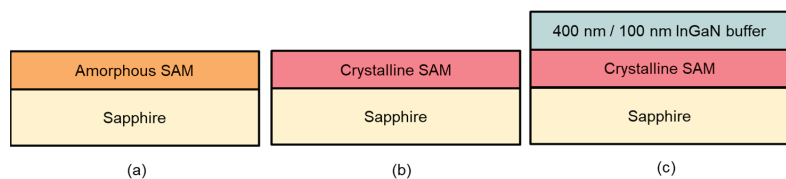
The group III-nitride material system has enabled numerous technologies including electronic and optoelectronic devices. InGaN-based LEDs can be used for emitters of different wavelengths by varying the indium content in the film. A higher indium concentration in the quantum well is required for longer emission wavelengths. An increasing indium content changes their bandgap from 0.7 eV to 3.4 eV, spanning the near IR to near UV range, respectively [1]. One of the most difficult aspects of the InGaN-based material synthesis is its lattice mismatch with the conventionally used GaN buffer layer, which is approximately 11% between GaN and InN [2–5]. Such a high lattice mismatch results in a high strain, causing dislocations in the crystalline structure and defect generation [1,2]. The use of a relaxed InGaN buffer layer reduces the lattice mismatch between the buffer layers and the active region of the emitters, enhancing the efficiency of the devices [6]. AlInGaP-based red emitters are conventionally used; however, size reduction results in a severe efficiency reduction [7–9], which is not a critical concern for nitride-based emitters [10–12]. Therefore, there is a critical need for a relaxed InGaN substrate technology. One of the methods to achieve relaxed InGaN is to grow an InGaN buffer layer on a suitable lattice-matched substrate such as ZnO (lattice-matched to In<sub>0.22</sub>Ga<sub>0.78</sub>N) [13–17] or ScAlMgO<sub>4</sub> (SAM) (lattice-matched to In<sub>0.17</sub>Ga<sub>0.83</sub>N) [18–20]. Using a modified flexible underlayer to achieve relaxed InGaN has been studied, such as the porosification of Si-doped GaN [21–24] and thermal decomposition of underlying high-composition InGaN [25,26]. These methods have successfully demonstrated relaxed InGaN buffer layers and achieved different extents of emission redshifts, however, they also had different constraints. Deposition on ZnO requires a very low deposition temperature (<600 °C), porous GaN based substrates require

additional fabrication steps, and thermal decomposition of high composition InGaN layer results in an increased dislocation density [14,18,26]. These constraints motivated us to pursue the study of accessible SAM substrates for high-composition InGaN synthesis. SAM has a lattice mismatch of 0% with  $\text{In}_{0.17}\text{Ga}_{0.83}\text{N}$  and  $\sim 2\%$  with GaN, making it a suitable candidate for hetero-epitaxial growth of III-nitride materials [18–20]. The high substrate cost of bulk SAM substrates—USD8900 for 2 in diameter substrates—is quite limiting for academic research [27]. The solid-phase epitaxy (SPE) of amorphous SAM on sapphire followed by crystallization is a cost-efficient way to solve this issue. A problem associated with the creation of thin layers of SAM is that the crystallization of the SAM layer with unoptimized annealing conditions leads to the appearance of scandium-deficient regions on the surface, which lead to the formation of undesirable spinel-phase  $\text{MgAl}_2\text{O}_4$  material [28]. The surface roughness of SPE-grown SAM is considerably higher than the other substrate technologies cited before due to its multi-crystallinity. In a previous study, Chen et al. demonstrated the synthesis of epitaxial SAM on a sapphire substrate with a preferred lower temperature of crystallization to constrain the formation of spinel-phase  $\text{MgAl}_2\text{O}_4$  [28].

In this work, we present an improved crystallization method for SAM layers grown on a sapphire substrate and present Metal-Organic Chemical Vapor Deposition (MOCVD) growth of InGaN layers on crystalline SAM. The surface roughness and crystallinity were optimized by annealing SAM at different temperatures for various durations. The InGaN layers grown on SAM on sapphire demonstrated a higher photoluminescence (PL) intensity and a longer peak wavelength of emission compared to the same layers grown on a co-loaded reference GaN on sapphire template.

## 2. Materials and Methods

InGaN on SAM on sapphire was achieved following a three-step process. Initially, an amorphous SAM was sputtered onto a sapphire substrate, which was then subjected to crystallization through annealing. Finally, InGaN films were deposited on the crystallized SAM film on sapphire using MOCVD (Figure 1). The amorphous SAM layer was deposited using on-axis radio frequency (RF) magnetron sputtering with a chamber pressure of 2.4 Pa and RF power of 45 W applied on the substrate at room temperature. The crystallization of the SAM layer was accomplished by annealing in a pre-heated furnace in air at different temperatures (1123 K–1223 K) for different time ranges (20–30 h). After annealing, the samples were cooled outside the furnace in ambient air.



**Figure 1.** Cross-sectional schematics of (a) amorphous SAM deposited with RF magnetron sputtering, (b) crystallization of the SAM by annealing in a tube furnace, (c) subsequent MOCVD growth of InGaN.

In the first set of experiments, the effect of pre-annealing sapphire was studied. The pre-annealing step improved the surface morphology and atomic step uniformity of the sapphire substrate [29,30]. Moreover, high-temperature treatment will result in a uniform oxygen-terminated surface that can improve the deposition of the SAM [31]. Pre-annealing of the sapphire substrate was performed at 1673 K for 10 h. A 40 nm thick amorphous SAM layer was deposited on the pre-annealed sapphire and unannealed sapphire. Both samples were then annealed for 10 h at 1173 K followed by 15 h at 1223 K for the layer crystallization. Further series of crystallization experiments were performed. The first was a time series where three samples with nominally the same amorphous SAM layer thickness of 75 nm were deposited on sapphire substrates. These samples were annealed

at 1223 K for 20 h, 25 h, and 30 h. In the second set of crystallization experiments, three different thicknesses of the SAM layers were studied: 25 nm, 75 nm, and 90 nm. All the samples in the second series were annealed at 1223 K for 25 h. In the third series, the temperature of one of the two annealing steps was varied as follows. A thickness of 40 nm was chosen for two samples that were annealed for a total of 25 h at different temperatures for the first 10 h and 1223 K for the remaining 15 h. The second annealing step of 1223 K for 15 h was designed to ensure crystallization, and by varying the temperature of the first 10 h of annealing, the volumetric ratio of spinel to SAM phases was compared to determine the ideal crystallization annealing condition.

After SAM crystallization, InGaN layers were grown using MOCVD with triethylgallium (TEGa), trimethylindium (TMI), and ammonia (NH<sub>3</sub>). The 100 nm and 400 nm thick InGaN layers were grown with a calibrated composition of  $x_{\text{In}} = 0.14$  on both SAM on sapphire as well as a reference GaN template on sapphire. These layers were grown with TMI and TEGa flows of 2.6 and 4.9  $\mu\text{mol min}^{-1}$  at 1138K, respectively, with an NH<sub>3</sub> flow of 89 mmol/min.

An atomic force microscopy (AFM) scan was performed to compare the surface morphology of the layers using a Bruker Icon AFM tool. The roughnesses of the films were evaluated and compared through the root-mean-square (RMS) Ra parameter. The thickness of the SAM layer was measured with X-ray reflectivity (XRR) using the Panalytical Empyrean X-ray diffractometer. The same equipment was utilized for  $\omega-2\theta$  and  $(\omega-2\theta)-\omega$  reciprocal space map (RSM) scans to evaluate the film crystallinity as well as the layer composition. SAM- and spinel-phase MgAl<sub>2</sub>O<sub>4</sub> peaks were identified with the indexes from previously reported structures [32,33]. The quality of the crystallized SAM layer was evaluated by comparing the spinel (311) to SAM (0009) peak-to-background intensity ratio, the SAM (0009) peak's full width of half maximum range (FWHM), and the spinel (311) peak's FWHM from the  $\omega-2\theta$  scans. Transmission electron microscope (TEM) studies are currently underway to investigate crystalline quality. Due to the thickness restriction on acquiring high-quality RSM on thin SAM films, RSM scans were performed on the reference InGaN on GaN template on sapphire to determine the calibrated indium content in 100 nm and 400 nm thick InGaN layers. The approximate indium content on different substrates was quantified with photoluminescence (PL) spectroscopy using a Horiba LabRAM HR Evolution Raman Spectrometer, using a blue 405 nm laser with an acquisition time of 0.5 s and 125 W/cm<sup>2</sup> power. The systematic variation of the experimental parameters is summarized in Table 1. Sputtered amorphous SAM film on Si along with a bulk SAM substrate were externally characterized using X-ray fluorescence (XRF). XRF was performed using a Rigaku Primus II WDXRF X-ray source with a rhodium X-ray tube in vacuum conditions across a 10 mm diameter measurement area.

**Table 1.** Phase content,  $\omega-2\theta$  FWHM, and roughness for crystallized SAM layers. The annealing temperature for part one (T1) and annealing time for part two (t2) were varied in different experiments. The time of annealing part one was 10 h (t1) and the temperature for annealing part two was 1223 K (T2).

Sample	Pre-Annealing	Thickness (nm)	T1 (K)	t2 (h)	Spinel-to-SAM Ratio	SAM FWHM (Arc-Seconds)	Spinel FWHM (Arc-Seconds)	RMS Roughness (nm) in 0.5 $\mu\text{m} \times 0.5 \mu\text{m}$ Scan	In Content
A	Yes	40	1173	15	0.220	1307	901	1.57	
B	No	40	1173	15	Semi-crystallized				
C	Yes	25	1223	15		0.203	1512	1188	1.25
D	Yes	75	1223	15	0.521	1033	900	1.75	
E	Yes	90	1223	15	0.408	1008	936	2.3	
F	Yes	75	1223	10	0.453	720	959	1.41	20.8%
G	Yes	75	1223	15	0.446	953	991	1.7	20.8%
H	Yes	75	1223	20	0.177	953	929	2	25.9%
I	Yes	40	1123	15	0.263	1059	994	1.48	20.9%

### 3. Results and Discussions

#### 3.1. XRF Results

The results of the film compositions (Wt%) and atomic percentages (At%) of sputtered amorphous SAM film on Si and bulk SAM substrate are summarized in Table 2. These results indicate that the stoichiometry of both the sputtered SAM film and the SAM substrate were fairly comparable, pointing to the possibility of using a crystalline thin SAM film as a substitute for SAM substrate.

**Table 2.** Stoichiometry of amorphous SAM film on Si and SAM Substrate.

	Amorphous SAM on Si Wt%	Amorphous SAM on Si At%	Bulk SAM Substrate Wt%	Bulk SAM Substrate At%
Sc	26.8	13.6	28.2	14.4
Al	17.6	14.8	16.3	13.8
Mg	15.5	14.5	15.7	14.8
O	40.1	57.1	39.8	57.0

#### 3.2. Effect of Pre-Annealing

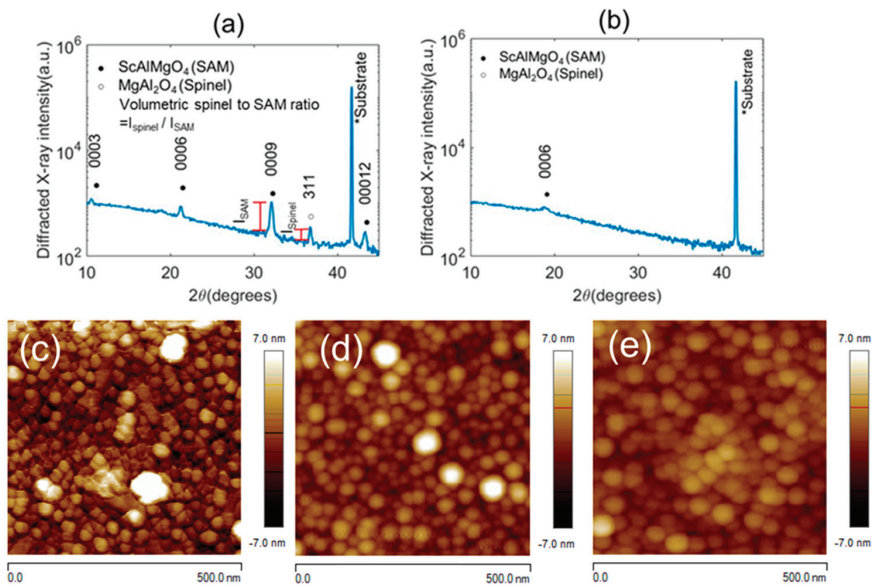
The pre-annealing experiment was performed to improve the sapphire substrate morphology and study its effect on the crystallization of sputtered SAM.

Sample A and B (Table 1) have the same thickness (40 nm) with the same deposition and annealing condition (1173 K for 10 h and 1223 K for 15 h). Sample A used pre-annealed sapphire substrate and Sample B used unannealed sapphire substrate.

Sample A had a SAM reflection with a high peak-to-background ratio in the thin-layer XRD measurements (Figure 2a). Sample B remained amorphous or partially crystallized (Figure 2b). The surface roughness of A increased from 1.16 nm to 1.57 nm after crystallization, as shown in the  $(500 \text{ nm})^2$  size AFM scans (Figure 2d,c). Sample B showed an RMS roughness of 1 nm (Figure 2e) after annealing, which was similar to the RMS roughness of amorphous Sample A, 1.16 nm (Figure 2d). The crystallized samples tended to have a higher roughness than amorphous layers. As mentioned before, the pre-annealing step improved the surface morphology, and the oxygen-terminated surface aided the formation of crystalline SAM film above the sapphire substrate [29–31]. An improved substrate morphology of sapphire resulted in an efficient crystallization of Sample A compared to Sample B.

#### 3.3. Effect of SAM Thickness

Samples C, D, and E were deposited with thicknesses of 25 nm, 75 nm, and 90 nm, respectively, on a pre-annealed sapphire substrate. The crystallization for all three samples was conducted at 1223 K for 25 h. The results are compared using XRD and AFM (Table 1). As the thickness varied from 25 nm to 90 nm, the RMS roughness changed from 1.25 nm to 2.3 nm. The spinel-to-SAM ratio also increased from 0.203 to 0.408. The reason for this behavior could be that the spinel was crystallizing faster than SAM for a given thickness, and the higher the thickness of the layer, the longer the crystallization duration [34]. For thinner 25 nm SAM layers (Sample C), the spinel and SAM phase both crystallized for the annealing duration of 25 h, whereas for the 90 nm SAM layer (Sample E), the spinel phase crystallized; however, the SAM phase did not crystallize efficiently. The high spinel-to-SAM volumetric ratio resulted in the formation of facets, which increased the surface roughness, degrading the morphology. Increasing the layer thickness from 25 nm to 75 nm resulted in a decrease in the FWHM of the  $\omega-2\theta$  of the SAM 0009 reflection from 1188 to 900 arc-seconds, which then nominally remained the same from 75 nm to 90 nm thick SAM layers. This trend could be related to the interfacial reaction between SAM and sapphire during the annealing process resulting in a lower quality of the SAM layer near the interface [28]. With the increasing thickness of the SAM layer on sapphire, the contribution of this poor-quality interfacial layer on the peak intensity of the SAM layer in the XRD scan was reduced, resulting in a lower FWHM of the SAM layer.



**Figure 2.** X-ray diffraction  $\omega$ - $2\theta$  scans of annealed SAM layer on (a) pre-annealed sapphire (Sample A) and (b) unannealed sapphire (Sample B). AFM images of (c) crystallized Sample A, with RMS roughness of 1.57 nm, (d) amorphous Sample A, with RMS roughness of 1.16 nm, and (e) Sample B (not fully crystallized), with RMS roughness of 1 nm.

### 3.4. Effect of Annealing Time

The effect of annealing at a fixed temperature (1123 K) for different durations was studied using 75 nm thick crystallized SAM on sapphire samples. Samples F, G, and H were annealed with durations of 20 h, 25 h, and 30 h, respectively. The RMS roughness increased from 1.41 nm to 2 nm with increasing annealing duration. The spinel-to-SAM volumetric ratio decreased from 0.453 to 0.177 with increasing duration. Although the spinel-to-SAM ratio decreased, the results are difficult to interpret due to the decrease in the overall intensity of both spinel (311) and SAM (0009) peaks, the reason for which is not well understood at this point. With a longer annealing duration, we speculate that the SAM crystallizes more effectively compared to a shorter annealing time due to a lower crystallization rate. The spinel-phase crystallization rate was faster than the SAM phase and the spinel X-ray reflections appeared with a relatively higher intensity than SAM when the sample was annealed for a shorter duration. Subsequent annealing steps resulted in the formation of more SAM-phase material, enhancing its relative intensity [34,35].

### 3.5. Effect of Annealing Temperature

A 25 h total annealing duration was chosen to proceed with the annealing temperature experiment. A high SAM thickness may increase the roughness of the film; however, an insufficient SAM thickness might fail to serve as a lattice-matched layer for the subsequently grown InGaN films. Thus, an intermediate-thickness 40 nm SAM layer was chosen in the following series, as surface roughness reduction was one of the main goals of this study. The temperature series was divided into a two-step annealing experiment for Samples A and I. The annealing temperature of the first 10 h was 1123 K (Sample A) and 1173 K (Sample I). In both cases, the first annealing step was followed by 15 h at 1223 K to ensure crystallization. Samples A and I were both pre-annealed and used the same thickness of SAM layer. After crystallization, Samples A and I had similar RMS roughness. Sample I had a slightly higher volumetric spinel-to-SAM ratio than Sample A, because the spinel phase may have formed at a faster rate compared to that of SAM at 1123 K (Table 1). The



SAM may require a higher annealing temperature to crystallize sooner; however, beyond an optimized temperature, Sc-deficient regions may start to appear. More data points are required to determine a clear trend for the annealing temperature. The optimized crystallization temperature for SAM will be investigated in future work.

### 3.6. MOCVD Growth of Thick InGaN Layers

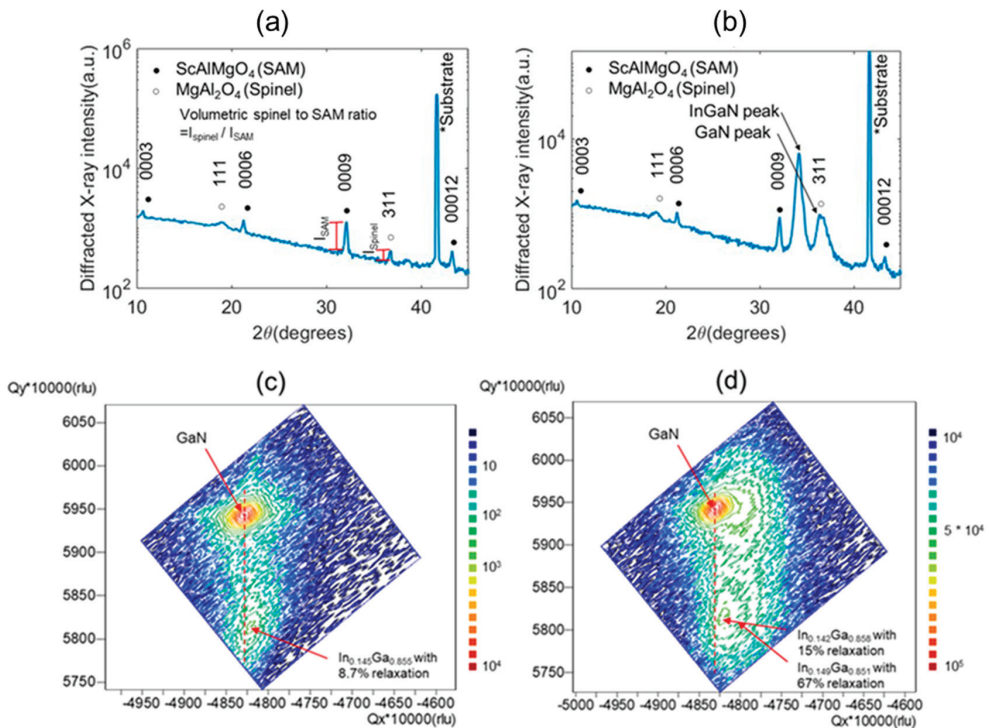
Samples F and H were placed in the MOCVD reactor to deposit a 100 nm thick InGaN layer. In addition, Samples G and I were utilized to deposit a 400 nm thick InGaN layer (Table 1). In both these experiments, reference GaN on sapphire templates were co-loaded to determine the indium content and InGaN relaxation extent on these samples with RSM ( $-1 -1 4$ ) reflection scans. The SAM layers had low thickness compared with the sapphire substrate and the InGaN layer, resulting in a relatively low intensity in the XRD RSM scans. SAM was required as a reference for the lattice constant to measure the InGaN lattice constant and its relative degree of relaxation. However, the low intensity of SAM introduced challenges in obtaining high-resolution RSM measurements on InGaN on SAM on sapphire samples. RSM scans were performed on InGaN on GaN on sapphires samples and PL was performed on both samples to provide a quantitative comparison of the indium concentration between the InGaN on GaN template and the InGaN on SAM on sapphire. The grown structure included a targeted 3–5 nm of GaN interlayer to smooth the morphology, as reported in reference [36]. The corresponding  $\omega$ - $2\theta$  diffraction patterns of the SAM Sample H before and after the MOCVD growth are shown in Figure 3a,b. The growth of the 100 nm InGaN layer on GaN on sapphire indicated the indium content of 0.145 with a degree of relaxation of 8.7%. The 400 nm thick layer showed two InGaN peaks: one corresponding to 14.2% indium content with a degree of relaxation of 15% and the second one with 14.9% indium content and a 67% degree of relaxation (Figure 3c,d). With a 400 nm InGaN thickness, the layer had exceeded its critical thickness on GaN on sapphire; hence, the second peak appeared with higher relaxation [37]. Both peaks of 400 nm InGaN had a higher degree of relaxation compared to the 100 nm InGaN layer owing to higher strain in the structure [38,39]. Comparing the surface morphology using RMS roughness for Samples F and H from Table 1, prior to the InGaN deposition, Sample H showed a significant reduction in the spinel-phase facets although with a slightly higher surface roughness, the reason for which is not well understood at this point (Table 1). However, Sample H demonstrated a lower spinel-to-SAM volumetric ratio of  $\sim 0.18$  compared to  $\sim 0.45$  for Sample F, which might be the reason for fewer formations of facets after the InGaN growth (Figure 4a,b). For the second MOCVD growth of the thicker 400 nm InGaN layer, prior to the MOCVD deposition, Samples G and I had a spinel-to-SAM volumetric ratio of  $\sim 0.45$  and  $\sim 0.22$ , respectively. After the InGaN deposition, the AFM scan showed similar roughness for Samples G and I; however, Sample I showed a smaller grain size than Sample G, which we speculate may be due to the lower spinel-to-SAM volumetric ratio (Figure 4c,d). This suggests that further lowering of the spinel-to-SAM volumetric ratio is necessary to suppress the spinel facets in SAM and improve the homogeneity in the subsequently grown InGaN layer.

The InGaN layer grown on SAM and GaN showed different PL wavelengths of emission (Figure 5a,b) suggesting different degrees of strain in the structure and different indium incorporation. Based on the strain information achieved from the RSM scans and PL emission wavelength, the indium compositions of InGaN on GaN on sapphire samples were estimated and compared to the indium composition measured in RSM scans for validation. Equations (1) and (2) were utilized [40,41], where  $E_g$  is the bandgap energy,  $R$  is the degree of relaxation, and  $x$  is the indium composition. The PL peak emission wavelength was converted to bandgap energy  $E_g$  using Equation (2) [41], where  $\lambda$  is the wavelength and  $h\theta$  is the photon energy, interpreted here as the bandgap energy of the InGaN layer. With this method, 100 nm InGaN on GaN on sapphire with a relaxation of 8% (from RSM) luminescing at 432 nm was determined to have an indium content of 14.5%, which is the same as the indium concentration measured with the XRD RSM scan shown in

Figure 3c. However, the RSM scan of 400 nm InGaN on GaN on sapphire layer (Figure 3d), as discussed above, demonstrated two separate indium peaks, thereby making the indium content estimation challenging. Due to a  $\sim 10\%$  larger lattice constant of InN compared to GaN [2], when thicker InGaN films are grown on GaN, the layer exceeds its critical thickness resulting in strain-relaxed films. The appearance of two separate peaks may be an indication of unintentionally relaxation-graded films, with a higher degree of relaxation for layers closer to the film surface, with RSM scans showing an averaged indium content and degree of relaxation across a range of thickness. Assuming the layers at the surface of the 400 nm thick InGaN on GaN on sapphire sample were 100% relaxed, a luminescence at 475 nm as depicted in Figure 5b should have  $\sim 16\%$  indium content, using Equations (1) and (2), which is nominally similar to that observed from the two InGaN peaks in the Figure 3d RSM scan. As the PL characterization was performed on the top surface of the wafer, consideration of full relaxation of the films close to the surface to determine the indium content accurately can be justified.

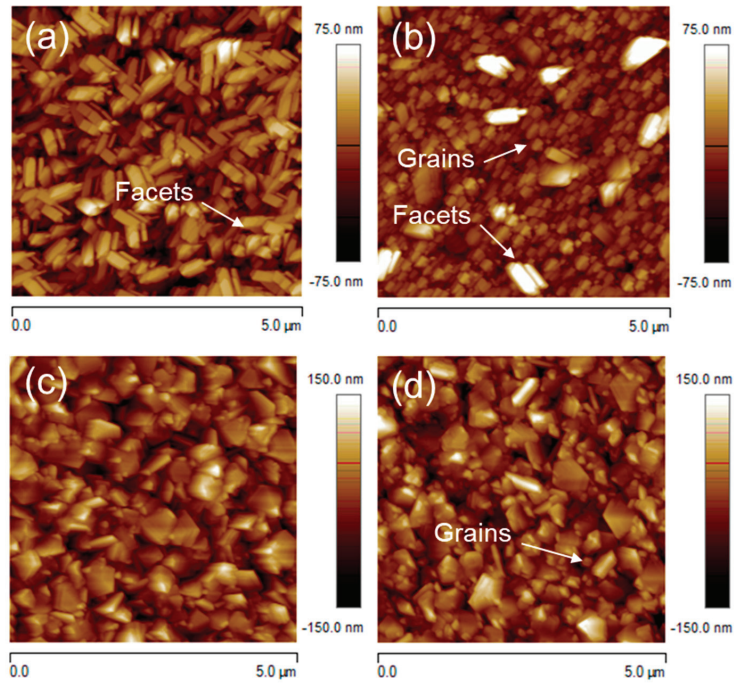
$$E_g(R, x) = 3.42 + (0.69R + 3.42)x^2 - (1.57R + 4.07)x. \quad (1)$$

$$\lambda(\mu\text{m}) = \frac{1.2398}{h\nu(\text{eV})} \quad (2)$$

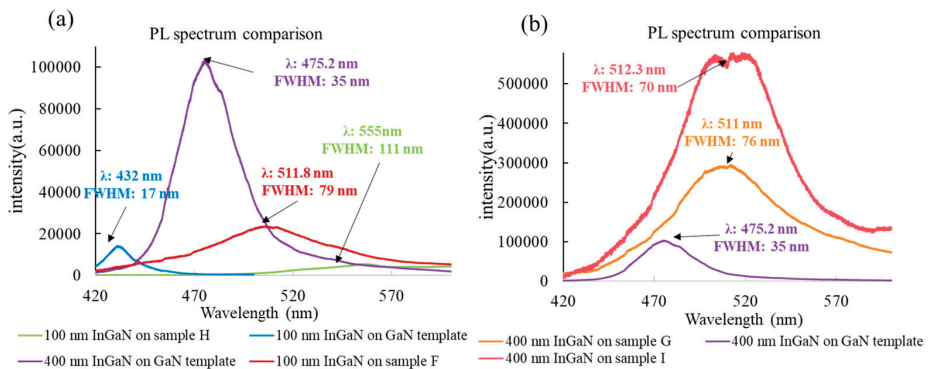


**Figure 3.**  $\rightarrow$  XRD  $\omega$ - $2\theta$  of (a) Sample H, (b) Sample H with 100 nm InGaN on 75 nm SAM layer on Al<sub>2</sub>O<sub>3</sub>; RSM ( $-1 -1 4$ ) of (c) 100 nm InGaN on GaN template; RSM ( $-1 -1 4$ ) of (d) 400 nm InGaN on GaN template.





**Figure 4.** AFM size  $5\ \mu\text{m} \times 5\ \mu\text{m}$  scan of (a) Sample F (100 nm InGaN layer), RMS roughness: 18.3 nm, (b) Sample H (100 nm InGaN layer), RMS roughness: 14.5 nm, (c) Sample G (400 nm InGaN layer), RMS roughness: 30.8 nm, (d) Sample I (400 nm) InGaN layer, RMS roughness: 31.3 nm.



**Figure 5.** PL spectrum of (a) 100 nm InGaN on SAM and GaN template with an intensity range of 0 to  $\sim 100,000$ . (b) 400 nm InGaN on SAM and GaN template with an intensity range of 0 to  $\sim 600,000$  (400 nm InGaN on GaN template was the common spectrum for both plots).

For the InGaN on SAM on sapphire, as mentioned above, without a GaN buffer layer, utilization of a thin crystalline SAM layer posed challenges in acquiring the exact film composition and degree of relaxation with XRD RSM scans. Therefore, some assumptions were made for the degree of relaxation parameter to estimate the indium content using Equations (1) and (2) while using the PL wavelength as the only measured entity. For the InGaN on SAM on sapphire samples, applying 8.7% relaxation to Equation (1) to calculate the indium content of the 100 nm thick InGaN films for Samples F and H, the results were 32.7% and 46.1%, which are impractical. In addition, SAM films are lattice-matched to

$\text{In}_{0.17}\text{Ga}_{0.83}\text{N}$  [18–20]; therefore, these films can be considered as grown 100 % relaxed. Therefore, the indium composition of Samples F and H were recalculated considering full relaxation ( $R = 1$  in Equation (1)), resulting in an indium composition of 20.8% for Sample F and 25.9% for Sample H. For the 400 nm thick InGaN on SAM on sapphire samples, Sample G and Sample I, the same assumption of 100% relaxation yielded indium concentrations of 20.8% and 20.9%, respectively.

The PL results of InGaN film on SAM on sapphire and the reference GaN on sapphire samples are summarized in Table 3. With a 100 nm InGaN layer grown on GaN on sapphire, a peak wavelength of 432 nm with a PL intensity of around 11,000 arbitrary units (a.u.) was measured, which will be considered as the baseline for comparison of the PL intensity of 100 nm InGaN samples grown on SAM. An increased thickness (400 nm) of the InGaN layer on GaN on sapphire depicted higher indium incorporation, thereby emitting a longer wavelength of 475 nm compared to 432 nm, with an improvement in the intensity (100,000 a.u.) of almost ten times. The thick (400 nm) InGaN on GaN on sapphire was the second reference sample for the comparison with thick (400 nm) InGaN grown on SAM. Thick (400 nm) InGaN layer grown on 40 nm SAM (Sample I) produced a two times higher PL intensity, a 1.3 nm redshift in the peak emission wavelength, and a 6 nm lower FWHM compared to Sample G (75 nm of SAM), as shown in Figure 5b. This improvement in the PL emission characteristics could be due to the lower volumetric spinel-to-SAM ratio of Sample I (0.263) compared to Sample G (0.446). Although these two samples showed similar surface roughness measured with AFM, more small-sized grains were formed in Sample I whereas Sample G had larger facets, which might be the reason for the improved crystalline quality and lower FWHM of Sample I compared to Sample G (Figure 4c,d).

**Table 3.** PL results of InGaN film on SAM on sapphire substrates along with reference InGaN on GaN on sapphire samples.

Sample Name	SAM Film Thickness (nm)	InGaN Film Thickness (nm)	Spinel-to-SAM Ratio	Peak Wavelength (nm)	PL FWHM (nm)
F	75	100	0.453	512	79
H	75	100	0.177	555	111
100 nm InGaN on GaN on sapphire	-	100	-	432	17
G	75	400	0.446	511	76
I	40	400	0.263	512	70
400 nm InGaN on GaN on sapphire	-	400	-	475	35

Although the PL emission of 400 nm InGaN on SAM on sapphire samples demonstrated a higher peak emission intensity, 100 nm InGaN grown on SAM showed a longer redshift, which is the intended target. The 100 nm InGaN layers on SAM on sapphire (Sample H) demonstrated the longest wavelength among all the samples with an indium composition of ~26%, but it also demonstrated a two times lower PL intensity compared with reference InGaN on GaN on sapphire (Figure 5a). Sample H was the only sample that demonstrated a lower intensity among all InGaN on SAM on sapphire samples compared with InGaN on GaN template. Further investigations are needed to understand this behavior. Comparing the 100 nm InGaN layers grown on SAM samples, Samples F (75 nm) and H (75 nm) emitted at different wavelengths with different intensities. While Sample F demonstrated a lower redshift of ~80 nm, a higher intensity of emission by approximately two times was observed, even with a poorer surface morphology. Owing to the higher indium incorporation, a drop in the emission intensity by half is still promising, considering the ~120 nm (555 nm compared to 432 nm) redshift for InGaN on Sample H compared to the GaN on sapphire. A more controlled experiment on Sample H needs to be performed to emit in the same range as Sample F to draw further conclusions about

the lower emission intensity. The key difference between F and H was that Sample H had a lower spinel-to-SAM ratio and less formation of spinel facets (Figure 4a,b). The SAM samples with improved homogeneity result in an overall smoother surface morphology, critical for the subsequently grown InGaN layers. This PL result further strengthens our assertion that a lower spinel-to-SAM volumetric ratio is important to achieve high-quality InGaN layers on the optimized SAM on sapphire substrates that we have developed, but in this specific case it resulted in a higher indium content, thereby making the quality comparison inconclusive.

The FWHM of the PL for the InGaN on SAM layers was higher than that for the InGaN on GaN templates. This might be caused by the high surface roughness of the underlying SAM layers, resulting in a stronger indium surface segregation, which leads to a non-uniform indium incorporation [42]. The FWHM of the PL for the InGaN on SAM layers on sapphire obtained in our experiments were comparable to the InGaN layers grown on ZnO substrates [43]. Both thicknesses of the InGaN layers on the SAM on sapphire samples demonstrated higher intensities (two times higher for 100nm InGaN on Sample F and six times higher for 400 nm InGaN on Sample I) and longer emission wavelengths (around 123 nm for 100 nm InGaN and around 37 nm for 400 nm InGaN) than those grown on GaN on sapphire templates. Although the high surface roughness of the InGaN on SAM on sapphire samples may contribute to the increase in the PL intensity, it still cannot account for the high level of intensity enhancement observed in our experiments. Prior reports have shown that roughening of the surface on the nanometer scale has conventionally either degraded the PL intensity or led to minor enhancements [44,45]. However, when the surface roughness increased from the nanometer scale to the micrometer scale, the PL intensity was enhanced by almost twice. In our experiment, compared to InGaN on GaN on sapphire, the InGaN on SAM on sapphire samples had a surface roughness degradation on the scale of tens of nanometers, changing from ~30 nm to ~10 nm, respectively, for a  $5 \mu\text{m} \times 5 \mu\text{m}$  AFM scan. A two to six times higher PL intensity observed in this work, therefore, cannot be accounted for by this nanometer-scale change in surface roughness. Therefore, we speculate that the high InGaN material quality may be the reason for the higher PL intensity observed for the InGaN on SAM on sapphire samples.

This is one of the highest reported redshifts for any relaxed InGaN pseudo-substrate technology so far and one of the few wherein the redshift is accompanied by an increased emission intensity [21]. Further investigations will be pursued to achieve device results on these substrates. These results demonstrate the potential of SAM on sapphire substrates as a viable candidate to achieve thick, high-indium-concentration InGaN layers for long-wavelength emitters.

#### 4. Conclusions

In this work, further optimization of SAM crystallization was investigated to suppress the spinel phase to obtain an improved surface morphology. Compared to the previous work [28], both the surface roughness and the volumetric ratio of the spinel to SAM phase have improved. From the thick InGaN layer growth, we identified that the spinel-to-SAM ratio was one of the key parameters to suppress spinel-phase facets that transfer onto the MOCVD-grown layer surface, increasing the overall surface roughness value. The higher PL intensity along with the redshift demonstration of the InGaN layers on SAM demonstrate the potential of sputtered and crystallized SAM as a promising substrate for longer-wavelength III-nitride emitters. The growth condition for the InGaN layers was not extensively optimized in this work. In the future, we will further investigate the optimized annealing temperature for SAM crystallization and design better growth conditions for the epitaxial growth of InGaN on SAM to grow the light-emitter structures.

**Author Contributions:** Investigation, G.W., S.S.P. and P.G.E.; Formal analysis, G.W. and Y.L.; Data curation, G.W., Y.L., J.K., Y.H. and J.C.; Methodology, G.W., Y.L., J.K., S.M. (Samuel Marks), R.L., C.L., S.S.P. and P.G.E.; Visualization, G.W.; Writing—original draft, G.W.; Writing—review and editing, G.W., S.M. (Swarnav Mukhopadhyay), S.S.P. and P.G.E.; Project administration, S.S.P. and P.G.E.;

Supervision, S.S.P. and P.G.E.; Validation, S.S.P. and P.G.E.; Funding acquisition, S.S.P. All authors have read and agreed to the published version of the manuscript.

**Funding:** This work was financially supported by the National Science Foundation Materials Research Science and Engineering Center (DMR-1720415).

**Institutional Review Board Statement:** Not applicable.

**Informed Consent Statement:** Not applicable.

**Data Availability Statement:** The data that support the findings of this study are available from the corresponding author upon reasonable request.

**Acknowledgments:** We would like to thank Brandon Erickson for helping with manuscript proof-reading. The authors gratefully acknowledge the use of facilities and instrumentation supported by NSF through the University of Wisconsin Materials Research Science and Engineering Center (DMR-1720415).

**Conflicts of Interest:** The authors declare that they have no conflict of interest.

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Article

# Plasma-Assisted Halide Vapor Phase Epitaxy for Low Temperature Growth of III-Nitrides

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**Abstract:** Developing growth techniques for the manufacture of wide band gap III-nitrides semiconductors is important for the further improvement of optoelectronic applications. A plasma-assisted halide phase vapor epitaxy (PA-HVPE) approach is demonstrated for the manufacture of undoped and In-doped GaN layers at  $\sim 600$  °C. A dielectric barrier discharge (DBD) plasma source is utilized for the low-temperature activation of ammonia. The use of the plasma source at a growth temperature of  $\sim 600$  °C increases the growth rate from  $\sim 1.2$  to  $\sim 4\text{--}5$   $\mu\text{m}/\text{h}$ . Furthermore, the possibility for the growth of InGaN at  $\sim 600$  °C has been studied. Precursors of GaCl and InCl/InCl<sub>3</sub> are formed in situ in the reactor by flowing HCl gas over a melt of metallic Ga and In, respectively. The In concentration was low, in the order of a few percent, as the incorporation of In is reduced by plasma due to the activation of chlorine-containing species that etch the relatively poorly bonded In atoms. Nevertheless, the approach of using plasma for ammonia activation is a very promising approach to growing epitaxial III-nitrides at low temperatures.

**Keywords:** PA-HVPE; GaN; InGaN; plasma activated ammonia; low-temperature growth

## 1. Introduction

III-N wide bandgap semiconductors such as GaN and its alloys with indium or aluminum are widely used for manufacturing LEDs, laser diodes, photovoltaics, and high-frequency high-power devices [1–3]. GaN has the potential for high pressure, high temperature, and high voltage applications due to its high critical electric field, good thermal conductivity, and high electron mobility [4,5].

Today, most white LED lamps are based on down conversion when phosphors absorb light from UV or blue LEDs and then re-emit photons at lower energies resulting in a white spectrum. However, the energy losses using down conversion can be about 20–30% depending on the wavelength due to the Stokes shift [6]. These losses can be avoided if a multi-chip design with red, green, and blue LEDs is used with color-mixing optics. Currently, there are red LEDs based on alloys of GaAsP and blue LEDs based on InGaN with relatively low In content demonstrating high quantum efficiencies exceeding 80% [7]. However, efficient green LEDs emitting around 550–600 nm are still difficult to manufacture. This phenomenon is known as the green gap [8]. The origin of the green gap is related to the degradation in crystalline quality and piezoelectric fields in strained InGaN quantum wells (QWs) due to an increase in lattice mismatch between In<sub>1-x</sub>Ga<sub>x</sub>N and the underlying GaN, which is roughly 1% for every 0.1 indium mole fraction “x” [9,10]. This gives rise to the poor structural quality of the material, especially for thicker layers and it will result in reduced efficiency of the InGaN-based LEDs. The problem is further complicated when growth is performed on foreign substrates such as on the commonly used sapphire (Al<sub>2</sub>O<sub>3</sub>) or silicon carbide (SiC) that have a significant lattice mismatch with GaN of  $\sim 16$  and 3%, respectively [11,12]. The lattice mismatch results in an increased density of threading dislocations that act as non-radiative recombination channels, which is a critical issue in the In-rich InGaN-based LEDs [13]. To reduce stress, it is advantageous to fabricate thick

**Citation:** Pozina, G.; Hsu, C.-W.; Abrikosova, N.; Hemmingsson, C. Plasma-Assisted Halide Vapor Phase Epitaxy for Low Temperature Growth of III-Nitrides. *Crystals* **2023**, *13*, 373. <https://doi.org/10.3390/cryst13030373>

Academic Editors: Peng Chen and Zhizhong Chen

Received: 31 January 2023

Revised: 16 February 2023

Accepted: 20 February 2023

Published: 22 February 2023



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lattice-matched InGaN layers of high crystalline quality that can be used as initial templates for further growth of InGaN-based device structures.

To overcome the abovementioned problems several different techniques to fabricate LEDs by growth on a relaxed InGaN layer have been suggested [14]. For example, highly relaxed thick layers of InGaN templates [15], growth on thermally decomposed InGaN layers [16], growth of InGaN on lattice-matched ScAlMgO<sub>4</sub> substrates [17,18], growth of relaxed InGaN on InGaN pseudo-substrates [19,20], and relaxed InGaN templates grown on porous GaN [21].

Molecular beam epitaxy (MBE) and metal-organic vapor phase epitaxy (MOVPE) are common methods for fabricating epitaxial layers and heterostructures for various III-N applications. However, due to low growth rates (<1 μm/h) these methods are not suitable for growing thick III-N layers that can be used as templates. Another problem is related to the tendency of In<sub>1-x</sub>Ga<sub>x</sub>N to phase-segregate into In-rich and Ga-rich alloy regions during the growth, especially as the indium fraction increases [22]. This is partly caused by a high surface mobility of the In atoms compared to the Ga atoms and the large disparity in the vapor pressures of these two metals. While halide vapor phase epitaxy (HVPE) is a more promising technique to produce thick GaN layers at ~1000 °C due to high growth rates in the range of 10–100 μm/h [23,24], it remains challenging to reduce the growth temperature to ~500–600 °C, i.e., to temperatures necessary to prevent thermal segregation of InGaN. This is because the cracking efficiency of ammonia, which is a typical precursor of nitrogen, sharply reduces at temperatures below 1000 °C, which results in low growth rates and poor crystal quality [25].

Thus, in this work, we report the development of a proof-of-concept method to grow GaN layers using a plasma-assisted HVPE (PA-HVPE) process. The implementation of the plasma source in the reactor chamber before the sample holder allows ammonia to be activated even at lower growth temperatures of ~570 °C, which results in an increase in growth rates by a factor of 2 up to 5 μm/h. We have also used metallic indium to form in situ precursors of InCl/InCl<sub>3</sub> with the aim of studying the possibility of In incorporation during HVPE growth.

## 2. Materials and Methods

For the experiments, we used a horizontal homemade HVPE reactor schematically shown in Figure 1. The HVPE system consists of a resistively heated oven with three zones. Each temperature zone can be controlled and heated up to 1050 °C. The system has two boats for in situ generation of GaCl and InCl<sub>3</sub>/InCl by flowing HCl over metal melts. The Ga and In metals have a purity of 7 N. Nitrogen was used as carrier gas and the pressure in the reactor during growth was 500 mbar. The HCl flow over the Ga melt was kept constant at 5 mL/min, and, for the In melt, the flow was varied in the range of 2–10 mL/min. The NH<sub>3</sub> and N<sub>2</sub> gas flows were kept constant at 80 mL/min and 1000 mL/min, respectively. The temperature of the metal melts can be varied by changing the position of the boats in the reactor. In this study, the temperature of the Ga melt was 700 °C, while the temperature of the In melt was varied in the range of 260 to 460 °C. As a substrate for the growth, both *c*-axis Al<sub>2</sub>O<sub>3</sub> with a thickness of 450 μm and GaN templates were used. The GaN templates were commercially available templates consisting of a 3 μm thick MOVPE GaN layer grown on *c*-axis Al<sub>2</sub>O<sub>3</sub> wafers with a thickness of 430 μm. Since the growth of high-quality GaN on foreign substrates, such as sapphire, requires several elaborate steps to form a nucleation layer [26], we have mainly carried out homoepitaxial growth on GaN templates in this work. The size of the samples was 1 cm × 1 cm.

For plasma generation, dielectric barrier discharge (DBD) was used, where the plasma was generated between two graphite electrodes with a 430 μm thick Al<sub>2</sub>O<sub>3</sub> wafer acting as a dielectric (Figure 2a). The gap distance *d* was 5 mm. The electronics for the plasma generation control consists of four 15 kV high-voltage switches connected in a so-called H-bridge, in which the polarity between the electrodes can be changed by alternately turning on and off each pair of switches (S1, S4) and (S2, S3). Two 15 kV MOSFET push-pull

high-voltage switches (BEHLKE HTS 151-03-GSM) and a high-voltage unit (Heinzinger EVO10000-200rev) were used. Plasma generation was carried out using a voltage of ~3–5 kV. The pulse width was limited to 10  $\mu$ s since longer pulses resulted in discharging and an unstable plasma. The pulse repetition frequency was limited to 5 kHz by the MOSFET push-pull high-voltage switches. Figure 2b schematically shows a typical pulse sequence with “on” and “off” times. The HVPE growth of GaN is commonly performed at atmospheric pressure. At such pressures, it was difficult to obtain a stable nitrogen plasma even at high temperatures. Therefore, the growth of the studied layers was done at a lower pressure of 500 mbar. To prevent arc-discharge due to parasitic deposition on the electrodes, the growth time was limited to 15 min.

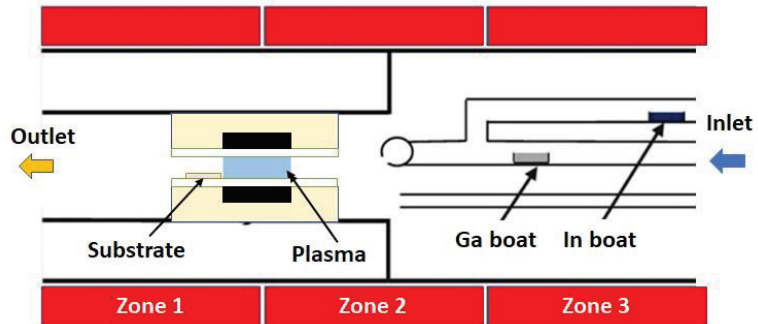


Figure 1. Schematic drawing of the HVPE reactor.

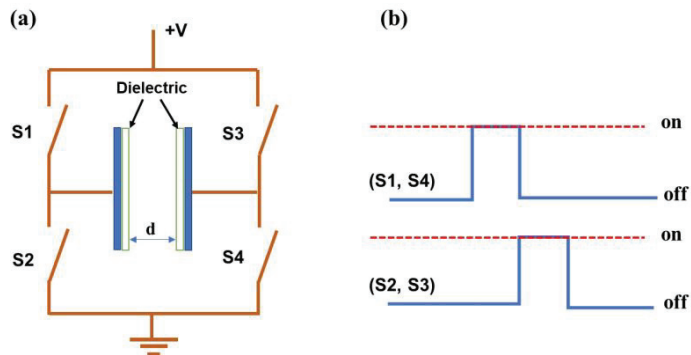


Figure 2. Schematic drawing of plasma generation DBD. (a) High-voltage H-bridge to switch polarity between electrodes with the electrode distance  $d$ . (b) The pulse sequence used to control H-bridge.

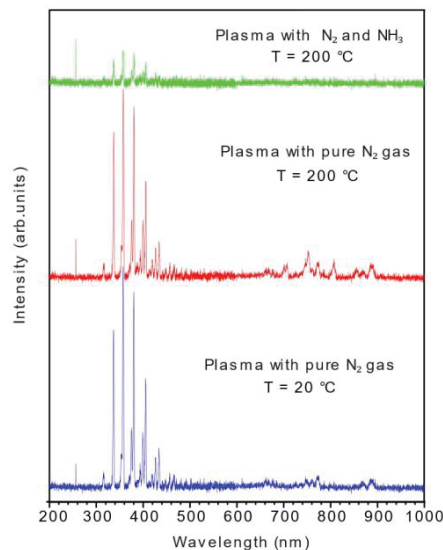
The thickness of the layers was estimated from the weight of the samples before and after growth to give quick feedback to the growth runs, but it was also confirmed by measurements using scanning electron microscopy (SEM) and white light reflectance spectroscopy (WLRS).

Optical characterization was performed by cathodoluminescence (CL) measurements at different temperatures from ~5 to 295 K using a MonoCL4 setup in situ SEM instrument LEO1550. For plasma and transmission spectra measurements, we used a Thorlabs fiber-based compact Czerny-Turner CCD spectrometer, model CCS200/M. Atomic force microscopy (AFM) measurements were performed using a Dimension 3100 SPM microscope with the VT-102 vibration isolation table. X-ray diffraction (XRD) measurements were done using a PANalytical X'Pert Pro diffractometer with Cu-K $\alpha$  radiation.



### 3. Results and Discussion

Figure 3 shows optical spectra of the nitrogen plasma generated between the electrodes inside the reactor with parameters used during the growth of samples. Measurements are shown for 20 and 200 °C for pure nitrogen (blue and red lines) and when ammonia with a flow of 80 mL/min was added in the chamber (green lines). At higher temperatures, the chamber was protected by an isolating shield, which prevented optical measurements. The plasma spectrum shows peaks in the range of 300–500 nm related to the transitions of the  $N_2$  s positive system (2PS) overlapping with  $N_2^+$  first negative system (1NS) originating from the transition between the excited states and the ground state of molecular ion  $N_2^+$  [27]. Electronic transitions in the region of 500–900 nm are related to the first positive system (1PS) of  $N_2$  [28]. The 1PS lines become more intense at 200 °C. We also observed at this temperature a weak sharp line at ~746.6 nm, which might correspond to the excited nitrogen atom transition at 746.83 nm.



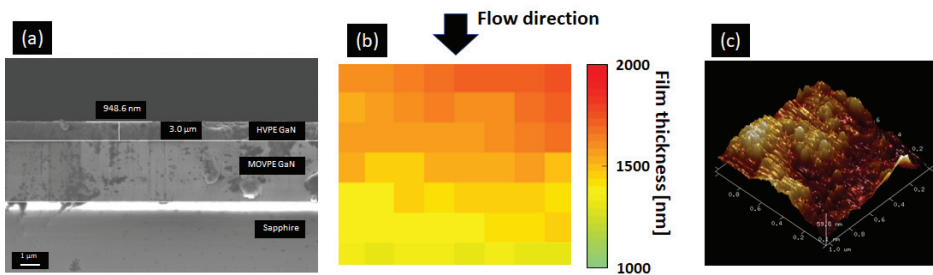
**Figure 3.** Spectra of nitrogen plasma at 20 °C (blue line) and 200 °C (red line). The top graph (green line) shows the plasma spectrum at 200 °C when ammonia gas was added to the nitrogen.

When the ammonia gas was added, the intensities of the transition peaks decrease as can be seen in Figure 3 for the plasma spectrum shown by the green line. In this case, the spectrum was dominated mainly by the 2PS transitions, while no additional lines were observed, although the transition at 746.6 nm was still present in the spectrum. We also observed a sharp peak at ~256.6 nm in all measured plasma spectra. The origin of this peak has not yet been identified; however, it is not related to the response function of the instrument, but to some unknown species in the plasma.

First, the HVPE growth of GaN layers at a low temperature of ~600 °C was performed without and with plasma generation. The thickness of the layers increased from 0.17  $\mu\text{m}$  to 0.5  $\mu\text{m}$ , which means a significant increase in the growth rate from ~0.6  $\mu\text{m}/\text{h}$  to 2  $\mu\text{m}/\text{h}$  by activation of ammonia using the plasma source. The deposition in this particular case was done directly on a sapphire substrate to avoid any influence on the layer properties from the MOVPE GaN templates. When growth is performed on sapphire, the growth rate is not constant and is lower before coalescence.

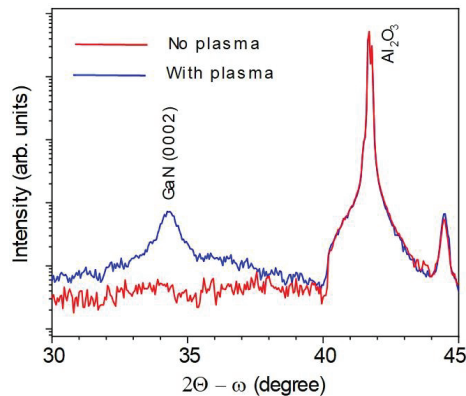
Using the GaN templates, the growth rate at ~600 °C increases to ~4–5  $\mu\text{m}/\text{h}$  for the samples produced with ammonia activated by plasma, while attempts to grow GaN layers without plasma generation resulted in much lower growth rates of ~1.2  $\mu\text{m}/\text{h}$ .

SEM measurements confirmed that the estimation of thickness from the weight gives a reasonable average value. For the sample in Figure 4a, the HVPE layer thickness determined from the weight measurements was  $0.96\ \mu\text{m}$ , and from the SEM image was  $0.95\ \mu\text{m}$ . Figure 4b shows a thickness map of a layer grown at  $620\ ^\circ\text{C}$  on a GaN template. For this layer, the average thickness of  $\sim 1.6\ \mu\text{m}$  was determined from the weight measurements, which correlates with the thickness map, where the variation in thickness was obtained in the range of  $1.3\text{--}1.7\ \mu\text{m}$ . There is a gradient in the thickness over the sample ( $\sim 25\%$ ) in the direction of the gas flow. Thus, for scaling up the process and deposition of larger areas, the system requires rotation of the sample and/or higher carrier gas flows. The roughness is  $\sim 14\ \text{nm}$  for the root mean square (RMS) as estimated from AFM measurements in Figure 4c.



**Figure 4.** (a) Cross-section SEM image shows the thickness of the HVPE layer. (b) WLR thickness map. The thickness varies in the region  $1300\text{--}1740\ \text{nm}$ . The top of the figure is closest to the plasma source. (c) AFM image taken over  $1\ \mu\text{m} \times 1\ \mu\text{m}$  area.

The structural quality of the GaN layers grown directly on sapphire was examined by XRD (see Figure 5). The GaN layer grown with plasma generation shows a reflection peak from the (0002) plane and, thus, an alignment to the  $c$ -axis, while the sample grown without ammonia activation shows only a sapphire-related peak.

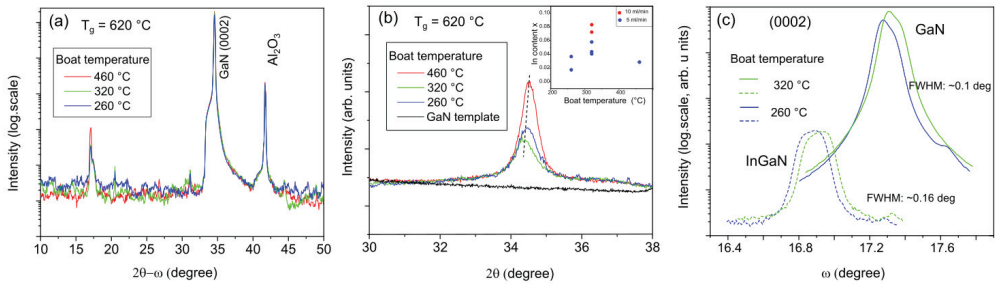


**Figure 5.** XRD spectra measured for the GaN layers grown at  $620\ ^\circ\text{C}$  directly on sapphire (0001) substrates with plasma (blue line) and without plasma (red line) generation of nitrogen precursor. The peak at  $\sim 44.3$  degrees is related to the holder.

We have investigated the possibility of indium incorporation in GaN using the PA-HVPE process with different temperatures of the boat with metallic indium, with different HCl flows over the boat with indium. The process was also studied using growth temperatures of  $570$  and  $620\ ^\circ\text{C}$ . The XRD patterns measured for the symmetric (0002) reflection are shown in Figure 6a for samples grown at  $620\ ^\circ\text{C}$  at three different temperatures of the metallic indium. The dominating diffraction peak is related to GaN, which also involves a

reflection from the GaN template. Therefore, to distinguish signals from the HVPE layers and the MOVPE GaN template, grazing incidence XRD (GIXRD)  $2\theta$  scans with an incident angle of 0.5 degrees were acquired (Figure 6b). Clearly, for the samples grown at different temperatures of the metallic indium, the XRD peak position shifts towards lower angles, which indicates the incorporation of indium in GaN. Note that the thickness of all layers was  $\sim 1 \mu\text{m}$ , which means that the layers can be considered to be fully relaxed [25]. In this case, the lattice constant  $c$  can be determined from the X-ray (0002) peak position according to the Bragg law and the indium molar fraction  $x$  can be calculated from Vegard's law:

$$c_{\text{InGaN}} = xc_{\text{InN}} + (1 - x)c_{\text{GaN}}, \quad (1)$$

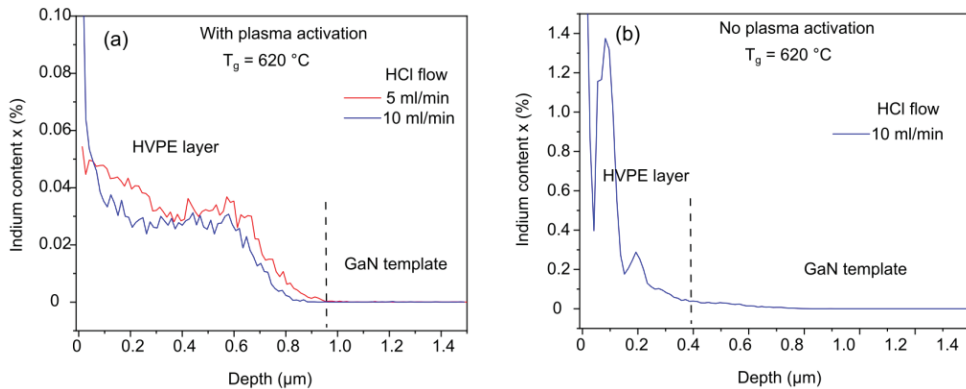


**Figure 6.** (a) XRD patterns measured for the In-doped GaN layers grown at 620 °C on GaN templates using plasma activation of ammonia and different temperatures of the boat with metallic In melt of 460 °C (red line), 320 °C (green line) and 260 °C (blue line). (b) Grazing incidence 2 theta scans performed with a small incident angle of 0.5 degrees shown for the same samples as in (a) and for the GaN template for reference. The inset shows estimated the indium content vs. The boat temperature. (c) XRD omega rocking curves for InGaN and GaN (0002) reflections for samples grown with In boat temperatures of 260 °C (blue lines) and 320 °C (green line).

To estimate the indium concentration in the layers from XRD data, we have used values of 5.702 and 5.185 Å for the lattice parameter  $c$  of InN and GaN, respectively [29]. The obtained  $x$  values are plotted in the inset of Figure 6b for different growth parameters. The highest indium concentration of  $\sim 8\%$  was obtained for the medium boat temperature of  $\sim 320$  °C and HCl flow of 10 mL/min. However, the XRD method to assess indium composition in InGaN depends on the lattice parameters, which have a spread of values according to the literature [29], which can arise to inaccuracies. The rocking curves are rather broad with full widths at half maximum (FWHM) of  $\sim 0.1$  and  $\sim 0.16$  degrees for (0002) GaN and InGaN reflections, respectively (see Figure 6c), which indicates structural imperfections. This is an additional problem contributing to the determination of lattice parameters and, thus, to correctly estimating In content from XRD measurements. Nevertheless, GIXRD has been shown as a feasible technique to study InGaN films with various In% on Si substrate [30].

Furthermore, SIMS analysis shows that, although indium indeed incorporates in the HVPE layers at 620 °C, the estimated concentration was lower than that obtained from XRD data. The depth profiles of indium content for samples grown at 620 °C with HCl flows of 5 and 10 mL/min and with the ammonia activated by plasma are shown in Figure 7a in the linear scale. For comparison, the indium concentration profile is also plotted for the layer grown with the same parameters but without plasma generation in Figure 7b. Clearly, the growth rate is twice as high with plasma-assisted growth. The activated ammonia concentration is higher after the plasma source and that gives rise to a higher growth rate of GaN. At the same time, plasma has a negative effect on indium concentration because plasma simultaneously activates chlorine-containing species. The relatively poor bonding ability of In compared to Ga in InGaN means that In can be more easily etched by the highly reactive plasma-activated chlorine-containing species and that will result in a lower In

concentration [31,32]. In addition, it is also known that the growth of InGaN does not occur when InCl is used since the equilibrium constant of the reaction between InCl and NH<sub>3</sub> is small [33]. Since the InCl<sub>3</sub> in our system is passed through the plasma, we cannot rule out that some of the In precursors are decomposed to InCl. Thus, to improve the incorporation of In in the layers, the precursors InCl<sub>3</sub> and GaCl should bypass the plasma.



**Figure 7.** (a) SIMS depth profile for indium concentration for samples grown with ammonia activated by plasma. (b) SIMS profile for the sample grown with the same parameters as in (a) but without activation of ammonia by plasma. The indium boat temperature was 320 °C. The dashed lines are a guide to the eye.

The band gap shift caused by different concentrations of indium in the InGaN layers grown using plasma-activated ammonia can be observed in transmission measurements. Then, the optical band gap can be estimated from the absorption coefficient  $\alpha$ . For the direct band gap semiconductors  $\alpha$  is related to the band gap energy  $E_g$  as follows:

$$\alpha^2 E^2 \sim (E - E_g), \quad (2)$$

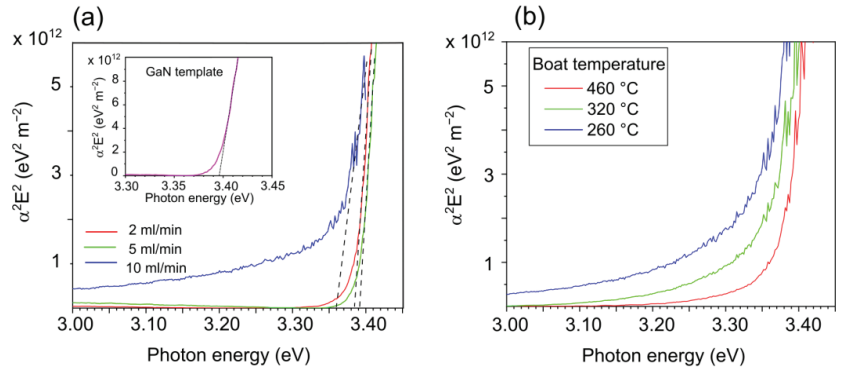
where  $E$  is the photon energy. Graphs of  $\alpha^2 E^2$  as a function of photon energy in the vicinity of the band edge are shown in Figure 8a for samples grown with different HCl flows through the boat with indium. The reference spectrum for the GaN template is also shown in the inset. The shift in the absorption edge is clearly seen in Figure 8b for the samples grown using different temperatures of the indium melt. The energy of the band gap can be estimated by extrapolating the linear part of  $\alpha^2 E^2$  to zero as indicated in Figure 8a by dashed lines. The extracted values of  $E_g$  are plotted in Figure 9a,b for the same samples as in Figure 8. Note, the optical band energy of 3.396 eV estimated for the GaN template is slightly higher than the 3.39 eV for relaxed GaN, which is common for layers under compression when grown on sapphire [34].

The energy of the bandgap for alloy In<sub>x</sub>Ga<sub>1-x</sub>N can be approximated by Vegard's law:

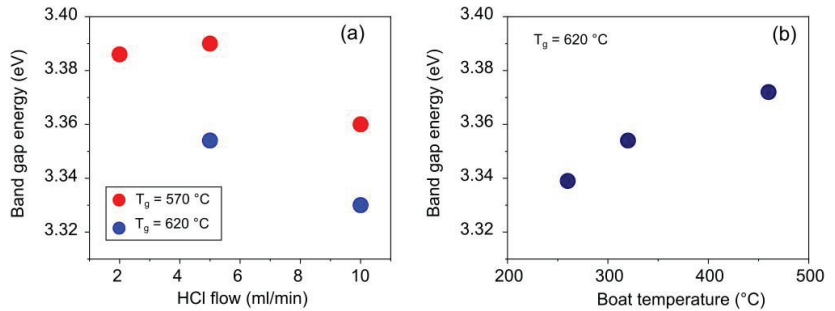
$$E_g(\text{In}_x\text{Ga}_{1-x}\text{N}) = xE_g(\text{InN}) + (1 - x)E_g(\text{GaN}), \quad (3)$$

which allows the calculation of the indium composition  $x$ . Using the bandgap energy of 3.39 and 0.7 eV for GaN and InN [25], respectively, and the InGaN bandgap energy from the absorption data, we have determined that the indium concentration does not exceed 3% in the layers grown with plasma-activated ammonia. Taking into account nonlinearity in the InGaN band gap with bowing parameter in the range between ~1.3 and 3.8 eV [35,36], the indium concentration can be lower. This result correlates well with the data obtained by the SIMS analysis. Indium concentrations determined by different techniques are collected in Table 1. The discrepancy in the determination of indium content has several causes. First, the estimation of indium fraction by SIMS can give an error due to the matrix effect as

SIMS is mainly used for the determination of the concentrations of impurities [37]. Second, the extraction of lattice constant  $c$  from the XRD patterns can be also inaccurate due to broad XRD peaks and material imperfection. Thus, there is a moderate overestimation in In content determined by GIXRD compared to absorption spectra. Similar observations have also been reported when comparing In% determined by various techniques [30].



**Figure 8.** (a) Squared absorption coefficient plotted as a function of photon energy for layers grown at 570 °C at three different flows of HCl through the boat with indium. Temperature of the boat kept constant at 320 °C. The inset shows the spectrum for the GaN template for reference. The dashed lines are a guide to the eye. (b) Graphs for layers grown at 620 °C for different temperatures of the boat with metallic indium. HCl flow over indium melt was kept to 5 mL/min.

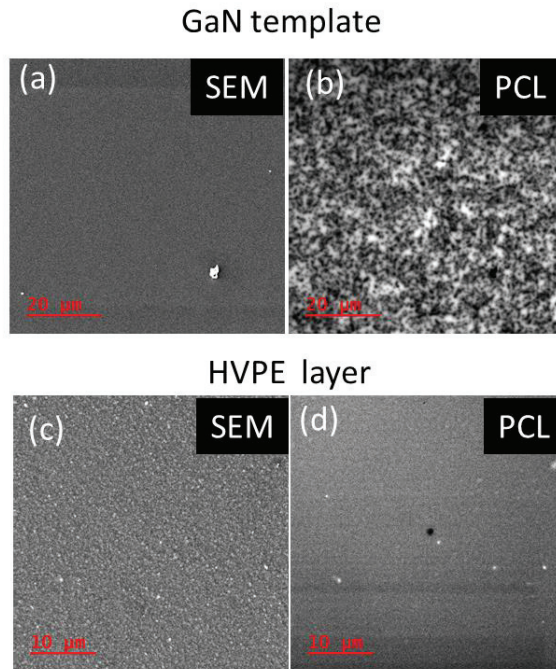


**Figure 9.** The band gap energy estimated from the absorption measurements for samples grown (a) with different HCl flows through the boat with indium and (b) at different temperatures of the boat with indium.

**Table 1.** In content estimated by different techniques for layers grown with different process parameters.

In Boat Temperature (°C)	In Content % (XRD)	In Content % (Absorption)
260	3.7	2.3
320	5.8	1.7
460	2.8	1.0
HCl (mL/min), $T_g = 570$ °C		
2	-	0.5
5	8.3	0.4
10	6.3 (SIMS 0.03)	1.5
HCl (mL/min), $T_g = 620$ °C		
5	5.8 (SIMS 0.04)	1.7
10	7.2	2.6

The emission properties have been studied by low-temperature CL simultaneously with SEM measurements. The morphology of the studied layers produced with plasma generation shows a rougher surface compared to the MOVPE GaN layer (template) (see Figure 10a,c). At the same time, panchromatic CL (PCL) images at 5 K demonstrate that threading dislocations observed as dark spots in the image for the GaN template (Figure 10b) are likely overgrown during the HVPE process judging from the PCL image, which demonstrates uniform contrast (Figure 10d). A similar tendency to overgrow threading dislocations has been observed previously in HVPE GaN layers [38]. However, the uniform contrast in Figure 10d can be also caused by the presence of strong nonradiative centers over the entire InGaN layer, which will prevent the decoration of threading dislocations.

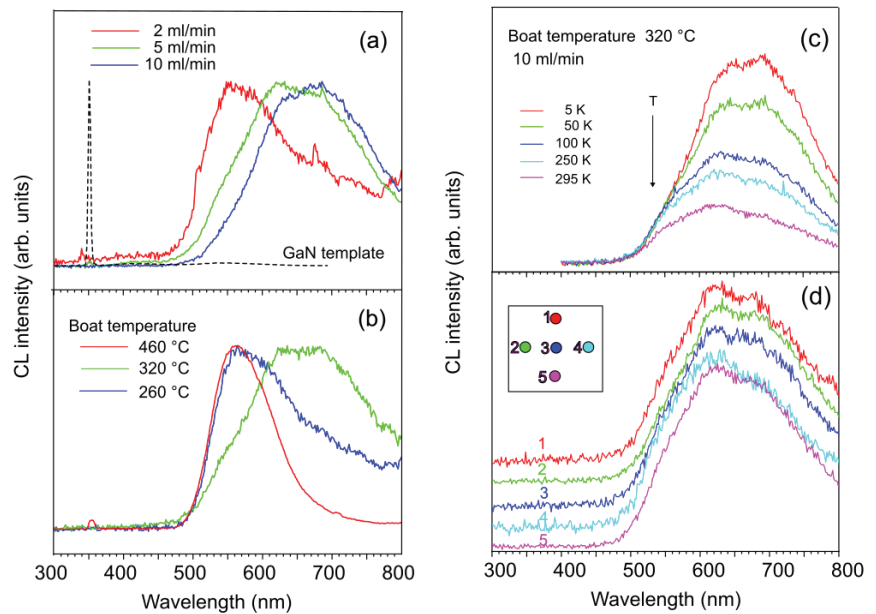


**Figure 10.** (a) SEM and (b) panchromatic CL images for the GaN template. (c) SEM and (d) panchromatic CL images for the InGaN layer grown with plasma-activated ammonia at  $T_g = 620$  °C with HCl flow of 5 mL/min and at the indium melt temperature of 320 °C.

Examples of CL spectra measured at 5 K for the samples grown with three different process parameters are shown in Figure 11. The reference CL spectrum for the GaN template is shown by the dashed line. CL spectra for all studied samples grown by using plasma-activated ammonia are dominated by defect luminescence. Increasing the HCl flow over the indium melt at a boat temperature of 320 °C results in the shift of the maximum of the defect luminescence to the lower photon energies for the samples grown at 570 °C (Figure 11a). The influence of the indium boat temperature on the luminescence is also noticeable as shown for the layer grown at 620 °C with a constant HCl flow of 5 mL/min (Figure 11b). CL spectra measured at different temperature for the layer grown with a constant HCl flow of 10 mL/min through the indium boat is presented in Figure 11c. The ratio of the integrated intensities for the defect emission at 5 K and room temperature is ~2.5. The layer shows rather uniform emission properties with the same peak position independently of the point of acquisition as shown in Figure 11d. Conversely, for different samples, the shift of the CL band maximum correlates with the increased concentration of indium precursor and with indium content determined by XRD. Similar luminescence was



observed for plasma-assisted MBE InGaN samples, where the emission shift was assigned to the increasing indium content [39]. In our case, however, the observed CL shift can hardly be attributed to the narrowing of the band gap of  $\text{In}_x\text{Ga}_{1-x}\text{N}$  with increasing  $x$ , as the variation of the optical band gap does not exceed 30 meV, while the shift of the CL bands is more than 300 meV and ranged between 2.2 eV and 1.85 eV. The observed emissions will be, thus, considered as related to defect luminescence in GaN, known as yellow (YL) and red (RL) bands. Similar RL has been observed in HVPE GaN samples but it is not so common for MOVPE GaN [40]. Although the position of the RL bands is around 1.8 eV, it can be caused by different defects with different properties, and the nature of the RL band is yet to be revealed. The YL1 band with the maximum at 2.2 eV is better studied and associated recently with a carbon-related defect ( $\text{C}_\text{N}$ ) rather than defects involving Ga vacancy [40]. YL1 is typical for MOVPE GaN layers where metal-organics are used as Ga precursor. In HVPE samples, the carbon concentration is usually very low. While YL1 is not pronounced in the undoped HVPE GaN, it appears under doping with carbon impurity [41]. Here, using graphite plasma electrodes for ammonia activation, carbon species can be produced, which explains the strong YL1 emission. The observed shift in the emission to red wavelengths and the enhancement in the RL band are correlated with an increased concentration of indium precursor (i.e.,  $\text{InCl}$  or  $\text{InCl}_3$ ). Considering that RL is typical for HVPE-grown GaN, our observation may indicate that the origin of the RL band is related to the chlorine-containing impurities.



**Figure 11.** (a) Low-temperature CL spectra for samples grown with different HCl flow rates through the boat with In. CL spectrum for the GaN template is shown by the dashed line for reference. (b) CL spectra at 5 K for layers grown at different temperatures of the indium boat. (c) CL spectra measured at different temperatures for the layer grown with the indium boat temperature of 320 °C and with a constant HCl flow rate of 10 mL/min. (d) CL spectra at room temperature measured at different points as schematically indicated in the inset for the same sample as in (c).

#### 4. Conclusions

We have demonstrated a PA-HVPE method for the growth of GaN layers at a low temperature of  $\sim 600$  °C. Plasma at a pressure of 500 mbar inside the growth chamber was generated using dielectric barrier discharge. The use of plasma allows ammonia to be activated even at low temperatures, which resulted in increased growth rates of up

to ~4–5  $\mu\text{m/h}$  at ~600 °C compared to ~1–1.5  $\mu\text{m/h}$  for the conventional HVPE process. We have investigated the possibility of using metallic indium to form  $\text{InCl}/\text{InCl}_3$  precursors directly inside the growth chamber. The effect of various process parameters on the In concentration in the InGaN layers has been studied. The incorporation of indium was confirmed by XRD, SIMS, and absorption measurements, but does not exceed a few percent. We have also found that, although plasma is very efficient to activate ammonia and to increase the growth rates at low temperatures, the concentration of indium significantly reduces due to the activation of reactive chlorine-containing species that etch In at the growth surface. To increase the efficiency of the indium precursor, further modifications of the gas inlets and the plasma source should be done. To avoid the negative effect of chlorine species on the structural quality and the incorporation of indium into InGaN layers, the supply of GaCl and  $\text{InCl}/\text{InCl}_3$  precursors should approach the growth surface without passing through the plasma source. Nevertheless, the suggested PA-HVPE process is very promising for activating ammonia and promoting the growth of thick III-nitrides layers at low temperatures.

**Author Contributions:** Conceptualization, G.P.; methodology, C.-W.H. and N.A.; software, C.H.; validation, G.P., C.-W.H. and C.H.; investigation, G.P., C.-W.H., N.A. and C.H.; data curation, C.H.; writing—original draft preparation, G.P.; writing—review and editing, C.H.; visualization, G.P. and C.H.; project administration, G.P. and C.H.; funding acquisition, G.P. and C.H. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research was funded by the Swedish Research Council (grant nos. 2018-04552, 2019-05154) and the Swedish Energy Agency (grant no. 46563-1).

**Data Availability Statement:** The data presented in this study are available on reasonable request from the corresponding author.

**Acknowledgments:** The authors are grateful for the technical support from Linköping University.

**Conflicts of Interest:** The authors declare no conflict of interest.

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Article

# Micro-Nanoarchitectonics of Ga<sub>2</sub>O<sub>3</sub>/GaN Core-Shell Rod Arrays for High-Performance Broadband Ultraviolet Photodetection

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**Abstract:** This study presents broadband ultraviolet photodetectors (BUV PDs) based on Ga<sub>2</sub>O<sub>3</sub>/GaN core-shell micro-nanorod arrays with excellent performance. Micro-Nanoarchitectonics of Ga<sub>2</sub>O<sub>3</sub>/GaN core-shell rod arrays were fabricated with high-temperature oxidization of GaN micro-nanorod arrays. The PD based on the microrod arrays exhibited an ultrahigh responsivity of 2300 A/W for 280 nm at 7 V, the peak responsivity was approximately 400 times larger than those of the PD based on the planar Ga<sub>2</sub>O<sub>3</sub>/GaN film. The responsivity was over 1500 A/W for the 270–360 nm band at 7 V. The external quantum efficiency was up to  $1.02 \times 10^6\%$  for 280 nm. Moreover, the responsivity was further increased to  $2.65 \times 10^4$  A/W for 365 nm and over  $1.5 \times 10^4$  A/W for 270–360 nm using the nanorod arrays. The physical mechanism may have been attributed to the large surface area of the micro-nanorods coupled with the Ga<sub>2</sub>O<sub>3</sub>/GaN heterostructure, which excited more photogenerated holes to be blocked at the Ga<sub>2</sub>O<sub>3</sub> surface and Ga<sub>2</sub>O<sub>3</sub>/GaN interface, resulting in a larger internal gain. The overall high performance coupled with large-scale production makes it a promising candidate for practical BUV PD.

**Keywords:** ultraviolet photodetectors; Ga<sub>2</sub>O<sub>3</sub>/GaN heterostructure; core-shell micro-nanorod arrays

**Citation:** Tang, R.; Li, G.; Hu, X.; Gao, N.; Li, J.; Huang, K.; Kang, J.; Zhang, R. Micro-Nanoarchitectonics of Ga<sub>2</sub>O<sub>3</sub>/GaN Core-Shell Rod Arrays for High-Performance Broadband Ultraviolet Photodetection. *Crystals* **2023**, *13*, 366. <https://doi.org/10.3390/cryst13020366>

Academic Editors: Dmitri Donetski, Peng Chen and Zhizhong Chen

Received: 3 January 2023

Revised: 2 February 2023

Accepted: 15 February 2023

Published: 20 February 2023



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## 1. Introduction

Broadband ultraviolet photodetectors (BUV PDs) have attracted significant attention as an emerging technology, and they have been widely used in land invasion, forest fire and ozone hole security monitoring, satellite and security communications, and other fields [1–4]. Over the past few decades, significant developments in fabricating BUV PDs have been achieved based on wide-band-gap semiconductors, such as MgZnO/ZnO, AlGaIn/GaN [5–10]. However, high Al/Mg-content AlGaIn/MgZnO layers with high crystal quality are difficult to achieve by epitaxial growth, as the process of alloying makes the fabrication complex and introduces high defect density, thereby increasing the dark current and limiting the performance of PDs [11–17]. Alternatively, Ga<sub>2</sub>O<sub>3</sub> can avoid the complex and unmanageable alloying process owing to its intrinsic solar-blind region band gap. Furthermore, Ga<sub>2</sub>O<sub>3</sub> exhibits high thermal stability (MP 1730 °C), chemical stability and excellent thermal conductivity. Accordingly, Ga<sub>2</sub>O<sub>3</sub>-based PDs gained vast attention in the past few years [18–28]. Moreover, Ga<sub>2</sub>O<sub>3</sub>/GaN heterostructures have a broadband ultraviolet bandgap. More importantly, the intrinsic conduction band difference between Ga<sub>2</sub>O<sub>3</sub> and GaN is 0.1 eV, which facilitates the flow of electrons. The intrinsic valence-band barrier between Ga<sub>2</sub>O<sub>3</sub> and GaN is approximately 1.4 eV, which can effectively block hole transport, resulting in a large internal gain. Therefore, Ga<sub>2</sub>O<sub>3</sub>/GaN heterostructures are considered to be promising materials for BUV PDs. Guo et al. fabricated a super-high-performance self-powered UV PD based on the GaN/Sn:Ga<sub>2</sub>O<sub>3</sub> p–n junction. The responsivity at 254 nm reached up to 3.05 A/W without consuming external power [29].

Lin et al. proposed a typical UV PD based on the “sandwich” structure (graphene/ $\beta$ -Ga<sub>2</sub>O<sub>3</sub>/GaN heterojunction). Using rectifying effect of the p-GaN/ $\beta$ -Ga<sub>2</sub>O<sub>3</sub> diode, the photodetector showed an extremely low dark current density of  $1.25 \times 10^{-8}$  A/cm<sup>2</sup>, and the responsivity is up to 12.8 A/W by the hot carrier multiplication in graphene under Solar-blind ultraviolet illumination [30]. Kalra et al. demonstrated epitaxial  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>/GaN-based vertical metal–heterojunction–metal (MHM) broadband UV-A/UV-C PDs, the PD exhibited the responsivity (R) of 3.7 A/W at 256 nm, and the UV-to-visible rejection  $>10^3$ , and a photo-to-dark current ratio of  $>100$  [31].

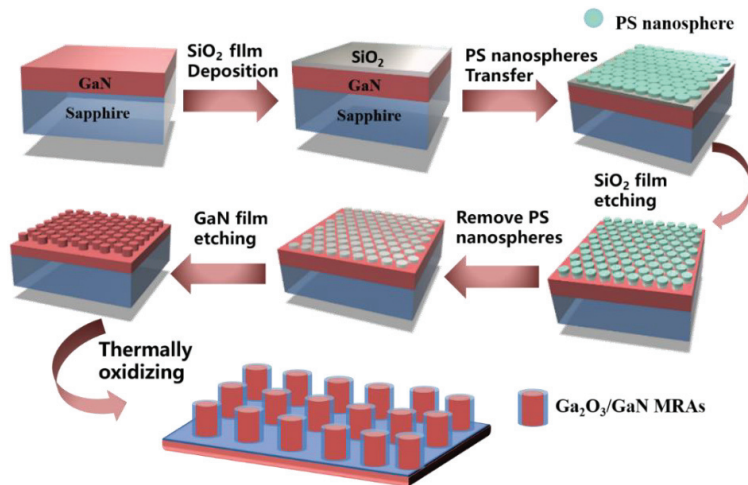
Although there are many reports on BUVD based on Ga<sub>2</sub>O<sub>3</sub>/GaN heterostructures, they are mostly thin-film structures [29–33]. The Micro-Nanoarchitectonics of Ga<sub>2</sub>O<sub>3</sub>/GaN rod arrays are featured with a higher surface-to-volume ratio display superior optical absorption ability and higher recovery efficiency. Specifically, the higher surface area induces more photogenerated carriers and enhances recombination of nonequilibrium carrier via the high surface states, leading to excellent response characteristics. He et al. [34] grew Ga<sub>2</sub>O<sub>3</sub>/GaN nanowires by partially thermally oxidizing GaN nanowires grown using molecular beam epitaxy (MBE). The fabricated PD based on vertical Ga<sub>2</sub>O<sub>3</sub>/GaN nanowire arrays showed a broadband spectral response from 276 to 366 nm with a high responsivity exceeding 550 A/W at  $-5$  V bias and a fast response speed in the millisecond range. Wang et al. [35] fabricated monoclinic  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> vertically aligned nanorod arrays (NRAs) by hydrothermal and post-annealing methods. The fabricated solar-blind PD based on  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> NRAs exhibited a high responsivity of 550 A/W under a bias of 5 V. Moreover, the PD exhibited self-powered characteristics, that is, a responsivity of 10.80 mA/W at 0 V bias and response time of 0.38 s. Although significant developments have been achieved based on Micro-Nanoarchitectonics Ga<sub>2</sub>O<sub>3</sub>/GaN rod arrays, there are still many areas that could be further optimized. For example, most of the reported structures are based on relative complex vertical structures, and the preparation methods of Ga<sub>2</sub>O<sub>3</sub>/GaN heterostructures are mainly MBE [36–39], metal-organic chemical vapor deposition (MOCVD) [40–42], pulsed laser deposition (PLD) [43–45], atomic layer deposition (ALD) [46–48] and so on. These methods require precise control. It is worth noting that thermal oxidation, that is, the high-temperature thermal oxidation of GaN to obtain Ga<sub>2</sub>O<sub>3</sub>, is relatively simple and suitable for mass production [49–61]. Furthermore, the metal-semiconductor-metal (MSM) structure takes advantage of the high light–electron conversion of nano/micro-rod arrays and possesses the unique advantage of easier fabrication compared to other vertical sandwich structures. More importantly, such an MSM geometry constructed two electrodes on the nano/microarrays to increase the electrode effective area and thus effectively collect photogenerated carriers, further improving the performance of PDs.

In this study, Micro-Nanoarchitectonics of Ga<sub>2</sub>O<sub>3</sub>/GaN core-shell rod arrays were prepared by high-temperature oxidization of GaN M-NRAs. MSM PD based on Ga<sub>2</sub>O<sub>3</sub>/GaN core-shell microrod arrays (MRAs) was fabricated. The PD showed excellent performance; an ultrahigh responsivity of 2300 A/W for 280 nm and over 1500 A/W for the 270–360 nm band was obtained at a 7 V bias. The external quantum efficiency was approximately  $1.02 \times 10^6\%$  at 280 nm, respectively. The physical mechanism was attributable to the large surface area of the MRA arrays and Ga<sub>2</sub>O<sub>3</sub>/GaN heterojunction band structure, which blocked more holes at the surface of the M-NRA and Ga<sub>2</sub>O<sub>3</sub>/GaN heterojunction interface, resulting in a larger internal gain compared to the planar Ga<sub>2</sub>O<sub>3</sub>/GaN film-based PD. This mechanism is consistent with the results of PD fabricated using NRAs. It is worth highlighting that the features of inexpensive manufacturing and easy scalability are particularly attractive for mass production.

## 2. Materials and Methods

To take advantage of the internal gain brought by the special band structure of Ga<sub>2</sub>O<sub>3</sub>/GaN heterojunction, the Micro-architectonics of Ga<sub>2</sub>O<sub>3</sub>/GaN with core-shell structure were fabricated. Figure 1 is a schematic of the Ga<sub>2</sub>O<sub>3</sub>/GaN core-shell MRAs fabrication. GaN/sapphire samples with approximately 5  $\mu$ m-thick unintentionally doped GaN epitax-

ial layer were used in this study. The GaN/sapphire wafers were ultrasonically cleaned in acetone and isopropyl alcohol for 15 min and then dipped into a diluted hydrochloric acid water solution (HCL:H<sub>2</sub>O = 1:1) for 5 min to eliminate the native oxide. A SiO<sub>2</sub> film with a thickness of 200 nm was deposited on GaN using plasma-enhanced chemical vapor deposition (SENTECH SI500D). Subsequently, the polystyrene microsphere solution and alcohol were mixed in a 1:1 ratio, and then the polystyrene microspheres were transferred to the surface of the sample. A highly ordered self-assembled monolayer of microspheres with a diameter of 1.7 μm was arranged on the sample. To reduce the size of the microspheres and increase the distance between them, the samples were treated with oxygen plasma for 10 min. The polystyrene microsphere template was then transferred to the SiO<sub>2</sub> film by etching the SiO<sub>2</sub> film using inductively coupled plasma (ICP) with CF<sub>4</sub> gas for 120 s. After the ICP etching process, the polystyrene nanospheres were eliminated by dipping the sample in tetrahydrofuran for 2 h and sonicating for 30 s. Subsequently, the SiO<sub>2</sub> template was transferred to the GaN film through etching of the GaN film by ICP with Cl<sub>2</sub> and BCl<sub>3</sub> gases. Then, the sample was dipped in the BOE solution to eliminate the SiO<sub>2</sub> mask, and GaN MRAs with a cone morphology were fabricated. Subsequently, the sample was placed in an oxidizing furnace. The heating time from room temperature to 1000 °C was approximately 55 min in an oxygen-gas environment. GaN was oxidized in a quartz tube furnace injected with 50 sccm of oxygen gas at 1000 °C for 45 min at atmospheric pressure. Finally, the samples were removed from the oxidizing furnace when the temperature was reduced to 200 °C in a nitrogen protection environment. An interdigitated metal contact (Ti/Al) with a thickness of 30/100 nm was patterned using standard photolithography (Karluss MA6/BA6), DC magnetron sputtering, and lift-off processes. Each device comprised 10 pairs of interdigital electrodes with lengths, widths, and spacings of 300, 6, and 6 μm, respectively. Consequently, the effective illumination area was  $3.42 \times 10^{-4}$  cm<sup>2</sup>. The fabricated PD was finally annealed by rapid thermal annealing under an N<sub>2</sub> atmosphere at 200 °C for 120 s. The contrast PD based on the planar Ga<sub>2</sub>O<sub>3</sub>/GaN film was fabricated using a direct high-temperature oxidization process from a GaN film, as described above.



**Figure 1.** Schematic of the Ga<sub>2</sub>O<sub>3</sub>/GaN MRAs fabrication.

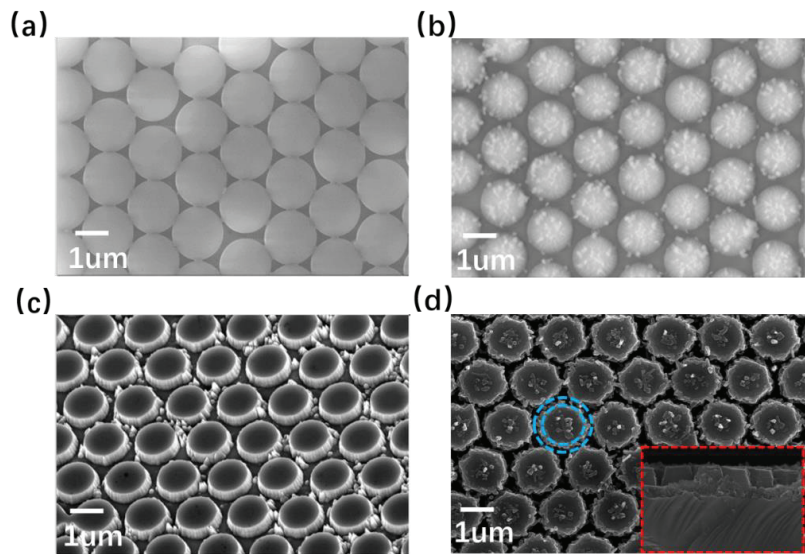
To characterize the material properties, the surface and cross-sectional morphology, microstructure, and the elemental mapping were determined using a ZEISS SIGMA high-resolution field emission scanning electron microscope (FE-SEM). Phase formation and crystallinity were monitored using a Helios Nano-Lab 460HP high-resolution transmission electron microscope (HR-TEM). The I–V characteristics were measured using a Keithley 2410 source meter and Keithley 6514 programmable electrometer. A 450 W Xe arc lamp,



mechanical chopper, and lock-in amplifier were applied to measure the photocurrent response spectra. The system was calibrated using a standard silicon detector. The devices were all illuminated perpendicularly to the front metal/semiconductor contact side. All measurements were performed at room temperature.

### 3. Results

Figure 2a shows the surface morphology of the polystyrene microspheres. A highly ordered self-assembled monolayer of microspheres with a diameter of  $1.7\ \mu\text{m}$  was arranged on the sample. Other sizes of the polystyrene microspheres can also be used to fabricate the GaN rod arrays with different sizes. The diameter of the microspheres was reduced to  $1.3\ \mu\text{m}$  and the spacing of the microspheres increased after oxygen plasma treatment, as shown in Figure 2b. GaN rod arrays with different sizes and distances can also be prepared flexibly by adjusting the power and duration of oxygen plasma processing. Figure 2c shows the surface morphology of the GaN MRAs, and the highly ordered GaN MRAs with a diameter of about  $1.3\ \mu\text{m}$  was obtained. This size is similar to the size of the polystyrene microspheres after plasma treatment. Figure 2d shows the surface morphology of the oxidized  $\text{Ga}_2\text{O}_3/\text{GaN}$  MRAs. The diameter of the  $\text{Ga}_2\text{O}_3/\text{GaN}$  MRAs was approximately  $1.35\ \mu\text{m}$ . The height of the  $\text{Ga}_2\text{O}_3/\text{GaN}$  MRAs was approximately  $750\ \text{nm}$ , as shown in the inset of Figure 2d. Clearly, the  $\text{Ga}_2\text{O}_3/\text{GaN}$  MRAs show a core-shell structure, in which the outer shell is  $\text{Ga}_2\text{O}_3$  with a  $200\text{--}300\ \text{nm}$  thickness and the core is GaN with an  $850\text{--}1050\ \text{nm}$  thickness. Some  $\text{Ga}_2\text{O}_3$  grains with several hundred nanometers in size were observed on the top surface of the MRAs, which was also confirmed in our previous study. The X-ray diffraction (XRD) spectrum of the sample and morphology of the planar  $\text{Ga}_2\text{O}_3/\text{GaN}$  film were similar to those previously reported and are not shown here [54,55,59–61].



**Figure 2.** (a) Surface SEM image of microspheres. (b) Surface SEM image of microsphere after oxygen plasma treatment. (c) Surface morphology of the GaN MRAs after etching the GaN film. (d) Surface morphology of the oxidized  $\text{Ga}_2\text{O}_3/\text{GaN}$  MRAs. The inset shows the cross-sectional SEM image of  $\text{Ga}_2\text{O}_3/\text{GaN}$  MRAs.

To assess the photoresponse characteristics of the planar  $\text{Ga}_2\text{O}_3/\text{GaN}$  film and Micro-architectonics of  $\text{Ga}_2\text{O}_3/\text{GaN}$  core-shell rod arrays, MSM PD based on a planar  $\text{Ga}_2\text{O}_3/\text{GaN}$  film (sample A) and  $\text{Ga}_2\text{O}_3/\text{GaN}$  MRAs (sample B) were fabricated. The device structure diagram of sample B is shown in inset of Figure 3b. The MSM structure, that is, the



two electrodes constructed directly on the MRAs, had a large electrode area, which enabled the efficient collection of photogenerated carriers. Moreover, owing to the intrinsic high valence-band barrier between Ga<sub>2</sub>O<sub>3</sub> and GaN (1.4 eV), the holes generated in GaN will be blocked at the interface of Ga<sub>2</sub>O<sub>3</sub>/GaN heterojunction underneath the electrode, resulting in a greater internal gain. The larger metal electrode area will cause more holes to be blocked at the interface of Ga<sub>2</sub>O<sub>3</sub>/GaN heterojunction, resulting in greater internal gain. The spectral response from 200 to 400 nm at applied bias of 7 V was investigated. The spectral responsivity values via wavelength are calculated using the relation [29]:

$$R = \frac{I_{\text{ph}} - I_{\text{Dark}}}{P_{\lambda}} \quad (1)$$

where  $I_{\text{ph}}$  and  $I_{\text{Dark}}$  are the currents measured under illumination and dark conditions, respectively, and  $P_{\lambda}$  is the incident power density at a specific wavelength of  $\lambda$ , which was calibrated using a standard silicon detector. The  $R$  dependences on wavelength under the applied bias of 7 V for samples A and B are shown in Figures 3a and 3b, respectively. Both PDs exhibited a wide-spectrum response in the UV region. When the illumination wavelength exceeds 370 nm, the responsivity of sample A decreases rapidly, which corresponds to the spectral response cutoffs of GaN material. Sample B has an obvious spectral response at 370–400 nm, which is attributable to the damage of GaN crystal structure by etching process during the preparation of GaN rod arrays, forming many surface defects in GaN and inducing the defect response. Therefore, it is necessary to further optimize the preparation process in the future. As shown in Figure 3a, the peak responsivity was 6.3 A/W at 260 nm for sample A, and the responsivity at the range of 250–360 nm exceeded 2 A/W. For sample B, the peak responsivity was 2300 A/W at 280 nm, the peak responsivity is enhanced by approximately  $4 \times 10^2$  times compared with sample A (6.3 A/W), and the responsivity at the 270–360 nm band exceeded 1500 A/W, as shown in Figure 3b. It is also superior to some reported values [34,35]. Both of the two samples have high responsivity, indicating that the two PDs have a large external quantum efficiency (EQE), which is defined as the number of electrons generated per incident photon and can be obtained using the following equation [27]:

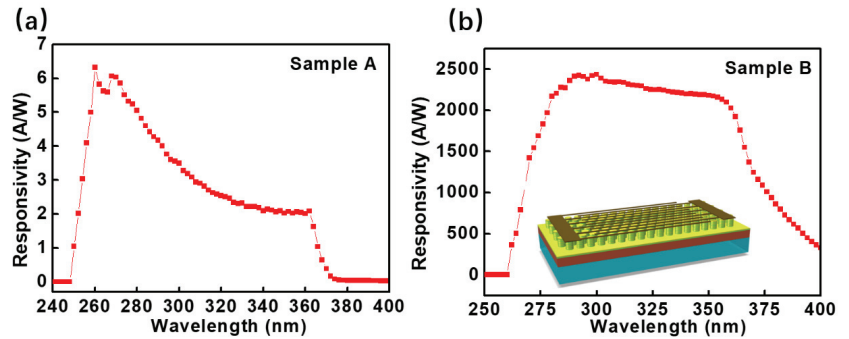
$$\text{EQE} = \frac{Rh\nu}{q\lambda} \quad (2)$$

where  $R$ ,  $h$ ,  $c$ ,  $q$ , and  $\lambda$  are the responsivity, Planck's constant, speed of light, electron charge, and wavelength of the incident optical light, respectively. It is observed that sample A exhibited an EQE of approximately  $3 \times 10^3\%$  for 260 nm and sample B exhibited an ultrahigh EQE of approximately  $1.02 \times 10^6\%$  for 280 nm. Compared with sample A, the internal gain of sample B is significantly increased. Obviously, it cannot be explained by the increase in light absorption efficiency owing to the large surface area of MRAs. This is assignable to the larger surface area of the MRA coupled with the Ga<sub>2</sub>O<sub>3</sub>/GaN heterostructure. This is discussed in detail later in this study.

Detectivity ( $D^*$ ), which usually describes the smallest detectable signal, is another key figure of merit of PDs. The detectivity ( $D^*$ ) can be expressed as [27]

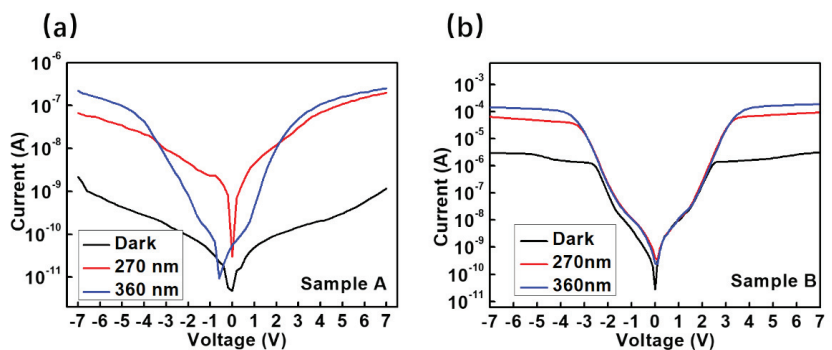
$$D^* = \frac{R}{\sqrt{2eI_{\text{dark}}/S}} \quad (3)$$

where  $S$  ( $3.42 \times 10^{-4} \text{ cm}^2$ ) is the effective area under illumination with the shot noise from  $I_{\text{Dark}}$  regarded as the major component of the total noise. The detectivity  $D^*$  of sample A was calculated as  $4.47 \times 10^{12}$  Jones for 260 nm. The detectivity  $D^*$  of sample B was calculated as  $2.65 \times 10^{13}$  Jones for 280 nm and shows that the ability to detect weak signals is improved.



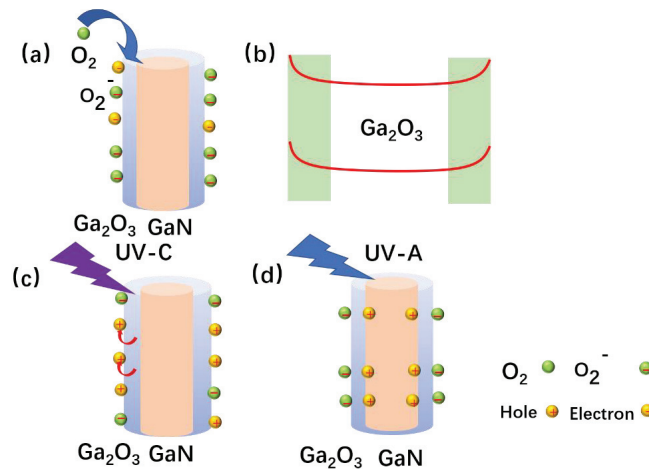
**Figure 3.** (a) Spectral responsivity values of sample A as a function of wavelength at 7 V bias, (b) spectral responsivity values of sample B as a function of wavelength at 7 V bias. The inset shows the device diagram of sample B.

Figure 4a,b shows the I–V characteristics of samples A and B under dark conditions and the illumination of 270 nm/360 nm light, respectively. For sample A, the dark current at 7 V bias is  $1.14 \times 10^{-9}$  A, and the photocurrents are  $1.99 \times 10^{-7}$  and  $2.44 \times 10^{-7}$  A at 270 nm and 360 nm light illuminations, respectively, while the photo-to-dark ratios for 360 nm and 270 nm/dark current both exceeded  $10^2$ . Such low light-to-dark ratio is mainly due to the rather weak intensity of the 270 nm and 360 nm light illuminations, which is separated from the xenon lamp light passing through the monochromator. When the bias voltage is in the range of  $-3\sim 3$  V, the photocurrent at 360 nm light illumination is less than that at 270 nm light illumination, indicating that the depletion region is mainly in the  $\text{Ga}_2\text{O}_3$  layer. As the bias voltage increases, the photocurrent for 360 nm increases rapidly, and exceeds the photocurrent for 270 nm, which indicates that the depletion layer of the device enters the GaN layer. The PD presents B-UV detection, which is consistent with the results of the response spectrum. For sample B, the dark current at 7 V bias is up to  $10^{-6}$  A, which is three orders of magnitude higher than that of sample A. The significant increase in dark current is attributable to the following reasons. The larger electrode area of sample B not only increased the photocurrent, but also inevitably led to larger dark current. Meanwhile, the etching process of the GaN film also caused a deterioration of the GaN crystalline quality, resulting in a greater current leakage. Therefore, the photocurrent was evidently higher than that of dark current until the bias voltage exceeding 3.2 V. The photo-to-dark ratios for 360 nm and 270 nm/dark currents both exceeded 10. It is necessary to further optimize the process to improve the light/dark ratio.



**Figure 4.** I–V characteristics of samples A (a) and B (b) in the dark and under 254 nm/365 nm UV illuminations.

To clearly explain the increased internal gain in sample B, the photodetection model and mechanism of sample B are schematically shown in Figure 5. As shown in Figure 5a,b, the microarchitectonics of  $\text{Ga}_2\text{O}_3/\text{GaN}$  core-shell rod arrays have a larger surface area, and more ambient oxygen molecules are adsorbed on the surface of the MRAs in the dark environment. The free electrons on the surface of the  $\text{Ga}_2\text{O}_3$  film were trapped by oxygen molecules, forming a depletion layer and the energy band bending near the surface of the MRAs. When the device was illuminated under UV-C light, the photogenerated holes in  $\text{Ga}_2\text{O}_3$  migrated to the surface of  $\text{Ga}_2\text{O}_3$  due to the bending band. Compared with the photogenerated electrons in  $\text{Ga}_2\text{O}_3$ , the photogenerated holes in  $\text{Ga}_2\text{O}_3$  that migrate to the surface of  $\text{Ga}_2\text{O}_3$ , were difficult to collect by the electrode, resulting in a large gain. When the device was illuminated under UV-A light, because negatively charged oxygen ions existed on the surface of the  $\text{Ga}_2\text{O}_3$  film after the reaction with  $\text{O}_2$ , the photogenerated holes in the GaN film were aggregated at the interface of  $\text{Ga}_2\text{O}_3/\text{GaN}$  owing to the capacitance effect. These holes were also difficult for the electrode to collect, resulting in an enhanced gain. Therefore, sample B exhibited a greater internal gain than sample A in BUV band range.

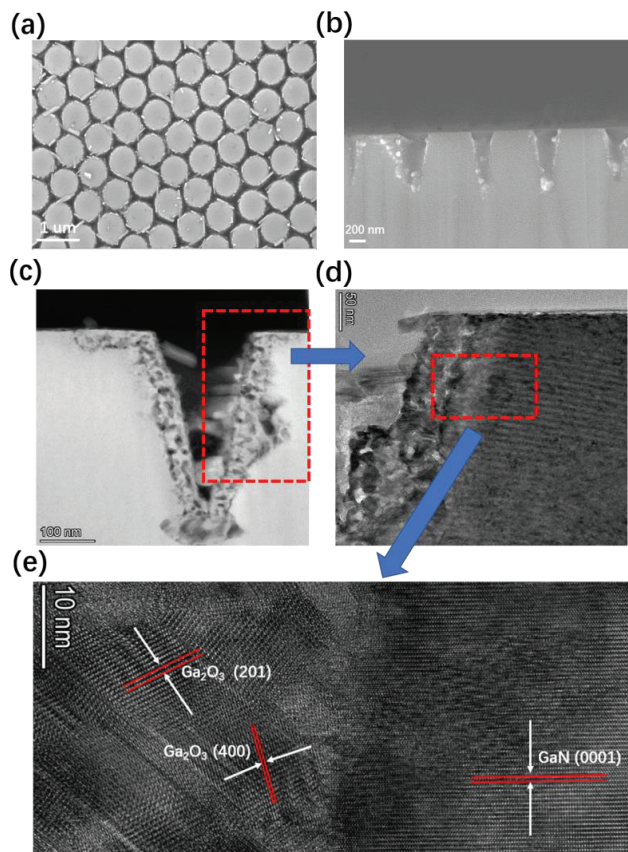


**Figure 5.** (a,b) Schematic of reaction of  $\text{Ga}_2\text{O}_3/\text{GaN}$  core-shell micron rod with oxygen and band of  $\text{Ga}_2\text{O}_3$  films after reaction with oxygen respectively (c) Schematic of holes transferred to the surface of  $\text{Ga}_2\text{O}_3$  film under UV-C illumination; (d) Schematic of photo-generated holes in GaN layer gathering at  $\text{Ga}_2\text{O}_3/\text{GaN}$  heterojunction interface owing to capacitance effect under UV-A illumination.

Moreover, the  $\text{Ga}_2\text{O}_3/\text{GaN}$  core-shell MRAs with higher surface-to-volume ratios effectively improved the light absorption efficiency and thus excited more photogenerated carriers. Because of the larger electrode area, these additional photogenerated electrons can be effectively collected and increase the photocurrent. In addition, more holes were blocked at the  $\text{Ga}_2\text{O}_3/\text{GaN}$  interface underneath the electrode, resulting in high responsivity. Since the  $\text{Ga}_2\text{O}_3/\text{GaN}$  heterojunction has the low conduction band barrier (0.1 eV) and high valence band barrier (1.4 eV), the photogenerated electrons in the GaN layer can pass through the  $\text{Ga}_2\text{O}_3/\text{GaN}$  heterojunction and be collected by the electrode. Meanwhile, the photogenerated holes in GaN are effectively blocked in the  $\text{Ga}_2\text{O}_3/\text{GaN}$  heterojunction, noting that these blocked photogenerated holes are mainly located at the  $\text{Ga}_2\text{O}_3/\text{GaN}$  heterojunction interface below the electrode. A larger metal electrode area can block more holes, thus leading to greater photoconductance gain. The designed structure effectively coupled the optical field enhancement effect with the internal gain of the heterojunction, resulting in ultra-high responsivity of the PDs.

Whether the increased gain caused by the oxygen adsorption, or the large electrode area coupled by the internal gain of the  $\text{Ga}_2\text{O}_3/\text{GaN}$  heterojunction, both are related to the

surface area of Ga<sub>2</sub>O<sub>3</sub>/GaN core-shell rod arrays. To further confirm the above mechanism, Ga<sub>2</sub>O<sub>3</sub>/GaN NRAs with larger surface areas were fabricated using the same method as described above, except that the polystyrene microspheres with a diameter of 1 μm was applied as the mask template and the thermal oxidation time was reduced to 30 min. Figure 6a,b shows the surface and cross-sectional topography of the NRAs. As shown in Figure 6a,b, the highly ordered Ga<sub>2</sub>O<sub>3</sub>/GaN NRAs were obtained, the diameter of the nanocolumn is approximately 700 nm and the height is approximately 400–450 nm. A thin layer of Ga<sub>2</sub>O<sub>3</sub> was identified in the outermost layer of the NRA. In order to demonstrate the formation of the Ga<sub>2</sub>O<sub>3</sub>/GaN core-shell structures, high-resolution HR-TEM inspections were performed. As shown in Figure 6c–e, the outmost shell with a thickness of 10–50 nm is confirmed, which corresponds to the β-Ga<sub>2</sub>O<sub>3</sub> (201) and β-Ga<sub>2</sub>O<sub>3</sub> (400), and the core area corresponds to GaN (0001). These results indicate that the GaN NRAs were oxidized at high temperature and form the polycrystalline Ga<sub>2</sub>O<sub>3</sub> film on the GaN surface.



**Figure 6.** (a) Surface morphology of the oxidized Ga<sub>2</sub>O<sub>3</sub>/GaN NRAs. (b) Cross-section SEM image of Ga<sub>2</sub>O<sub>3</sub>/GaN NRAs. (c,d) Low-magnification TEM image of the core-shell NRA. (e) HR-TEM image of the core-shell NRA.

To further confirm the formation of the nanoarchitectonics of Ga<sub>2</sub>O<sub>3</sub>/GaN rod arrays with core-shell structure by thermal oxidation, energy dispersive X-ray (EDX) and element mapping characterizations were performed on the cross section of Ga<sub>2</sub>O<sub>3</sub>/GaN NRAs. As shown in Figure 7a–e, it can be intuitively seen that Ga and O elements are mainly distributed in the outermost layer of the nanorods, which represents the formed Ga<sub>2</sub>O<sub>3</sub> thin film layer. The Ga and N elements are mainly distributed inside the nanorods, which

corresponds to the GaN layer inside. These results further demonstrate the formation of the Ga<sub>2</sub>O<sub>3</sub>/GaN core-shell structures. To assess the photoresponse characteristics of the nano-architectonics of Ga<sub>2</sub>O<sub>3</sub>/GaN core-shell rod arrays, the PD (sample C) was fabricated in these structures with identical preparation method. Figure 8 shows the responsivity spectrum of sample C. The PDs exhibited a wide-spectrum response in the BUV region. An obvious optical response at 370–400 nm is observed in sample C, which is the same as sample B, indicating the existence of interband response. The peak responsivity of sample C is in the UV-A band range, while the case for sample B is in the UV-C band as described above. This is mainly because the thickness of Ga<sub>2</sub>O<sub>3</sub> in sample C is ultrathin, only 10–50 nm, and the sample C mainly exhibits UV-A band response induced from GaN material. As shown in Figure 8, the peak responsivity was  $2.65 \times 10^4$  A/W for 365 nm at 7 V applied bias, and the responsivity at the 270–360 nm band exceeded  $1.5 \times 10^4$  A/W, which is a further order of magnitude enhancement than sample B. These results show that larger surface area leads to greater internal gain, which is consistent with the proposed mechanisms as aforementioned. Nevertheless, it is possible to further optimize the thickness of Ga<sub>2</sub>O<sub>3</sub> film on GaN by adjusting the oxidation time, and realize the tunable detection in UV band. Overall, we proposed a simple method to fabricate the B-UV PD with high responsivity, which enables the detection under weak light illuminations.

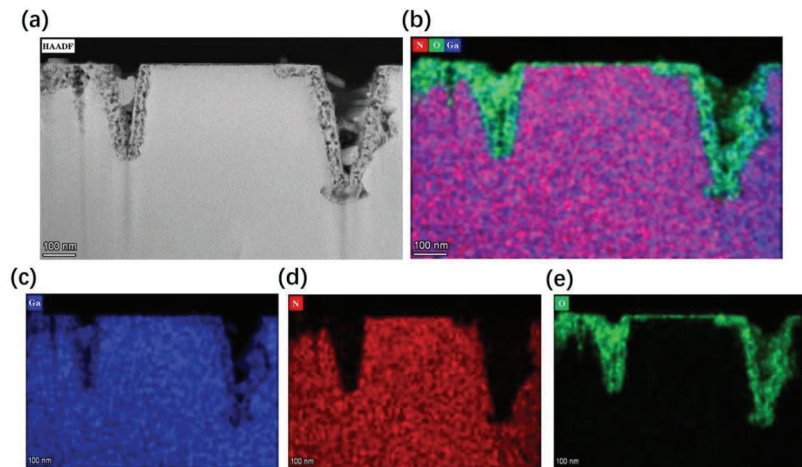


Figure 7. (a) Cross-section SEM image of Ga<sub>2</sub>O<sub>3</sub>/GaN NRA and (b) corresponding element mapping; (c–e) are distribution diagrams of Ga, N and O elements respectively.

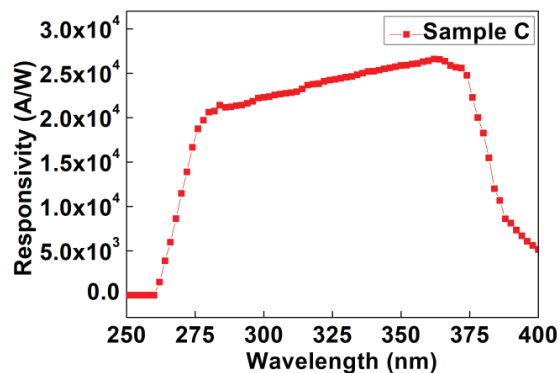


Figure 8. Spectral responsivity values of sample C as a function of wavelength at 7 V bias.



#### 4. Conclusions

In this study, we designed and demonstrated a BUUV PD based on Ga<sub>2</sub>O<sub>3</sub>/GaN core-shell MRAs and NRAs, which were fabricated using partially thermally oxidizing GaN MRAs and NRAs. The PD based on MRAs showed an ultrahigh responsivity of 2300 A/W for 280 nm and over 1500 A/W for the 270–360 nm band at 7 V. The detectivity and external quantum efficiency were approximately  $2.65 \times 10^{13}$  Jones and  $1.02 \times 10^6\%$  at 280 nm, respectively. The responsivity was further increased to  $2.65 \times 10^4$  A/W for 280 nm and over  $1.5 \times 10^4$  A/W for 270–360 nm using the nanorod arrays. Such high performance can be attributed to the blocking of photo-generated holes. Specifically, the large surface area of Ga<sub>2</sub>O<sub>3</sub>/GaN MRAs and NRAs led to the migration of photogenerated holes to the surface of Ga<sub>2</sub>O<sub>3</sub> film, which was caused by the band bending of Ga<sub>2</sub>O<sub>3</sub> surface induced by oxygen absorption mechanism and resulted in the large internal gains. Moreover, the larger metal electrode area can block more holes at the heterojunction interface of Ga<sub>2</sub>O<sub>3</sub>/GaN, which was caused by the larger valence-band barrier (1.4 eV). Overall, the proposed metal–semiconductor–metal structure enables a large surface area and is suitable for mass production.

**Author Contributions:** R.T., J.L. and K.H. conceived the idea and designed the experiments. J.L. and K.H. supervised the project. R.T., G.L. and N.G. explored the oxidation process and the devices' fabrication. R.T., G.L. and J.L. performed the device characterization and the simulation. R.T., X.H., J.L., K.H., J.K. and R.Z. analyzed the data and contributed to the mechanism investigation. R.T., J.L. and K.H. wrote the manuscript. All authors participated in the discussion and commented on the manuscript. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research was funded by Key Technologies Research and Development Program (2021YFB3600101); National Natural Science Foundation of China (62174141, 61974126, 51902273, and 61874090); Key scientific and technological Program of Xiamen (3502Z20191016); Natural Science Foundation of Fujian Province (No. 2021J01008).

**Conflicts of Interest:** The authors declare no conflict of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript; or in the decision to publish the results.

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Article

# MOCVD-grown $\beta$ -Ga<sub>2</sub>O<sub>3</sub> as a Gate Dielectric on AlGaN/GaN-Based Heterojunction Field Effect Transistor

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**Abstract:** We report the electrical properties of Al<sub>0.3</sub>Ga<sub>0.7</sub>N/GaN heterojunction field effect transistor (HFET) structures with a Ga<sub>2</sub>O<sub>3</sub> passivation layer grown by metal–organic chemical vapor deposition (MOCVD). In this study, three different thicknesses of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> dielectric layers were grown on Al<sub>0.3</sub>Ga<sub>0.7</sub>N/GaN structures leading to metal-oxide-semiconductor-HFET or MOSHFET structures. X-ray diffraction (XRD) showed the (201) orientation peaks of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> in the device structure. The van der Pauw and Hall measurements yield the electron density of  $\sim 4 \times 10^{18} \text{ cm}^{-3}$  and mobility of  $\sim 770 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  in the 2-dimensional electron gas (2DEG) channel at room temperature. Capacitance–voltage (C–V) measurement for the on-state 2DEG density for the MOSHFET structure was found to be of the order of  $\sim 1.5 \times 10^{13} \text{ cm}^{-2}$ . The thickness of the Ga<sub>2</sub>O<sub>3</sub> layer was inversely related to the threshold voltage and the on-state capacitance. The interface charge density between the oxide and Al<sub>0.3</sub>Ga<sub>0.7</sub>N barrier layer was found to be of the order of  $\sim 10^{12} \text{ cm}^{-2} \text{ eV}^{-1}$ . A significant reduction in leakage current from  $\sim 10^{-4} \text{ A/cm}^2$  for HFET to  $\sim 10^{-6} \text{ A/cm}^2$  for MOSHFET was observed well beyond pinch-off in the off-stage at -20 V applied gate voltage. The annealing at 900 °C of the MOSHFET structures revealed that the Ga<sub>2</sub>O<sub>3</sub> layer was thermally stable at high temperatures resulting in insignificant threshold voltage shifts for annealed samples with respect to as-deposited (unannealed) structures. Our results show that the MOCVD-grown Ga<sub>2</sub>O<sub>3</sub> dielectric layers can be a strong candidate for stable high-power devices.

**Keywords:** GaN; MOSHFET; Ga<sub>2</sub>O<sub>3</sub>; MOCVD; gate dielectric

**Citation:** Hasan, S.; Jewel, M.U.; Crittenden, S.R.; Lee, D.; Avrutin, V.; Özgür, Ü.; Morkoç, H.; Ahmad, I. MOCVD-grown  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> as a Gate Dielectric on AlGaN/GaN-Based Heterojunction Field Effect Transistor. *Crystals* **2023**, *13*, 231. <https://doi.org/10.3390/cryst13020231>

Academic Editors: Peng Chen and Zhizhong Chen

Received: 6 January 2023

Revised: 21 January 2023

Accepted: 23 January 2023

Published: 28 January 2023



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## 1. Introduction

GaN-based heterojunction field effect transistors (HFETs) have excellent properties such as high critical breakdown field, high current, and superior thermal/chemical stability, which are coveted for high power, both RF and high-frequency switching applications under harsh environments [1–4]. The high-frequency performance of HFETs is limited by a series of effects associated with charge leakage, trapping/de-trapping, and conduction characteristics at different locations of the devices [5]. One of the most significant performance-limiting phenomena is the injection of electrons from the gate electrode to the surface region of the semiconductor on the drain side of the gate electrode, which results in reliability issues as well as limitations on the input drive in power applications [6,7]. For high drain and gate bias, the magnitude of the electric field under the gate region can cause tunneling/leakage of electrons from the gate metal to the semiconductor. Thus, the tunneling/gate leakage effect becomes critical for radio frequency (RF) applications because the electric field oscillates with the total terminal (dc+RF) voltage [8]. During the high voltage portion of the RF cycle, a pulse of electrons will tunnel from the gate by acquiring sufficient energy and can cause gate breakdown [9,10]. The electron transport

on the surface is sluggish due to high effective mass, and dispersion is introduced due to the charging/discharging time constant [11]. The electrons escaping from the gate metal gather on the surface, creating a “virtual gate” effect that functions as an effective increase in gate length on the drain side can result in leakage current [7]. As a result, the conducting channel depletes of free electrons, and the device dc current and RF power decreases [7]. To overcome this problem, a dielectric material, often an oxide layer, is introduced between the metal gate and the semiconductor, creating metal-oxide-semiconductor-HFET (MOSHET) for high-frequency applications. Thus, the gate tunneling is reduced or eliminated with improved surface charge modulation by an insulating oxide layer under the gate [7,12].

The incorporation of the oxide layer improves the GaN-based HFET performance by minimizing the gate leakage current, maximizing the output power (as the input can be driven harder), improving the breakdown voltage, etc [13]. The interface between the semiconductor and oxide layer, however, plays an important role in transistor performance [14]. Chemically and thermally stable oxides with low density of interface states between the insulator (oxide) and semiconductor are required [15]. Several groups have reported the use of different dielectrics, such as aluminum oxide ( $\text{Al}_2\text{O}_3$ ) [16], hafnium dioxide ( $\text{HfO}_2$ ) [17], zirconium dioxide ( $\text{ZrO}_2$ ) [18], silicon dioxide ( $\text{SiO}_2$ ) [19], silicon nitride ( $\text{Si}_3\text{N}_4$ ), and hexagonal boron nitride (h-BN) [20], fabricated by several deposition methods, including atomic layer deposition (ALD) [14], pulsed laser deposition (PLD) [21], and plasma enhanced chemical vapor deposition (PECVD) [21].  $\text{SiO}_2/\text{hBN}$  has also been reported to be used as a substrate material for field effect transistors [22].

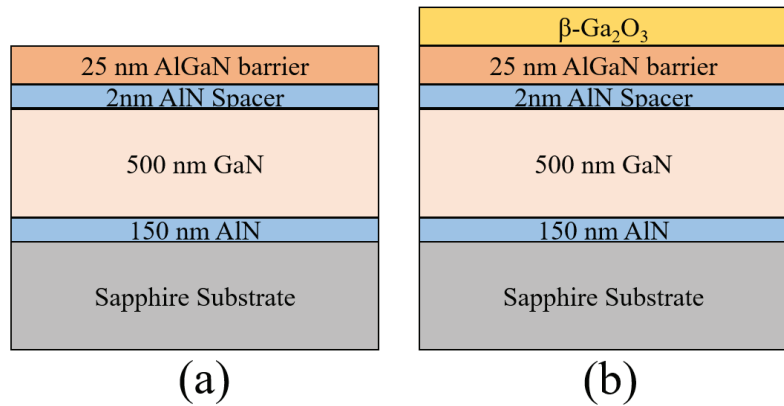
$\text{Ga}_2\text{O}_3$  is a promising material with potential dielectric applications for high-power devices because of its wide bandgap (4.4–5.3 eV) and high breakdown voltage ( $8 \text{ MVcm}^{-1}$ ) [23,24]. It has a moderate dielectric constant ( $k = 10.6$ ), which is higher than those of traditional dielectrics such as  $\text{SiO}_2$  ( $k = 3.9$ ), and  $\text{Si}_3\text{N}_4$  ( $k = 7.4$ ) [16]. This dielectric-constant value allows gate scaling and a smaller voltage for the same charge. The feasibility of using  $\text{Ga}_2\text{O}_3$  as a gate dielectric was demonstrated by employing ALD with compounds such as trimethylgallium, and triethylgallium as a Ga precursor and ozone or oxygen ( $\text{O}_2$ ) plasma as an oxygen precursor [23,25,26]. The  $\text{Ga}_2\text{O}_3$  layers grown by ALD for MOSHFETs are amorphous and prone to change their properties, especially threshold voltage, with annealing due to crystallization [27]. The use of crystalline metal-organic chemical vapor deposition (MOCVD) grown  $\beta\text{-Ga}_2\text{O}_3$  as a gate dielectric has so far not been reported. A comprehensive study of the electrical properties is necessary to determine the feasibility of MOCVD  $\text{Ga}_2\text{O}_3$  as a gate dielectric.

In this work, we study the electrical properties of  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}/\text{GaN}$  HFET with MOCVD-grown  $\beta\text{-Ga}_2\text{O}_3$  as a passivation/dielectric layer.  $\beta\text{-Ga}_2\text{O}_3$  layers of three different thicknesses of 10 nm, 20 nm, and 30 nm were grown on top of  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}/\text{GaN}$  creating MOSHFET structures. Furthermore, the variations in electrical properties, particularly the shift in threshold voltage, are studied for annealed and as-deposited MOSHFET structures with MOCVD-grown  $\beta\text{-Ga}_2\text{O}_3$ .

## 2. Experimental Methods

The epilayers used for devices studied in this paper were deposited in a vertical cold wall metal-organic chemical vapor deposition (MOCVD) system using nitrogen ( $\text{N}_2$ ) as a carrier gas on a 2-inch diameter c-axis sapphire substrate with  $0.2^\circ$  offcut. Trimethylaluminum (TMAI), triethylgallium (TEG), ammonia ( $\text{NH}_3$ ), and ultra-high purity oxygen were used as aluminum (Al), gallium (Ga),  $\text{N}_2$ , and oxygen ( $\text{O}_2$ ) precursors, respectively. First, a thin 150 nm aluminum nitride (AlN) buffer layer was grown on the sapphire substrate using the process described in [28,29]. Then, on top of the AlN layer, a 500 nm thick gallium nitride (GaN) channel layer with a V/III ratio of 8000 at a temperature of  $960^\circ\text{C}$ , a 2 nm AlN spacer, and a 25 nm thick barrier aluminum gallium nitride ( $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}$ ) layers with V/III ratio of 5000 at a temperature of  $1020^\circ\text{C}$  were grown at 100 Torr chamber pressure, creating heterojunction field effect transistor (HFET) structure [30–32]. The van der Pauw and Hall effect measurements show that the GaN layers used for our device structures

were highly resistive. Figure 1 shows the schematic of the FET epilayer structures used in this paper where, Figure 1a exhibits the schematic of the HFET structure. For this study, the  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> layers were grown on top of the HFET structure using the MOCVD process at 700 °C, 50 Torr chamber pressure, and a VI/III ratio of ~900. The details of the Ga<sub>2</sub>O<sub>3</sub> growth can be found elsewhere [33]. This creates a MOSHFET structure with the dielectric layer thickness varying from 10 nm to 30 nm, as shown in Figure 1b. The MOSHFET structure with 30 nm oxide thickness was annealed to gauge its electrical and thermal stability. Annealing was performed at 900 °C for 30 min in a 50/50 O<sub>2</sub>/N<sub>2</sub> (nitrogen was used as carrier gas) environment to avoid desorption from the Ga<sub>2</sub>O<sub>3</sub> layer.



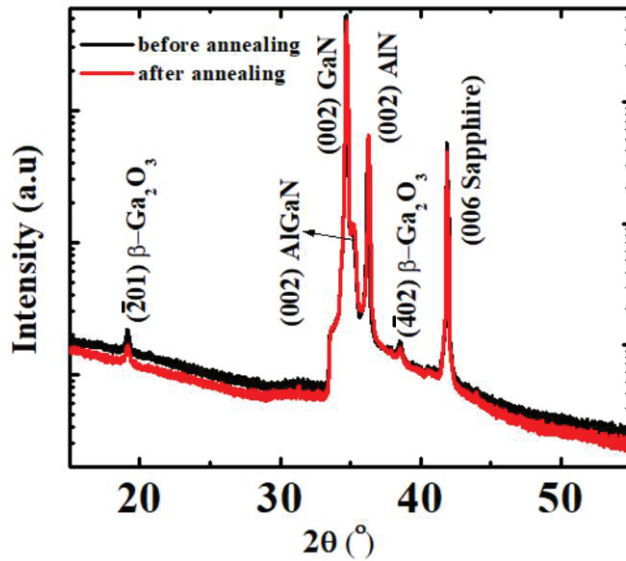
**Figure 1.** The epilayer structure of the (a) Al<sub>0.3</sub>Ga<sub>0.7</sub>N/GaN HFET, (b) Ga<sub>2</sub>O<sub>3</sub> MOSHFET.

We characterized the structural quality and electrical properties of all the device structures obtained in this work. A Rigaku Miniflex II Desktop X-ray diffractometer with Cu-K $\alpha$ 1 x-ray source ( $\lambda = 1.5406 \text{ \AA}$ ) operated at 30 mA current and 15 kV voltage was used to evaluate the structural properties of the epilayers. The capacitance–voltage (C-V) measurements were performed using a mercury probe controller model 802B connected with a HP 4284A Precision LCR Meter capable of measuring the impedance as a function of frequency. Gate leakage current was measured in the same mercury probe set up with Keysight B2910 Precision Source/Measure Units (SMU). The gate diameter of the mercury probe was 797  $\mu\text{m}$  with 0.1 pF stray capacitance. The van der Pauw/Hall effect measurements were performed on the samples using the MMR Technologies Inc. H-50 controller and MPS-50 programmable power supply with indium contacts.

### 3. Results and Discussions

Figure 2 shows the X-ray diffraction (XRD)  $2\theta$  scan of the MOSHFET structure (before and after annealing). The peaks at 18.8° and 38.2° are related to the (201) and (402) Ga<sub>2</sub>O<sub>3</sub> of the  $\beta$  phase [34]. The peak at 34.5° and the adjacent higher angle shoulder are consistent with the (002) and (002) reflection from the GaN channel and AlGaN barrier layers, respectively [35]. Note that the GaN channel layer was grown on 0.15  $\mu\text{m}$  AlN. The peak at 36.1° is due to the (002) AlN reflection. The peaks at 20.4° and 41.6° correspond to the (003) and (006) sapphire reflections [34]. The most common method of oxide dielectric deposition is ALD, which is mostly used for depositing amorphous materials [36]. The problem with amorphous layers is that, during the rapid thermal annealing (RTA) step required to form ohmic contacts to MOSHFETs, there occurs a phase transformation from amorphous to crystalline structure [27]. This transformation results in the formation of a microcrystalline structure with multiple grain boundaries, which creates leakage paths, rendering it unsuitable for device applications [27]. The process used for the MOCVD oxide deposition favors the growth of single-crystal  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> dielectric layers, as confirmed by the XRD data. Therefore, it is expected that, as Ga<sub>2</sub>O<sub>3</sub> is already in the crystalline

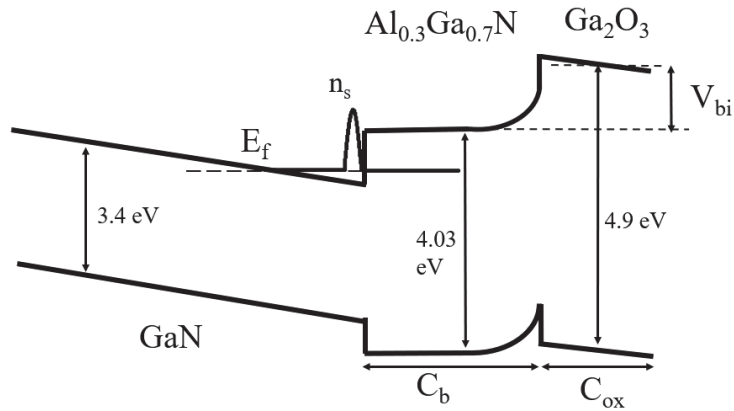
form, the thermal treatment will have a minimal impact on its electrical properties, as we demonstrate by the annealing experiments in the later description.



**Figure 2.** XRD  $2\theta$  scan of the MOSHFET structure (before and after annealing) confirming the presence of the peaks consistent with crystalline  $\text{Ga}_2\text{O}_3$  ( $\beta$  phase), GaN, AlGa<sub>3</sub>N, AlN, and sapphire substrate.

The origin of the highly conductive quantum confined two-dimensional electron gas (2DEG) at the AlGa<sub>3</sub>N/GaN interface is due to the lack of inversion symmetry along the [0001] axis of GaN coupled with AlN being relatively more electronegative [2]. The difference between spontaneous and piezoelectric polarization and band offset at the interface introduces a fixed polarization-induced sheet of carrier charges, indicated by the shift of Fermi level in the conduction band. Schrödinger and Poisson's equation-based charge distribution and band diagram can be calculated using different available tools [37]. However, a simpler approach using the Langer and Heinrich rule helps to estimate different parameters and understand the band structure at the heterojunction interfaces [38,39]. Figure 3 shows the schematical band diagram for the  $\text{Ga}_2\text{O}_3$  MOSHFET. The bandgaps for GaN, Al<sub>0.3</sub>Ga<sub>0.7</sub>N, and  $\text{Ga}_2\text{O}_3$  are 3.4 eV, 4.03 eV (using Vegard's law), and 4.9 eV ( $\beta$  phase), respectively [40]. The position of the Fermi level in GaN near the channel-barrier interface is in the conduction band; where  $n_s$  is the sheet carrier density,  $C_b$  is the Al<sub>0.3</sub>Ga<sub>0.7</sub>N barrier layer capacitance,  $C_{ox}$  is the  $\text{Ga}_2\text{O}_3$  layer capacitance. We can express the total gate capacitance ( $C_G$ ) using the series capacitance formula as below:

$$\frac{1}{C_G} = \frac{1}{C_b} + \frac{1}{C_{ox}} \quad (1)$$



**Figure 3.** The representative band diagram of GaN/AlGaIn MOSHFET with Ga<sub>2</sub>O<sub>3</sub> as a gate dielectric.

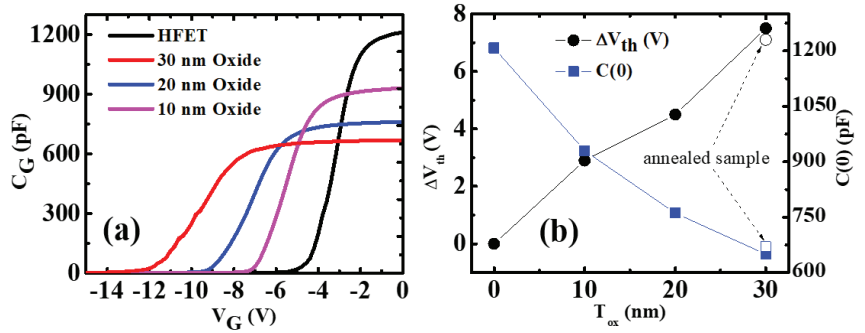
The capacitance–voltage (*C-V*) measurements of the MOSHFET structure were performed using a mercury probe gate contact to extract pertinent electrical parameters of the device structures, such as threshold voltage ( $V_{th}$ ), zero gate voltage capacitance, and 2DEG electron density. The total gate capacitance is given by Equation (1), i.e., the addition of the oxide dielectric layer capacitance in series with the barrier layer capacitance. The benefit of an oxide dielectric is to increase the gate breakdown voltage and/or reduce the gate leakage current by suppressing the surface states, sometimes superseded by the impact of different device electrical parameters such as threshold voltage and gate leakage current. The threshold voltage of the MOSHFET structure is given by the Equation [41]:

$$V_{th,MOSHFET} = V_{th,HFET} \left( 1 + \frac{d_i \epsilon_{s,b}}{\epsilon_i d_{s,b}} \right) \quad (2)$$

where  $V_{th,MOSHFET}$  and  $V_{th,HFET}$  are the threshold voltage of the MOSHFET and HFET (that without the oxide layer- otherwise identical), respectively.  $d_i$ ,  $d_{s,b}$ ,  $\epsilon_i$  and  $\epsilon_{s,b}$  are the thicknesses and dielectric constants of the insulator/oxide (indexed by  $i$ ) and semiconductor barrier (indexed by  $s,b$ ) layers, respectively. From equation (2), it is clear that if  $d_i$  increases,  $V_{th,MOSHFET}$  increases, whereas  $V_{th,MOSHFET}$  decreases with the increase in  $\epsilon_i$ . Thus, a higher dielectric constant and lower dielectric thickness are desirable for minimum threshold voltage shifts.

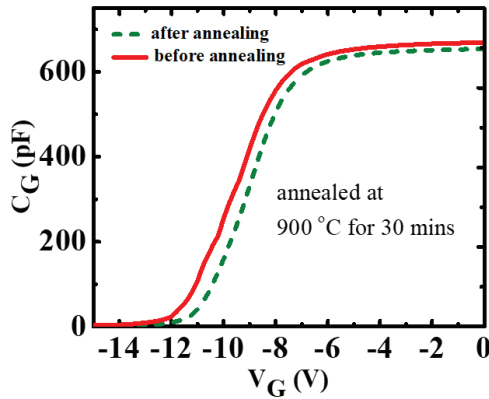
Figure 4 shows the capacitance voltage characteristics, threshold voltage and zero capacitance dispersion of our samples. Figure 4a shows the *C-V* data for HFET and MOSHFET structures with oxide thicknesses of 10 nm, 20 nm, and 30 nm. The addition of oxide on the HFET barrier adds capacitance in series with the existing barrier layer capacitance, which would lower the overall gate capacitance. The relative dielectric constants for the AlGaIn barrier layer (9.2) and that for the Ga<sub>2</sub>O<sub>3</sub> (10.6) are very close [42], and the AlGaIn barrier layers is undoped. Due to these reasons, we did not observe any change in the *C-V* curve shape near the zero-gate voltage position when increasing the negative gate voltage before depleting the channel. From equation (2), we observe that as the thickness of the oxide layer increases, the  $V_{th}$  should increase. The *C-V* measurements on the MOSHFET structure with MOCVD-grown Ga<sub>2</sub>O<sub>3</sub> gate dielectric confirm the increase in the  $V_{th}$  value. As the thickness of the Ga<sub>2</sub>O<sub>3</sub> layer increased, the  $V_{th}$  exhibited a negative shift. Thus, with the increase in dielectric layer thickness, a higher voltage is required to deplete the 2DEG. During the *C-V* measurement, when 2DEG starts to deplete, the capacitance decreases drastically, ultimately leading to pinching off of the channel. By further increasing the gate voltage beyond pinch-off, the depletion layer extends to the GaN channel. Figure 4b summarizes the above discussion.





**Figure 4.** C-V characteristics at 1MHz frequency of (a) HFET and  $\text{Ga}_2\text{O}_3$ -based MOSHFETs with different oxide thicknesses, (b) Threshold voltage and zero gate-voltage capacitance dispersion for HFET and  $\text{Ga}_2\text{O}_3$  MOSHFETs.

Figure 5 compares the C-V data for annealed and as-deposited MOSHFETs with a 30 nm thick  $\beta\text{-Ga}_2\text{O}_3$  as a gate oxide layer. The 30-min annealing at 900 °C was performed in the MOCVD reactor, used for the  $\text{Ga}_2\text{O}_3$  growth, as described in the experimental method section. As shown in Figure 2, the pre and post-annealed XRD was similar. As can be concluded from the C-V data, the annealing experiment did not result in any discernable change in the  $V_{th}$  and zero capacitance values, demonstrating the excellent thermal stability of the crystalline  $\beta\text{-Ga}_2\text{O}_3$ . The change in threshold voltage (open circle) and capacitance (open square) for the annealed MOSHFET structure are also shown in Figure 4b.



**Figure 5.** C-V data of at 1MHz frequency  $\text{Ga}_2\text{O}_3$ -based MOSHFET with 30 nm oxide thickness annealed (dashed line) and unannealed (continuous line).

The carrier density  $N_d$  was calculated using the Hall effect data and found to be on the order of  $10^{18} \text{ cm}^{-3}$ , the exact values of the carrier density can be found in Table 1. The built-in voltage  $V_{bi}$  (as shown in the band diagram: Figure 2) can be measured from  $1/C^2$  intercept with the x-axis and expressed by equation (3) [43]:

$$V_{bi} = \frac{qN_d x_d^2}{2\epsilon_s} + \frac{qN_d x_d}{\epsilon_{ox}} t_{ox} + \frac{Q_{ox}}{\epsilon_{ox}} t_{ox} \quad (3)$$



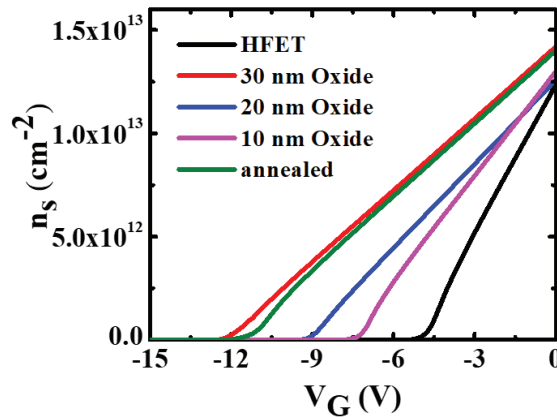
**Table 1.** The summary of the key electrical parameters measured/calculated from C-V and Hall measurements.

	$V_{th}$ (V)	$\mu$ ( $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ ) (Hall)	$R_{sh}$ ( $\Omega\text{cm}^{-2}$ ) (Hall)	$N_d$ ( $\text{cm}^{-3}$ ) (Hall)	$n_s$ ( $\text{cm}^{-2}$ ) (C-V)	$n_s$ ( $\text{cm}^{-2}$ ) (Hall)	$Q_{ox}$ ( $\text{Ccm}^{-2}$ ) (C-V)	$D_{it}$ ( $\text{cm}^{-2}\text{eV}^{-1}$ ) (C-V)	Leakage Current at -20 V ( $\text{A}/\text{cm}^{-2}$ )
HFET	-5	750	537	$6.8 \times 10^{18}$	$1.25 \times 10^{13}$	$1.55 \times 10^{13}$	None	None	$1.66 \times 10^{-4}$
10 nm	-7.9	772	630	$5.0 \times 10^{18}$	$1.28 \times 10^{13}$	$1.4 \times 10^{13}$	$-6.68 \times 10^{12}$	$7.47 \times 10^{12}$	$1.3 \times 10^{-6}$
20 nm	-9.5	770	650	$4.2 \times 10^{18}$	$1.24 \times 10^{13}$	$1.42 \times 10^{13}$	$-1.64 \times 10^{13}$	$7.57 \times 10^{12}$	$1.12 \times 10^{-6}$
30 nm	-12.5	776	685	$4.4 \times 10^{18}$	$1.4 \times 10^{13}$	$1.4 \times 10^{13}$	$-2 \times 10^{13}$	$4.98 \times 10^{12}$	$9.54 \times 10^{-7}$
annealed	-12.1	760	680	$4.5 \times 10^{18}$	$1.4 \times 10^{13}$	$1.4 \times 10^{13}$	$-3.06 \times 10^{12}$	$3 \times 10^{12}$	$8.33 \times 10^{-7}$

Here,  $t_{ox}$  and  $\epsilon_{ox}$  are the thickness and permittivity of the oxide layer,  $N_d$  is the carrier concentration,  $x_d$  and  $\epsilon_s$  are the depletion width and permittivity of the AlGaN barrier layer. If we set  $t_{ox} = 0$ , then the 2nd and 3rd term of Equation (3) becomes zero, and the equation represents the built-in voltage for conventional HFET structure. Using Equation (1) and the parallel plate capacitance formula for each series capacitor component, we can calculate the value of  $x_d$  at zero gate voltage. Inserting the determined value of  $x_d$ , and previously calculated/measured  $N_d$ ,  $t_{ox}$ , and known  $\epsilon_{ox}$ ,  $\epsilon_s$  into Equation (3), we can obtain the oxide charge  $Q_{ox}$ . The calculated values of  $Q_{ox}$  for all the samples is shown in Table 1. We observe a trend in the value of  $Q_{ox}$ ; as the oxide thickness increases, the value of  $Q_{ox}$ , become more negative which increases  $V_{th}$  shift supporting Equation (2). There may be impact of stress on the charge, but we did not isolate that in our calculation. Due to low thickness, we did not observe any signature peak of the dielectric  $\text{Ga}_2\text{O}_3$  or barrier AlGaN layer in Raman measurement (Figure S2 in Supplementary Section).

Figure 6 shows the 2DEG carrier density ( $n_s$ ) versus the gate voltage ( $V_G$ ) for 10, 20, and 30 nm gate oxide thicknesses calculated using the following equation:

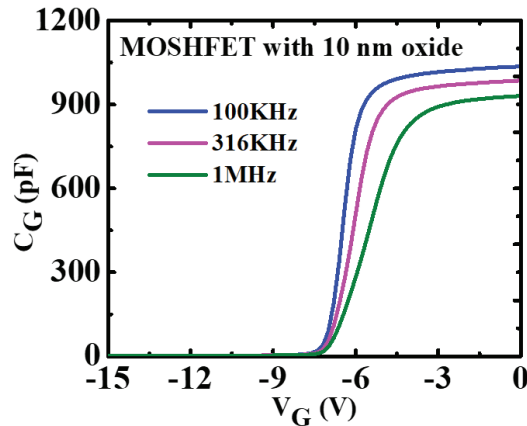
$$qn_s = (V_G - V_{th})C_G \quad (4)$$

**Figure 6.** 2DEG carrier density in FETs vs. applied gate voltage for different gate oxide thicknesses.

In all three cases, the zero-gate voltage value of sheet carrier density is very close in the range of  $(1.25\text{--}1.5) \times 10^{13} \text{ cm}^{-2}$ , a slightly higher value of  $n_s$  could be due to sample-to-sample variations. The sheet carrier concentrations measured using van der Pauw/Hall effect method are also in the range of  $(1\text{--}1.5) \times 10^{13} \text{ cm}^{-2}$ , which validates our calculations using the value from the C-V measurement by employing equation (4). The sheet carrier

concentration does not change with oxide layer thickness or annealing of the oxide layer. In previous studies for the ALD-grown amorphous oxide dielectrics-based MOSHFETs, it has been demonstrated that the annealing of the oxide layers drastically shifts  $V_{th}$ . As we can see in Figure 5, annealing of the crystalline  $\text{Ga}_2\text{O}_3$ -based MOSHFET, there is no noticeable change in the threshold voltage in contrast to the case for previously reported ALD-grown oxides [44]. To further validate the MOCVD oxide material property we can use Equation (1), to calculate the experimental dielectric constant for  $\beta\text{-Ga}_2\text{O}_3$ . The values of the gate capacitance,  $C_G$ , before and after annealing are  $1.64 \times 10^{-7} \text{ F/cm}^{-2}$  and  $1.67 \times 10^{-7} \text{ F/cm}^{-2}$  (for 1 MHz frequency measurement).  $C_b$  is the barrier capacitance of the MOSHFET, and the value is  $3.3 \times 10^{-7} \text{ F/cm}^{-2}$ . Based on  $C_{ox} = \frac{\epsilon_r \epsilon_0}{t_{ox}}$ , we get  $\epsilon_r = 10.9$  (using  $C_G = 1.67 \times 10^{-7} \text{ F/cm}^{-2}$ ), whereas the reference value is 10.6. Thus, it can be inferred that the MOCVD-grown oxide has a dielectric property that is very close to the previously reported literature value [42].

The interface trapped charge or interface traps stem(s) from dangling bonds at the semiconductor–insulator interface. The frequency-dependent High–Low method is commonly used to determine interface charge density ( $D_{it}$ ). Figure 7 shows the frequency-dependent CV measurement used to calculate the interface charge densities for MOSHFET with 10 nm oxide thickness (the frequency-dependent C–V measurements of MOSHFET with 20 nm, 30 nm oxide thickness along with the annealed sample are shown in the Supplementary Section Figure S1).



**Figure 7.** Frequency-dependent C–V characteristic of a MOSHFET with 10 nm thick gate oxide at frequencies of 100 kHz, 316 kHz, and 1 MHz.

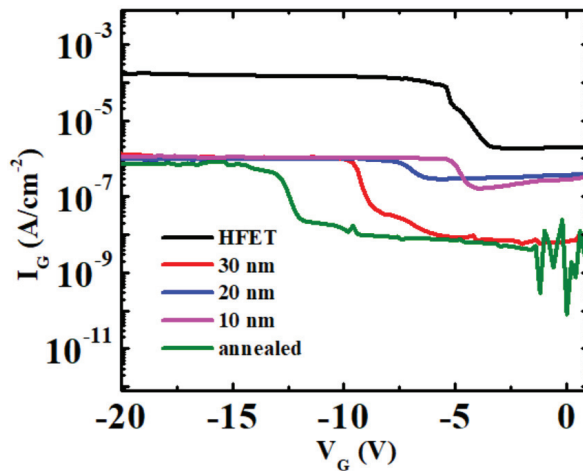
The High–Low frequency CV method compares a low-frequency C–V curve with one that is free of interface traps. The latter is usually referred to as a high-frequency C–V measurement, where interface traps with relatively long-time constants cannot respond, leading to decreased measured capacitance. At low frequencies, the interface traps can respond, if not deep, thus resulting in higher capacitance; 100 kHz and 1 MHz frequencies are the typical values can be used for CV-based calculations of the density of interface states ( $D_{it}$ ) of Nitride systems [45]. Consequently, from the difference between high- and low-frequency CV measurements, the  $D_{it}$  can be obtained based on Equation (5) at a specific applied gate voltage [46]:

$$D_{it}(V_G) = \frac{C_{ox}}{q} \left( \frac{C_{LF}}{C_{ox} - C_{LF}} - \frac{C_{HF}}{C_{ox} - C_{HF}} \right) \quad (5)$$

where  $C_{ox}$  is the capacitance of the oxide dielectric layer calculated using the parallel plate capacitor formula,  $q$  is the unit elementary charge,  $C_{LF}$  is the MOSHFET low-frequency

capacitance value and  $C_{HF}$  is the MOSHFET high-frequency capacitance value. The total trap densities for all the samples are tabulated in Table 1. For all samples, the calculated interface trap densities are in the range  $(3\text{--}7.57) \times 10^{12} \text{ cm}^{-2}\text{eV}^{-1}$ ; these values are close to the typically calculated values of MOSHFETs (typical values are in the order of  $\sim 10^{11} \text{ cm}^{-2}\text{eV}^{-1}$ – $10^{13} \text{ cm}^{-2}\text{eV}^{-1}$ ) [27]. The  $D_{it}$  value is expected to be lower for the processed devices due to the mesa isolation [47]. Our data revealed no specific correlation between the oxide thickness and interface trap densities. Ideally, this is the case, but the total number of bulk defects in the oxide under the gate would depend on the thickness, more data are needed to find any correlation. It is observed that the annealed sample showed a slightly smaller trap density, which can correlate to the higher  $n_s$ , the origin of which is not yet explored.

To further investigate the  $\beta\text{-Ga}_2\text{O}_3$  viability as a gate dielectric leakage current measurements were performed for all the samples. Figure 8 shows the gate leakage current in the HFET and different thicknesses  $\beta\text{-Ga}_2\text{O}_3$  MOSHFET structure. There is a significant reduction in leakage current for the MOSHFET structure compared to the HFET structure in the off-stage. The leakage current at  $-20 \text{ V}$  for HFET is  $\sim 10^{-4} \text{ A/cm}^2$ , and it reduces to  $\sim 10^{-6} \text{ A/cm}^2$  for MOSHFET. This remarkable improvement in the gate leakage current shows that  $\beta\text{-Ga}_2\text{O}_3$  can be used as an effective dielectric layer for GaN/AlGaN MOSHFETs. Table 1 summarizes the key electrical parameters of the GaN/AlGaN-based HFET and GaN/AlGaN/ $\beta\text{-Ga}_2\text{O}_3$ -based MOSHFET determined in this work.



**Figure 8.** Gate leakage current characteristics for HFET and for different gate oxide thicknesses MOSHFET.

#### 4. Conclusions

We have demonstrated MOCVD-grown single-crystal  $\text{Ga}_2\text{O}_3$  thin films as a gate dielectric on AlGaN/GaN HFETs. We have found that an increase in the thickness of the dielectric layer has an impact on threshold voltage  $V_{th}$ , shifting it to more negative values and reducing the zero capacitance as additional  $C_{ox}$  is added in series. The sheet carrier densities for HFET and MOSHFETs were determined to be  $\sim 10^{13} \text{ cm}^{-2}$ , well within the typical range-of  $10^{12} \text{ cm}^{-2}$ – $10^{13} \text{ cm}^{-2}$  for AlGaN/GaN-based devices. The leakage current was reduced by approximately 2 order from  $\sim 10^{-4} \text{ A/cm}^2$  for HFET to  $\sim 10^{-6} \text{ A/cm}^2$  for MOSHFET at  $-20 \text{ V}$ . Moreover, the addition of the oxide layer did not change the sheet carrier concentration but had an impact on the calculated value of oxide charge  $Q_{ox}$ . The calculated  $Q_{ox}$  value was found to be negative and mainly responsible for depleting the 2DEG. As the thickness of the  $\text{Ga}_2\text{O}_3$  layer increases, the  $Q_{ox}$  becomes more negative, following a trend similar to the change in  $V_{th}$  with increasing gate oxide thickness. The

charge density in the oxide–AlGa<sub>N</sub> barrier interface was found to be of the order of  $\sim 10^{12}$  cm<sup>2</sup>eV<sup>-1</sup>. The thermal stability, as confirmed by the annealing experiment, suggests that the MOCVD-grown single-crystal Ga<sub>2</sub>O<sub>3</sub> layer could be more suitable for the gate dielectric application compared to the ALD-grown oxide due to threshold voltage stability. The moderate interface trap density and good thermal stability indicate that MOCVD-grown  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is an excellent candidate for gate dielectric as well as a passivation layer for III-Nitride-based high-power RF MOSHFET devices.

**Supplementary Materials:** The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/cryst13020231/s1>. Figure S1. Frequency-dependent CV measurements of MOSHFET with (a) 20 nm thick gate oxide (b) 30 nm thick gate oxide, and (c) annealed 30 nm thick gate oxide. Figure S2. (a) Raman spectra of HFET and MOSHFET (30 nm oxide), (b) Raman spectra of Ga<sub>2</sub>O<sub>3</sub> on sapphire to identify the Ga<sub>2</sub>O<sub>3</sub> signature peak positions.

**Author Contributions:** S.H. Conceptualization of this study, Experimentation, Data curation, Methodology, Writing—original draft, M.U.J.: Revision, Experimentation, S.R.C.: Revision, Experimentation, Editing, D.L.: Revision, Experimentation, Editing, V.A.: Revision, Editing, Ü.Ö.: Revision, Editing, H.M.: Revision, Editing, I.A.: Conceptualization of this study, Visualization, Editing, Revision, Principal Investigator of this study. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research was funded by National Science Foundation (NSF), grant number 2124624.

**Data Availability Statement:** The data generated during and/or analyzed during the current study are available from the corresponding authors on reasonable request.

**Acknowledgments:** This research was supported by National Science Foundation (NSF) award No. 2124624 managed by Dominique M. Dagenais.

**Conflicts of Interest:** The authors declare that they have no conflict of interest.

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Article

# Effect of Amorphous Photonic Structure Surface Mounted on Luminous Performances of White LED

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**Abstract:** We fabricated amorphous photonic structures (APSs) with different periods and hole diameters. The GaN-based white light emitting diodes (LEDs) at nominal correlated color temperatures (CCTs) of 5000 and 6000 K were surface mounted by these APSs. The electroluminescence (EL) measurements showed less luminous efficiency (LE) and higher CCT than the ones of the virginal white LEDs. However, the LEs of many APS-mounted white LEDs increased compared to white the LEDs without APSs at the same CCTs. A finite-difference time-domain (FDTD) simulation was carried out on the APSs surface-mounted white LEDs and bidirectional scattering distribution functions (BSDFs) of different emissions were transferred to a Monte Carlo ray tracing simulation. The simulated LEs and CCTs conformed well to the experimental ones. The effects of the blue emission transmission and phosphor concentration were simulated to predict the absolute LE enhancement methods for white LEDs. At last, the hopeful APSs for high Les' general lighting were discussed.

**Keywords:** white light emitting diode (WLED); amorphous photonic structure (APS); luminous efficiency (LE); correlated color temperature (CCT); Fresnel loss; finite-difference time-domain (FDTD)

**Citation:** Huang, F.; Chen, Y.; Nie, J.; Shen, C.; Yuan, J.; Guo, Y.; Dong, B.; Liu, L.; Chen, W.; Chen, Z.; et al. Effect of Amorphous Photonic Structure Surface Mounted on Luminous Performances of White LED. *Crystals* **2023**, *13*, 6. <https://doi.org/10.3390/cryst13010006>

Academic Editor: Robert F. Klie

Received: 31 October 2022

Revised: 25 November 2022

Accepted: 17 December 2022

Published: 20 December 2022



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## 1. Introduction

Phosphor-based white light-emitting diodes (LEDs) are low-cost and popular lighting devices because of their high luminous efficiency, long lifetime, and environmental protection. Although the luminous efficiency of white LEDs with an InGaN active layer in the laboratory have been achieved more than 300 lm/W [1], the commercial ones usually showed a lower efficiency below 200 lm/W. In a phosphor-coated white LED, the interplay between multiple scatterings, emissions, and absorptions of light would be concerned carefully [2]. To reduce the back-scattering and inelastic scattering of blue and yellow lights, some techniques, such as scattered photon extraction (SPE), remote phosphor, multi-layered phosphor, and enhanced light extraction by internal reflection (ELiXIR) are developed [3–6]. The phosphor layer features include the encapsulant and phosphor materials, volume or mass concentration and size distribution of particles, matrix blending, and so on, which can adjust the global performances of the phosphor layer [7–9]. The efficient matching of refractive indexes among the encapsulant, package structure, chip, and phosphor is the key issue in light extraction [10,11]. The light extraction efficiency (LEE) nearly approaches 100% when the resin with a refractive index above 1.8 encapsulated the GaN-based LED [11]. Such high index resin is not available due to its reliability. To improve the LEE of white LEDs is still important and significant in the fields of general lighting and backlight of liquid crystal display. With the maturation of the material and processes of the white LED encapsulation, even several percent enhancement of LEE becomes very difficult [12].



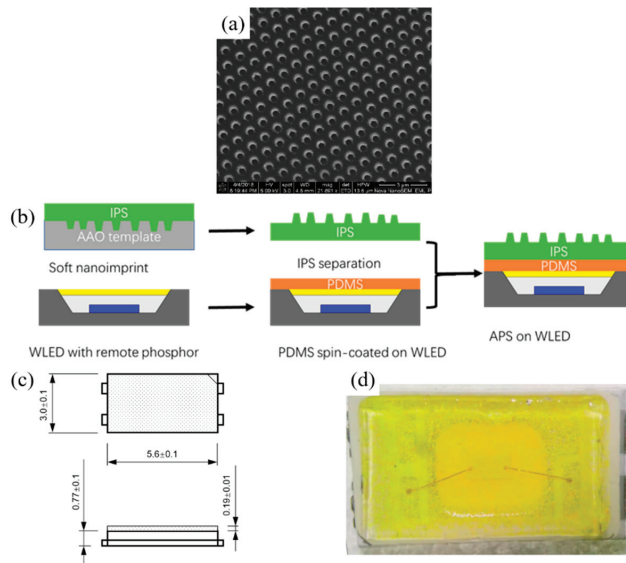
Recently, some nanostructures were applied on the white LED packaging to improve the color conversion efficiency, directionality, and spontaneous emission rate (SER) [13–22]. Quantum dot (QD) material is a type of good phosphor for white LEDs because of its high quantum yield, narrow spectral width, and high SER [13–15]. However, the agglomeration, self-absorption of luminescence, and surface state of the QDs lead to low efficiency in the encapsulant. Dang et al. presented a nonporous (NP) GaN by a simple electrochemical (EC) etching technique, where the QDs do not agglomerate and Förster resonance energy transfer may occur by being immediately proximal to the active layer [13]. The metallic nanostructures cause the surface plasmon coupling to both QD and quantum wells to enhance color conversion [15,22]. The ZnO nanorod is fabricated on the AZO seed layer using the aqueous solution method, which increases the luminous flux of white LED by 60% [16]. The directionality of light emission can be determined by dielectric Vogel spiral arrays or rare-earth phosphor-patterned films [17,18]. The directional emissions are beneficial to imaging and projecting devices. Due to the scattering of the phosphor, the total internal reflection (TIR) at the light extraction surface is not paid much attention. Many people find that flat devices show similar LEEs compared to the structured devices [2,10,23,24]. However, the TIR and Fresnel losses still remain on the light extraction surface [11,16,25–27], which should be alleviated to enhance the LEE of white LEDs.

There are some reports on mounting photonic structures onto the light extraction surface of monochromatic LED packages [28–30]. It is found that the LEE of blue LEDs can be improved even if it has reached over 90% [29]. The moth-eye technique can eliminate the Fresnel reflection effectively [31]. Some moth-eye structures are amorphous photonic structures (APSs) that show short-range order only. So, it is expected that the LEE will be improved when the white LED package surface is mounted with APSs. Moreover, APSs show a strong light extraction ability for a broad spectrum because of its antireflective structures and coherent scattering [32–34]. However, it has not been used in the white LED yet, which consists of a narrow blue emission and a broad yellow emission. In APS optimization, the finite-difference time-domain (FDTD) is used [35]. However, the FDTD simulation is limited to be operated on several microns by the computation capacity. It should combine with other simulators, such as Monte Carlo ray tracing to complete the large-size white LED package simulation [36]. In this work, we proposed an easy and feasible method that nanoscale intermediate polymer stamp (IPS) APSs were transferred to the silicone surface of white the LED package by the surface-mounting method, which was well used in the white LED package by Lumileds Co. [37]. Combined with the nanoimprint technique, it will open a door to apply the nanostructures in the white LED structures. The different periods and hole diameters of APSs were used on the different correlated color temperatures (CCTs). Although all the APS-mounted white LEDs showed less luminous efficiency (LE) than the virginal white LEDs, the LEEs of some APS-mounted white LEDs were enhanced when compared to the same CCT white LEDs without APSs. Moreover, some light output powers (LOPs) were enhanced by surface-mounted APSs. At last, the FDTD combined with ray tracing simulations were carried out, which explained the LE reduction with the APSs and predicted the LE enhancement with appropriate APS structures.

## 2. Material and Methods

APS structures were fabricated from commercial nanoporous anodic aluminum oxide (AAO) templates, typically as shown in Figure 1a. The templates were the silicon replicas of the original AAO structures on aluminum sheets. In this work, the quasi-periods of AAO templates were about 450 and 800 nm. The hole diameters were 400, 300, and 200 nm for the 450 nm-period AAO templates and the depths were about 500 nm, which corresponded to APS-1, APS-2, and APS-3. The hole diameters were 600 and 700 nm for the 800 nm-period AAO templates and the depths were about 600 and 700 nm, respectively, which corresponded to APS-4 and APS-5. Figure 1b shows the schematic diagram of APS transferring and surface-mounting process. First, the APS was transferred to the intermediate poly-

mer stamp (IPS) using nanoimprint technology. The detailed processes of nanoimprint and demolding would be found in [29]. Subsequently, PDMS (Sylgard184, Dow Corning 10:1 ratio with the curing agent) acting as the adhesive coating was spin-coated onto the commercial white LED packages (length = 5.6 mm, width = 3.0 mm, height = 0.77 mm, model: HV56301ZMQ20DC from Hualian Electronics Corp., Ltd., Xiamen, China). The schematic diagram and feature size of the white LED package is shown in Figure 1c. The IPS and PDMS covered the surface of white LED and the thickness of IPS and PDMS was about 0.19 mm. The nominal CCTs of the white LEDs were 5000 and 6000 K, respectively. Finally, the IPS was bonded onto the white LED using PDMS adhesive. The whole device was then heated for 30 min at 100 °C to cure the PDMS. The top-view photo of the completed device is shown in Figure 1d.



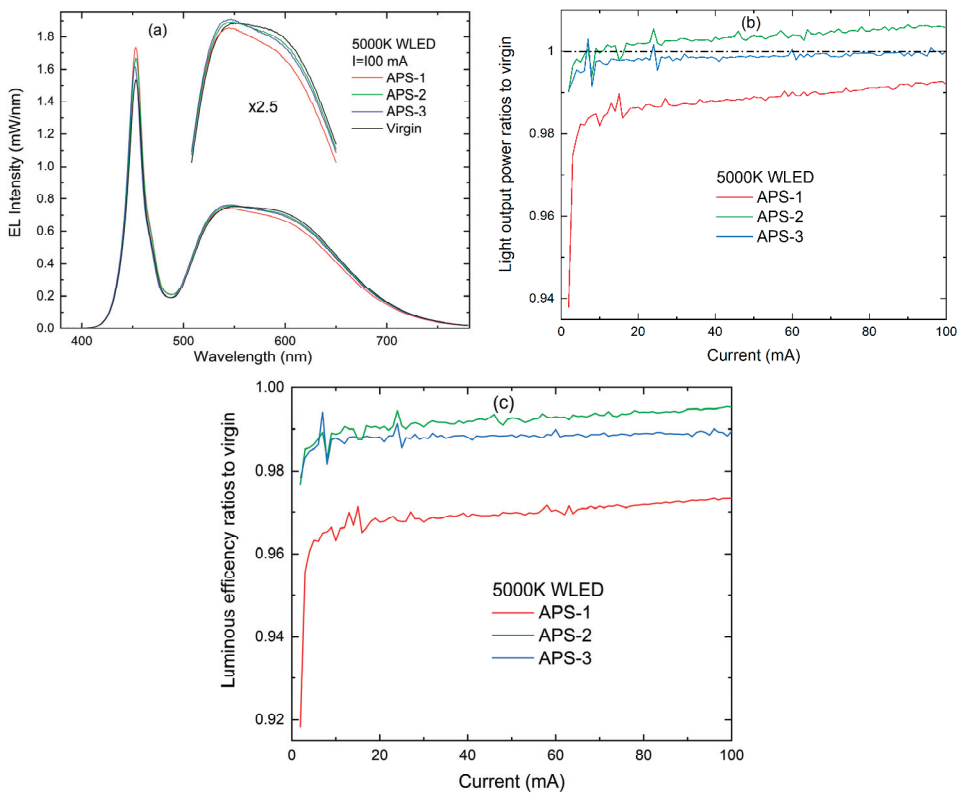
**Figure 1.** (a) SEM images of typical APS imprinted using AAO template. (b) The schematic diagram of APS transferring and surface-mounting process. (c) The schematic diagram and feature size of the white LED with and without package. (d) The top-view photo of the completed device.

The surface morphology of the APSs was examined using a scanning electron microscope (SEM, Nova Nano SEM 430, FEI, New York, USA). The electroluminescence (EL) spectra of the LEDs with and without APSs were measured using an Everfine HAAS-2000 spectroradiometer under the constant mode by using an integrating sphere (Everfine Co., Huangzhou, China). The integral duration is set as the constant of 100 ms. The white LED was located on the copper support. In the measurement, the increase in the junction temperature was less than 2 °C and could be ignored. Three-dimensional FDTD simulations were carried out to study the effect of APSs on the light extraction using Lumerical software (FDTD Solutions v8.21, Vancouver, BC, Canada) [35]. However, FDTD simulation dealt with light propagation in a small area due to the computation capacity and cannot work well in the phosphor layer. So, the Monte Carlo ray-tracing method was combined with an asymmetric bidirectional scattering distribution function (BSDF) [36]. After obtaining a BSDF for certain APSs using FDTD simulation, the corresponding APS surface was defined by the BSDF in a ray-tracing simulation.

### 3. Results and Discussion

Figure 2 shows the EL results of white LEDs at 5000 K with and without APSs mounting. The nominal CCTs of the virginal white LEDs are 5000 K. The APSs include APS-1,

APS-2, and APS-3, which correspond to the patterns of AAO400, AAO 300, and AAO200, respectively, in [29]. The periods of the APSs are about 450 nm. Figure 2a shows that all the integral intensities of blue emissions increase, while the ones of yellow emissions decrease with the APSs mounted. The white LEDs with APS-1 show more yellow emission reductions and more blue emission increase than those with APS-2 and APS-3. It is found that the spectral shapes are also modified by APSs. The EL intensities at the short-wavelength side of the yellow emissions are higher than the virginal ones. Figure 2b,c show the LOPs and LEs ratios to the virgins with different currents. It can be seen that the LOPs of the white LED with APS-2 are enhanced about 0.5% and the ones with APS-3 are similar to the virginal ones. However, the white LED with APS-1 shows that its LOP reduces significantly. Additionally, the LOP ratios increase with current monotonously. In Figure 2c, all the LEs of white LEDs decrease when the APSs are mounted. The white LEDs with APS-2 and APS-3 show about a 1% reduction in LEs, while APS-1 shows a more than 3% reduction.



**Figure 2.** EL results of white LEDs of 5000 K mounted with and without APSs. (a) EL spectra at current of 100 mA. Current dependencies of (b) light output power ratios to virgin and (c) luminous efficiency ratios to virgin for different APSs. The periods of the APSs are about 450 nm. In the inset of (a), four magnified segments are shown as 2.5 times of those in the original ones.

The blue emissions are enhanced by APSs mounting, which is due to the Fourier power spectra of APSs within a certain spatial frequency, as described in our previous work [29]. As for the decreasing yellow emissions, it may be due to the quenching of yellow emission by APSs or the less blue emissions to excite the yellow phosphor. Using the multistage FDTD simulations [29], the LEE enhancements of the monochromatic LEDs with wavelengths of 450, 525, and 580 nm were calculated as 3.7%, 1.2%, and 1.6% by APS-1, respectively. So, the yellow emissions decreasing is caused by less blue emission

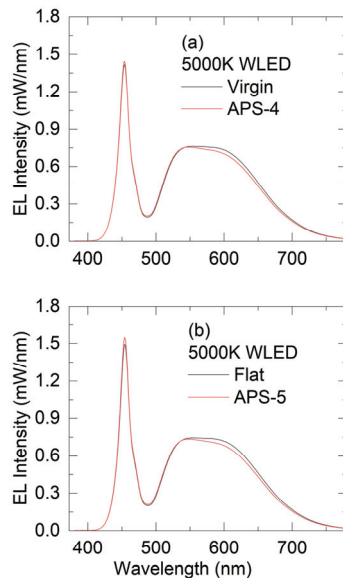
excitation. It also indicates APS-1 may be a candidate nanostructure for broadband LEE enhancement. The LEE enhancements of blue LEDs mounted with APS-1, APS-2, and APS-3 are 3.0%, 2.3%, and 1.3%, respectively [29], which demonstrates the reduction in yellow emission. As for the increasing yellow emission at the short-wavelength side, it may be due to the smaller hole diameters of APS-2 and APS-3 than those of APS-1. Although the blue emission excitation for yellow phosphor reduces with APS-2 and APS-3, the more yellow emission at short-wavelength side is extracted from the package. The enhancement of blue emission and part yellow emission lead to the LOPs with APS-2 and APS-3 not decreasing, as shown in Figure 2b. However, because the photopic vision function of blue light is much lower than that of the yellow one, all the LEs in Figure 2c show the reduction of 1–3%. With the current increasing, the CCT increases monotonously (not shown here), which means an increase in the blue emission content in the spectrum of white LED. For the virginal LED and LEDs with APSS, the increasing current would result in the droop effects on LOPs and LEs. However, considering the ratios to the virginal LEDs, the ratios of LOPs and LEs increase monotonously because there are more blue emissions with the increasing current and the APSS would further enhance the blue emission.

The EL measurements were also carried out on the white LEDs at 5000 K with APS-4 and APS-5 and 6000 K with APS-1. The LEs, LOPs, and CCTs of white LEDs with and without different APSS at the current of 100 mA are obtained and calculated, as listed in Table 1. All the LEs of white LEDs decrease when the APSS are mounted. The low CCTs of white LEDs with suitable APS seemly correspond to small LE variations. The LOPs of white LEDs with APSS change little compared to the flat ones. With APS-2 and APS-3, they show the LOP enhanced or unchanged compared to the virginal LEDs. The CCT increases when the APSS are mounted. APS-1 causes more CCT increase than APS-2 and APS-3. It is also seen that the nominal 6000 K white LED with APS-1 shows more CCT increase than the 5000 K one with the same APS. Combined with LEs and LOPs results, the blue emission increase seems to overlap the yellow emission decrease in LOPs, which agrees with the early report when the color conversion efficiency is high [38]. It is reasonable that the CCT increases with APSS because the blue emission contents increase in the white LEDs' spectra. Similarly, the smaller loss of yellow emission LOP will cause the smaller CCT increase. Lower nominal CCTs correlate to the smaller blue emission content in the white LED spectrum, which means a smaller effect of APS-1 on LE and CCT. It can be supposed that the smaller blue emission contents and appropriate APSS would enhance the LEs and decrease the CCT increment after APS is mounted on the white LED packages.

**Table 1.** LEs, LOPs, and CCTs of white LEDs with and without different APSS at the current of 100 mA.

Structures		LE (lm/W)	LOP (mW)	CCT (K)
APS-1	without	153.66	154.1	6304
	with	148.06	153.0	7354
APS-2	without	164.74	158.5	4940
	with	160.08	157.2	5615
APS-3	without	165.47	159.6	4823
	with	165.07	160.5	5240
APS-4	without	167.84	158.4	4779
	with	166.12	158.4	5198
APS-5	without	166.40	158.7	4712
	with	163.55	155.9	4942
APS-5	without	164.54	157.4	4820
	with	160.62	154.4	5119

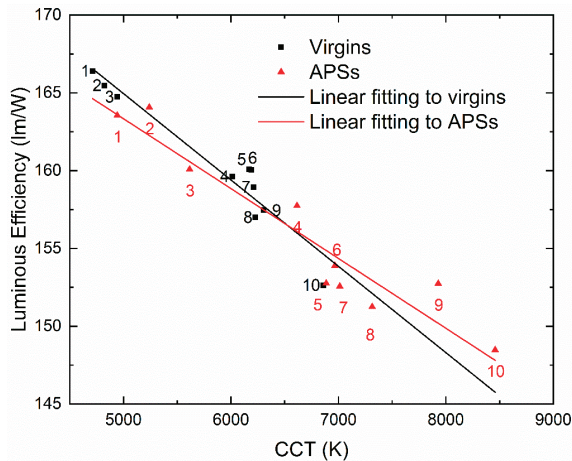
Figure 3 shows the EL spectra of white LEDs with and without APSs at CCTs of 5000 K. The periods of the APSs are 800 nm. The hole diameters are 600 and 700 nm for APS-4 and APS-5, respectively. The operating current is 100 mA. Compared to the EL spectra in Figure 2, the peak intensities of blue emissions increase insignificantly, while the ones of yellow emissions decrease similarly to with APS-2 and APS-3 after the APSs are mounted. So, both LOPs and LEs decrease for the white LEDs with APS-4 and APS-5. The CCTs also increase, whose changes are lower than 300 K. It indicates that the APSs with 800 nm period cannot enhance the blue light extraction significantly. The small blue light extraction enhancement would not cause significant yellow emission reduction. The yellow emission reduction may be due to the destructive interference. The non-iridescent structural colors in an APS come as a result of coherent scattering [34], while the other wavelength lights may not be extracted from the semiconductors due to the destructive interference. As for the small CCT changes of white LEDs by APS-4 and APS-5, it is due to the very small blue emission increase. If the APSs cause the yellow emission coherent scattering and the blue emission decreasing, the LOPs and LEs will be enhanced.



**Figure 3.** EL spectra of white LEDs mounted with and without (a) APS-4 and (b) APS-5 at CCTs of 5000 K. The periods of the APSs are about 800 nm.

The commercial white LEDs at the nominal CCTs of 5000 and 6000 K show a standard deviation of 200 K. So, ten typical white LEDs with APSs and their virgins are chosen to inspect the effects of the APSs on luminous performances. Their LEs and CCTs are plotted in Figure 4. It is obvious that all the white LEDs with APSs show lower LEs and higher CCTs than their virgins. With the CCT increase from 5000 K, the LEs seem to decrease monotonously. The record LE of white LEDs is 303 lm/W at about 5000 K [1]. More yellow emissions show higher LEs of white LEDs at the same LOPs. However, the red phosphor is less efficient than the yellow one, so the LEs will decrease when the CCT is lower than about 4500 K. Figure 4 shows that, at the same CCTs, many white LEDs show higher LEs with APSs than those without APSs, such as red points 2 and 4. The red points 9 and 10 also show higher LEs if the CCTs of the virginal white LEDs extrapolate to 8500 K. According to the linear fitting results, when the CCT is higher than 6500 K, the white LEDs with these APSs will show LE enhancements to the virgins at the same CCT. It indicates that the blue light emission enhancement by APSs can benefit the LE increases in white LEDs at the same CCTs. However, the absolute LE increases in white LEDs are impossible with the

above APSs because the CCT increases compared to the virgins. The experimental data points fluctuate along the fitting lines, which indicates the different effects of APSs and phosphor contents on the blue and yellow emissions. More blue and yellow emissions than the virginal ones originate from the emission enhancement by APSs. The yellow emission coherent scattering APSs may be concerned in light extraction.

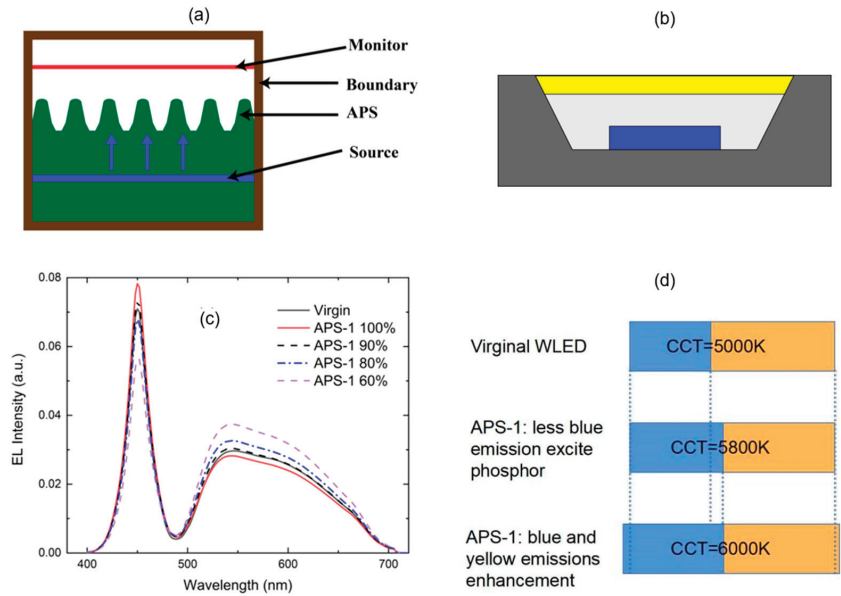


**Figure 4.** Relationship between luminous efficiencies and CCTs for white LEDs with and without APSs. The data are chosen with APS-1, APS-2, APS-3, APS-4, and APS-5 at the nominal CCTs of 5000 and 6000 K. The same numbers of black and red data points correspond to the same white LEDs with and without APSs. The fitting lines show same color as the experimental data.

In general, the LEs can be improved with appropriate APSs and corresponding virginal white LED spectra. At the same CCTs, the white LEDs with APSs can be easily achieved with higher LEs than those without APSs. However, the absolute enhancement of LE does not compare the same white LEDs with and without APSs. Here, we carried out the FDTD and ray tracing simulations to explore the LEs enhancement method. Because FDTD cannot simulate the phosphor effects and ray tracing cannot deal with the nanostructures [35,36], the BSDF of APS-1 was calculated by FDTD, which was then used in a ray tracing simulation. Figure 5a shows the schematic diagram of FDTD model according to our previous study [29]. The light source emitted the plane wave and it propagated from IPS through APS and then into the air. The refractive index values of IPS and air were set as 1.41 and 1.00, respectively. The lateral dimensions of the computational domain were set as  $6 \mu\text{m} \times 6 \mu\text{m}$ , considering the limitation of computer memory and computation capacity. The boundary condition in the top simulation area was set as a perfectly matched layer boundary condition and the four lateral boundaries were set as periodic boundary conditions. Figure 5b presents the LED model in the ray tracing simulator. The blue rectangular represents the LED chip and the yellow layer above represents the phosphor. In the ray tracing simulator, we figured out the emission of phosphor from the SPD of white LED without APS. In Figure 5c, the EL spectra of white LEDs are simulated, where the virginal and APS-1 white LEDs are simulated according to the experimental ones. The percentages of 100%, 90%, 80%, and 60% correspond to the blue emission transmission ratios to the real one with APS-1 by FDTD. The yellow emission transmissions remain unchanged. Then, the modified BSDFs are transferred to a ray tracing simulator. The blue emission reductions using nanostructures cause significantly yellow emission enhancements. It is observed that the simulated EL spectra of virginal and APS-1 (100% transmission) white LEDs are similar to the experimental ones. With the whole effects of APS-1, the LE decreases about 4% and the CCT increases from 6336 to 7589 K compared to the virginal ones. These results also agree with the experiment ones, whose LE decreases about 3.6% and the CCT increases



from 6304 to 7354 K, as listed in Table 1. It means the FDTD combined with ray tracing with the BSDFs is suitable for the white LEDs with and without APSs.



**Figure 5.** (a) The schematic diagram of white LED with APS in the FDTD simulation. (b) The white LED model in the ray tracing simulator. (c) Simulated EL spectra of white LEDs with APS with different blue emission transmission ratios. (d) The diagrammatic sketch of LE enhancement of white LED by APS-1 mounted.

APS-1 90% means a 10% reduction in blue emissions transmission of APS-1, which leads to a small increase in blue and yellow emission LOPs compared to the flat ones, as shown in Figure 5c. With a further decrease in blue emissions transmission for APS-1 80%, blue emission LOP reduces a bit and the yellow one increases significantly. As for APS-1 60%, both blue emission reduction and yellow emission enhancement are significant. The LEs of APS-1 80% and APS-1 60% samples are 10% and 25% enhancements compared to the virgin ones. Moreover, the CCTs decrease to 5868 and 4978 K, respectively. The absolute LEs enhancement requires more blue emissions to excite the yellow phosphor instead of light extraction from APS-1 directly. It is notable that the blue emission transmission reductions are set artificially, which is also difficult to find such APSs in practice. However, it can be found that the new APSs should change its period and size to decrease the blue emission transmission.

At last, the LE enhancement with APSs at the same CCTs can be discussed by a diagrammatic sketch, as shown in Figure 5d. It is supposed that the blue emission is 40% of LOP for 6000 K white LED, while 30% for 5000 K white LED. If their virginal LOPs are same, the virginal LE for 5000 K white LED is higher than that for 6000 K when APS-1 is mounted to the 5000 K LED package, more blue emission will be extracted directly. Less emission blue excitation led to yellow emission reduction. In the semiconductor, APS-1 reassigns the blue emission to extraction and excitation for phosphor. The total LOP does not change in the semiconductor with APS-1. Because the blue emission increases, the CCT will increase, which is supposed as 5800 K. Furthermore, the blue and yellow extracted emissions to air will be enhanced by APS-1. As mentioned above, the blue emission enhanced more than the yellow one as the CCT increased to 6000 K. Both the LOP and LE increase compared to those of the virginal white LEDs at 6000 K.



With the phosphor concentration increasing further, the scattering in the phosphor is more significant. So, the blue emissions reaching the surfaces of light extraction become less. The luminous flux will be enhanced absolutely compared to the virginal one, which is similar to the small transmission ratios of the blue emissions through APS-1 in Figure 5c. However, the quenching effect will appear when the phosphor concentration becomes high, because the self-absorption of phosphor and back scattering to chip will be significant. In the further research, the higher CCT white LEDs will be tried by sophisticated phosphor assembly. On the other hand, the yellow emission coherent scattering APSs may be hopeful to enhance the LEs for white LEDs. The broadband transmission of most yellow emissions and some blue emissions will be better for the absolute LE enhancements. The effective APSs need more design and experiments.

#### 4. Conclusions

In summary, the APSs with different periods and hole diameters were fabricated and surface mounted on the white LEDs at nominal CCTs of 5000 and 6000 K. The EL measurements on these white LEDs were performed. All the white LEDs with APSs show less LE and higher CCT than the ones of the virginal white LEDs. However, the LEs of many APS-mounted white LEDs enhanced compared to the white LEDs without APSs at the same CCTs. Some LOPs of the white LEDs are enhanced by APSs surface mounted. At last, FDTD combined with Monte Carlo ray tracing simulations were carried out on the APSs surface-mounted white LEDs using BSDF transferring. The simulation results of EL spectra, LEs, and CCTs conform well to the experimental ones. The simulations on the effects of the blue emission transmission and phosphor concentration predict that the absolute LE enhancement for white LEDs requires high phosphor concentrations for the existing APSs beneficial to blue light extraction or the optimal APSs for yellow emission coherent scattering. The APSs with the structural color are more hopeful for high LE general lighting.

**Author Contributions:** Conceptualization, Z.C.; Data curation, F.H., Y.C., J.N., C.S., J.Y., Y.G., B.D. and L.L.; Funding acquisition, Z.C.; Investigation, C.S., J.Y. and Y.G.; Methodology, Y.C.; Project administration, B.S.; Resources, J.N., L.L. and W.C.; Supervision, W.C. and B.S.; Writing—original draft, F.H. and Y.C.; Writing—review and editing, Z.C. All authors have read and agreed to the published version of the manuscript.

**Funding:** This work was supported by National Key Research and Development Program [grant number 2021YFB3600100]; National Natural Science Foundation of China [grant numbers 62174004, 61927806]; and Guangdong Basic and Applied Basic Research Foundation [grant number 2020B1515120020].

**Institutional Review Board Statement:** Not applicable.

**Informed Consent Statement:** Not applicable.

**Data Availability Statement:** The data presented in this study are available on request from the corresponding author.

**Conflicts of Interest:** The authors declare no conflict of interest.

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Article

# Investigation of the Effect of ITO Size and Mesa Shape on the Optoelectronic Properties of GaN-Based Micro LEDs

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**Abstract:** In this paper, in order to explore the influence of indium tin oxide (ITO) size and mesa shape on the performance of GaN-based micro light emitting diodes (Micro LEDs) on sapphire substrates, Micro LEDs of different sizes with ITO area smaller than or equal to the light-emitting area were designed and fabricated. The experiment results show that when the ITO area of the Micro LED is equal to the area of the light-emitting area, its optoelectronic performance is significantly better than that of the Micro LEDs whose ITO area is smaller than the area of the light-emitting area. When the light-emitting area size is 40  $\mu\text{m}$ , the wall-plug efficiency (WPE) of the two structures of Micro LEDs can differ by more than 50%. Based on above experiment results, this paper designed and fabricated Micro LEDs with different sizes of square and circular mesa with the same ITO area as the light-emitting area. The experimental results show that the WPE of the circular mesa Micro LED is slightly higher than that of the square mesa Micro LED at low current density. However, as the current density and chip size increase, the performance of the Micro LED with a square mesa is better.

**Keywords:** GaN; Micro LED; ITO; wall-plug efficiency; micro-electronics devices

**Citation:** Fang, A.; Xu, H.; Guo, W.; Liu, J.; Chen, J.; Li, M. Investigation of the Effect of ITO Size and Mesa Shape on the Optoelectronic Properties of GaN-Based Micro LEDs. *Crystals* **2022**, *12*, 1593. <https://doi.org/10.3390/cryst12111593>

Academic Editor: Ikai Lo

Received: 6 October 2022

Accepted: 2 November 2022

Published: 9 November 2022

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## 1. Introduction

In recent years, with the maturity of III-V compound semiconductor devices and integrated circuit technology [1–3], miniature portable electronic products have begun to emerge. Among them, Micro LEDs are widely used in smart phones, visible light communication, implantable devices and other fields due to their unique advantages [4,5]. However, the conventional LED structure has problems such as the difficulty of achieving good ohmic contact on the P-GaN surface, and the dense current distribution under the P electrode, which will lead to uneven current and heat distribution of the LED, which will degrade the optoelectronic performance of the LED and affect the reliability of the device [6]. Therefore, ITO films with high light transmittance, good electrical conductivity and easy-to-form good ohmic contact with P-GaN [7,8] are widely used as extended electrodes to improve the above problems. In recent years, scholars have continued to improve the structure and preparation methods of ITO films to further improve the optoelectronic properties of LEDs: in 2010, Cheng, L. et al. used photoresist as a mask for inductively coupled plasma etching (ICP) to transfer the twisted shape of the photoresist to the ITO surface; the study found that more scattering occurred on ITO with a rougher surface, and moreover, the performance of LEDs increased [9]. In 2018, J. Xu et al. deposited a thin layer of Al after sputtering ITO, and alloyed Al atoms with ITO atoms after thermal annealing; when the overall thickness of the film is 395nm, the light transmittance reaches 93.2%, and the optical output power of the device is increased by 13% compared with the pure ITO film [10]. For Micro LEDs, the mesa structure is an important factor affecting the optoelectronic performance of the device. The improvement of the light-emitting mesa mainly focuses on the treatment of the side wall [11]. In 2010, Chen P.H. et al. proposed to engrave nano-textures on the sidewall of the LED mesa to improve the light extraction efficiency, which increased the output power of the LED by more than 45% [12]; In 2010,

P.H. Chen et al. proposed an alternative approach to investigate these defects directly after MESA formation, by coupling optical characterization techniques together with time-of-flight secondary ion mass spectrometry (TOF-SIMS) on AlGaInP square shaped pixels of different sizes formed by BCl<sub>3</sub>-based reactive ion etching (RIE) [13], which provides convenience for the processing of mesa sidewall defects.

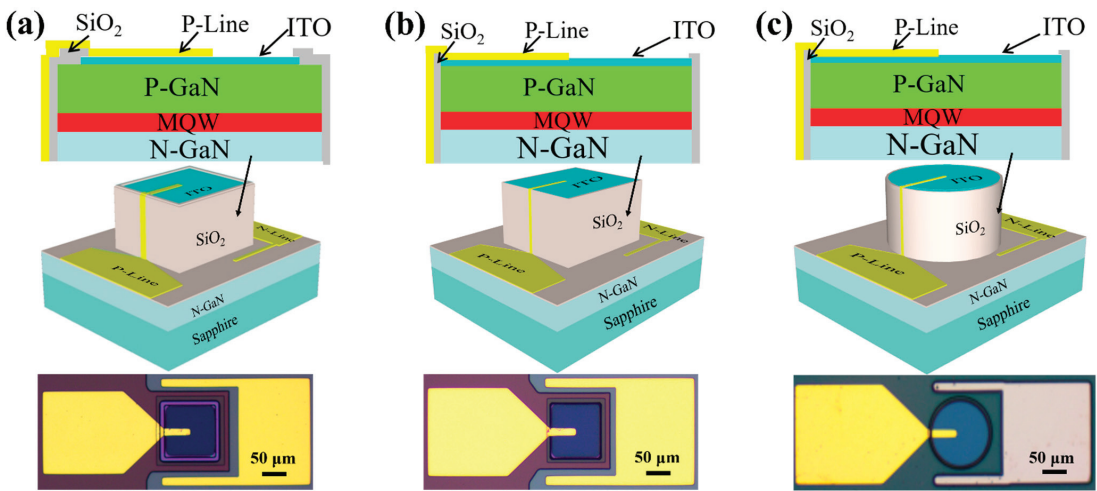
Although the research on ITO and mesa is relatively advanced, most of the studies focus on the improvement of the preparation process and the influence of the surface mechanism [14–16], and there are few studies on the specific size of ITO and the shape of the mesa in Micro LEDs. Therefore, this paper proposes Micro LEDs with an ITO area less than or equal to the area of the light-emitting area and square and circular mesa, to explore the influence of the size of the ITO relative to the area of the light-emitting area and the shape of the mesa on the optoelectronic property of Micro LEDs.

## 2. Materials and Methods

A GaN-based LED commercial epitaxial layer grown on sapphire was used, from bottom to top comprised of: 3.4 μm U-GaN; 2.3 μm N-GaN; 150 nm InGaIn/GaN multiple quantum wells (MQW) layer; 43 nm P-GaN. For the Micro LED with ITO area equal to the mesa area, in order to prevent the shrinkage of ITO from affecting the final area, we firstly deposited 110 nm ITO and 1.5 nm Al on the epitaxial layer by electron beam evaporation. Secondly, we annealed at 580 °C for 5 min to achieve good ohmic contact between ITO and P-GaN. Then, we etched the epitaxial layer 1.2 μm to N-GaN layer by inductively coupled plasma (ICP) etching to form light-emitting mesa. For the Micro LED with ITO area smaller than the light-emitting area, the above two steps were done in reverse. Then, for both kinds of Micro LED, 1000 nm-thick SiO<sub>2</sub> was grown by PECVD as the passivation layer (PV). Because SiO<sub>2</sub> is hydrophilic and photoresist is hydrophobic, HDMS treatment was used to remove the -OH on the surface of SiO<sub>2</sub>, so that the surface of SiO<sub>2</sub> could form hydrophobicity to adhere to the photoresist well. The PV pattern was obtained by photolithography and etching. Cr/Al/Ti/Pt/Au multilayer metal as P/N electrode with a thickness of 2.4 μm was deposited by electron beam evaporation. Finally, the wafer was thinned to about 200 μm by mechanical grinding method. A 39-layer distributed Bragg reflection (DBR) layer was fabricated by alternating SiO<sub>2</sub> and TiO<sub>2</sub> on the back of the wafer to improve the optical extraction efficiency.

Figure 1a is the Micro LED with the size of ITO smaller than the size of the light-emitting area. The ITO of this structure is 2 μm away from the boundary of the light-emitting area, and the ITO shrank inward by 2–3 μm during the process preparation. Therefore, the distance between the ITO boundary and the sidewall was maintained at 4–5 μm, so the overall area of the ITO was smaller than the mesa area, which had some impacts on the light output of the device. To investigate the effect of ITO size change on the performance of Micro LED, a novel Micro LED sample with the ITO size equal to the light-emitting area size was designed for this paper, as shown in Figure 1b.

In order to explore the influence of different mesa shapes on the optoelectronic characteristics of Micro LEDs, square and circular mesa Micro LEDs with the same light-emitting area were designed and fabricated. The schematic diagram of the structure of the circular mesa Micro LED is shown in Figure 1c.

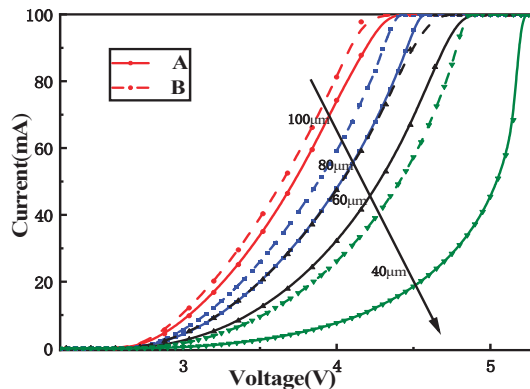


**Figure 1.** Micro LED (a) with ITO smaller than light emitting area (b) with ITO equal to light emitting area (c) with circular mesa (ITO equal to light emitting area).

**3. Results and Discussion**

*3.1. Influence of Different ITO Sizes on Optoelectronic Properties*

Structure A and B represent Micro LEDs whose ITO size is smaller than and equal to the area of the light-emitting area, respectively. Figure 2 shows the I-V characteristic curves of the two structures under different light-emitting area sizes; it can be seen that at the same light-emitting area size, the series resistance of A is smaller than that of B, which is because of the increase of ohmic contact area between the P-GaN and ITO, which reduces the voltage of the device. As the size of the light-emitting area of the Micro LED decreases, the series resistance increases; as the contact area between the P-GaN and the ITO decreases with the decrease, this results in an increase in the contact resistance.



**Figure 2.** I-V curves of Micro LEDs with ITO size smaller than (A) and equal to (B) the light-emitting area size.

Figure 3 shows the variation curves of the WPE of the two structures with the current density under different light-emitting sizes. Because under the dual action of Auger recombination and carrier leakage, the rise in luminous power will be limited, while the current and voltage can be kept in a high range, so the WPE shows a downward trend. The WPE of B is higher than that of A, because the larger ITO area of B not only means larger



light-emitting area and more photons emitted compared with the conventional structure A, but also means larger ohmic contact area and lower voltage. In addition, under the same light-emitting size, the larger the ITO is, the smaller the series resistance is (Figure 2). According to Formula (3), the value of voltage-temperature coefficient  $S$  decreases with the decrease of series resistance, so the thermal stability of B is better, which makes the current spreading and the optoelectronic performance of structure B better.

$$S = \left| \frac{dV_F}{dT} \right| = \frac{nk}{q} \ln \left( \frac{I_F}{I_S} \right) + \frac{dR_s}{dT} I_F \tag{1}$$

where,  $I_S$  is the reverse saturation current,  $q$  is the electronic quantity,  $k$  is the Boltzmann constant,  $T$  is the absolute temperature and  $n$  is the ideal factor.  $I_S$  is a function of temperature. Under the condition that all impurities in the semiconductor material are ionized and the intrinsic excitation can be ignored,  $I_S$  can be summarized as:

$$I_S = Ae \left( \sqrt{\frac{D_n}{\tau_n}} \frac{n_i^2}{N_A} + \sqrt{\frac{D_p}{\tau_p}} \frac{n_i^2}{N_D} \right) = CT^3 \exp \left( -\frac{eV_{g0}}{KT} \right) \tag{2}$$

$A$  is the knot area,  $C$  is a constant related to junction area and impurity concentration and  $V_{g0}$  is the potential difference between the conduction band bottom and the valence band top of the PN junction material at absolute zero. Substituting Formula (2) into Formula (1),  $S$  can be summarized as:

$$S = \left| \frac{dV_F}{dT} \right| = \frac{nk}{q} \ln \left( \frac{C}{I_F} \right) + \frac{3nk}{q} \ln T + \frac{3nk}{q} + \frac{1.5kT + E_a}{2kT^2} I_F R_s \tag{3}$$

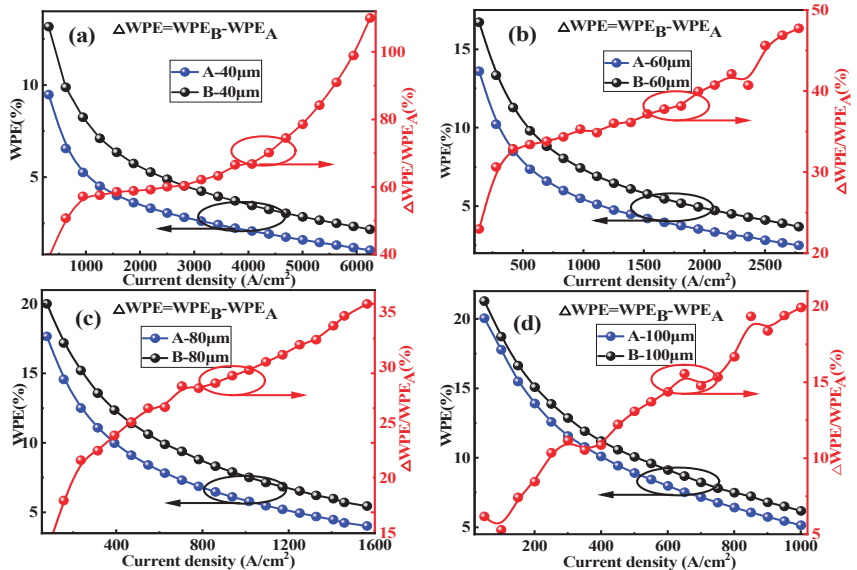


Figure 3. WPE vs. current densities of Micro LED A and B (a) 40  $\mu\text{m}$  (b) 60  $\mu\text{m}$  (c) 80  $\mu\text{m}$  (d) 100  $\mu\text{m}$ .

Figure 3 also shows the variation of the novel structure (B) compared with the conventional structure (A) under four kinds of size. It can be seen that as the chip size decreases, the ITO area has a greater impact on the optoelectronic performance of the Micro LED. Where the size of the light-emitting area is 40  $\mu\text{m}$  and 100  $\mu\text{m}$ , the WPE of the novel structure improves by up to 110% and 18% as shown in Figures 3a and 3d, respectively. A mathematical model can be used to describe this phenomenon. If the size of the light-

emitting area is “L” and the distance between the ITO boundary and the boundary of the light-emitting area is “a” (approximately equal to 2  $\mu\text{m}$ ), then the area ratio of the ITO to the light-emitting area is “ $(L - a)^2/L^2$ ”. Thus, the larger the size “L”, the closer the ratio to “1”, and the smaller the effect of the shrinkage of ITO on the current spreading is. Therefore, the performance of small size Micro LED can be significantly improved on account of the growth of the ITO area.

### 3.2. Influence of Different Mesa Shapes on Optoelectronic Properties

In this paper, C and D represent the square mesa Micro LED and circular mesa Micro LED in this comparative experiment, respectively. The specific dimensions of Micro LED with two structures are shown in Table 1.

**Table 1.** Specific dimensions of C and D.

Group	Length of C (L)	Area of C	Diameter of D (R)	Area of D
I	30 $\mu\text{m}$	900 $\mu\text{m}^2$	34 $\mu\text{m}$	908 $\mu\text{m}^2$
II	40 $\mu\text{m}$	1600 $\mu\text{m}^2$	45 $\mu\text{m}$	1590 $\mu\text{m}^2$
III	80 $\mu\text{m}$	6400 $\mu\text{m}^2$	90 $\mu\text{m}$	6362 $\mu\text{m}^2$
IV	100 $\mu\text{m}$	10,000 $\mu\text{m}^2$	113 $\mu\text{m}$	10,028 $\mu\text{m}^2$

Figure 4 shows the variation curves of WPE and luminous power of Micro LEDs with different mesa shapes under different current densities. As a whole, the WPE is almost the same for C and D; the luminous power of C is a little bit higher than that of D at high current density. However, with the increase in device size and current density, the square Micro LED has better optoelectronic performance. The WPE of the square mesa Micro LED is larger than that of the circular one, because the side surface area of the square light-emitting area is about 13% larger than that of the circular one, which leads to more light-emitting from the sidewall of C, thereby increasing the luminous power. As the current density increases further, more light emits from the sidewall, and the optoelectronic performance gap between the two structures will be widened, and as the size of the light-emitting area increases, the Micro LED with a square mesa will have better stability than the Micro LED with a circular mesa.

To further explore the performance differences of Micro LEDs with different mesa shapes in different sizes, the thermal characteristics of devices with two structures were tested under the current of 20 mA. Figure 5 shows the thermal resistance of Micro LEDs with square and circular mesa of different sizes. The thermal resistance of the square mesa Micro LED is slightly higher than that of the circular one when the size is small, which is the reason why the WPE of the D-I is slightly higher than that of C-I. With the increase in chip size, the thermal resistance of the two structures achieves the same level, that is, the thermal characteristics of the two structures are not the main factor affecting WPE in the case of large mesa size; the difference of luminous power caused by the light-emitting from the sidewall is the main reason for the difference in the optoelectronic performance of devices with two kinds of structures. Therefore, in Micro LEDs of small size, thermal factors are the cause why the square mesa cannot achieve a better optoelectronic performance than the circular one. However, with the increase in chip size, the Micro LED of the square mesa has a better optoelectronic performance due to the better luminous power.

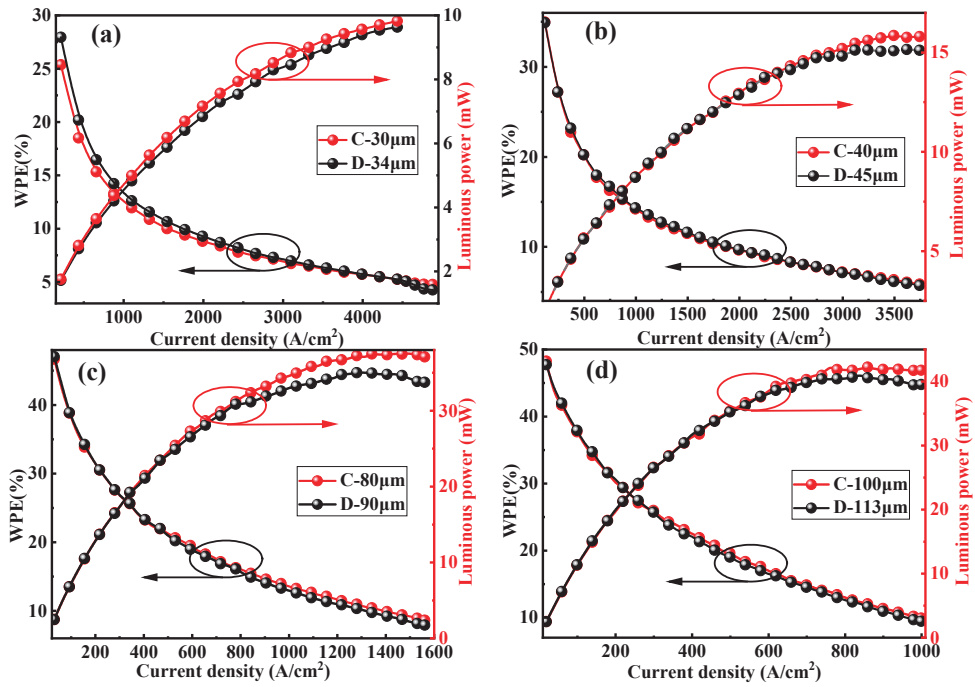


Figure 4. WPE and luminous power of C and D at different current densities, (a)–(d) correspond to experimental group I–IV (The size of the mesa increases gradually).

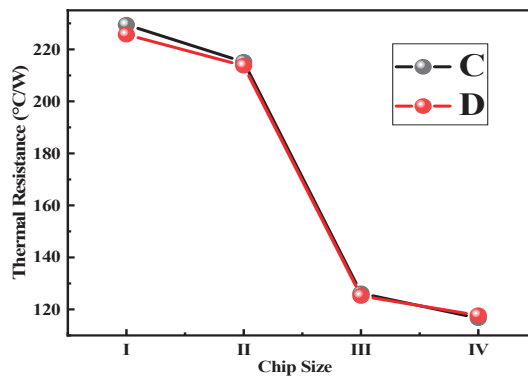


Figure 5. Thermal resistance of C and D with different mesa sizes at 20 mA current.

#### 4. Conclusions

In this paper, Micro LEDs with a light-emitting area size of 40–100  $\mu\text{m}$  and an ITO size smaller than or equal to the light-emitting area size were designed and fabricated respectively. After testing and analyzing these Micro LEDs with different structures, it is found that when the area of ITO is equal to the area of the light-emitting area, the optoelectronic performance of the Micro LED is obviously better than that of conventional Micro LEDs with the area of ITO smaller than the area of the light-emitting area. When the area of the light-emitting area is 40  $\mu\text{m}$ , the improvement of WPE by the new structure exceeds 50%, and with the increase in the current density, there is still a trend to improve WPE. According to this experimental result, we can improve the overall performance of the device by increasing the contact area between ITO and P-GaN, especially in small size

Micro LEDs. Furthermore, Micro LEDs with square and circular mesa of different sizes were designed and fabricated, which has the structure that the area of ITO is equal to the area of the light-emitting area. It is found that the WPE of the Micro LED with a square mesa is slightly higher than that of the Micro LED with a circular mesa at a high current density on account that the light emits from sidewall, which is instructive for us to choose the mesa shape of Micro LED as Micro LED usually works under high current density. And as the size of the light-emitting area increases, the Micro LED with a square mesa will have better stability than the Micro LED with a circular mesa. In the future display array fabrication, we can extract the light from the sidewall of Micro LED on the square mesa to the pixel position, which will be of great help to the future research of Micro LED display array. In general, the square mesa Micro LED with the ITO size equal to the area of the light emitting area exhibits better optoelectronic properties, which provides a new idea for further reducing the size of the Micro LED and improving the performance of the Micro LEDs in the future.

**Author Contributions:** Conceptualization, W.G. and A.F.; methodology, A.F.; formal analysis, A.F. and H.X.; investigation, A.F., J.C. and M.L.; writing—original draft preparation, A.F. and H.X.; writing—review and editing, A.F., H.X. and J.L.; supervision, W.G. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research was funded by National key R&D program of China (No. 2017YFB0402803).

**Institutional Review Board Statement:** Not applicable.

**Informed Consent Statement:** Not applicable.

**Data Availability Statement:** Not applicable.

**Conflicts of Interest:** The authors declare no conflict of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript; or in the decision to publish the results.

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## Article

# Nickel-Assisted Transfer-Free Technology of Graphene Chemical Vapor Deposition on GaN for Improving the Electrical Performance of Light-Emitting Diodes

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**Abstract:** With the rapid development of graphene technology, today graphene performs well in the application of light-emitting diode (LED) transparent electrodes. Naturally, high-quality contact between the graphene and the GaN underneath is very important. This paper reports a process for nickel-assisted transfer-free technology of graphene chemical vapor deposition on GaN. The nickel film plays the dual role of etching mask and growth catalyst, and is removed by the subsequent “penetration etching” process, achieving good direct contact between the graphene and GaN. The results show that the graphene effectively improves the current spreading of GaN-based LEDs and enhances their electrical performance. This scheme avoids the wrinkles and cracks of graphene from the transfer process, and is not only suitable for the combination of graphene and GaN-based LEDs, but also provides a solution for the integration of graphene and other materials.

**Keywords:** GaN; LEDs; graphene; transparent electrode; CVD; transfer-free

**Citation:** Tang, P.; Xiong, F.; Du, Z.; Li, K.; Mei, Y.; Guo, W.; Sun, J.

Nickel-Assisted Transfer-Free Technology of Graphene Chemical Vapor Deposition on GaN for Improving the Electrical Performance of Light-Emitting Diodes. *Crystals* **2022**, *12*, 1497. <https://doi.org/10.3390/cryst12101497>

Academic Editors: Peng Chen and Zhizhong Chen

Received: 7 October 2022

Accepted: 19 October 2022

Published: 21 October 2022

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## 1. Introduction

With the development of science and technology, light-emitting diodes (LEDs) play an increasingly important role in our daily life. Since the birth of gallium nitride (GaN)-based LEDs, they have greatly promoted the development of lighting and display fields. However, there are still problems in the development, such as the difficulty of heavy doping of p-type GaN. This means that the conductivity of p-type GaN is relatively poor, so that the current is difficult to spread to achieve sufficient current injection. For this reason, transparent electrodes came into being. Indium tin oxide (ITO) is the most representative transparent electrode material, which has excellent electrical conductivity and high transparency in the visible band [1–4]. Nevertheless, from the perspective of sustainable development, ITO is inferior to graphene because of the scarcity of indium [5,6]. In addition, graphene performs better than ITO on flexible substrates. These factors make graphene one of the most viable potential transparent electrode materials [7].

In the growth of graphene, metals play a crucial catalytic role. The catalytic mechanism is mainly divided into two types [8]: one is the carbon segregation and precipitation mechanism represented by nickel, under which more layers of graphene are grown; the other is the surface adsorption mechanism represented by copper, under which the number of graphene layers grown is lesser. Both of these mechanisms are widely used in the growth of graphene.

However, the vital role played by metal catalysts in graphene growth means that the growth of high-quality graphene is often inseparable from metals. As a result, as-grown graphene is always attached to the surface of metal substrates [9–11], which is

difficult to use in electronic devices directly. There are some solutions to this problem: for example, graphene can be transferred from the metal substrates to the target substrates, but in this process greater or lesser contamination and defects will inevitably be introduced. In addition, graphene can be directly grown on the target substrates, but without metal catalysis the growth of graphene is often more difficult [12,13].

To solve this problem, in this paper we propose a nickel-assisted transfer-free technology of CVD graphene on GaN. In this method, nickel film is used to catalyze the growth of high-quality graphene, and it is removed by the penetration etching process to realize the contact of graphene with the target substrates, so as to avoid the transfer process. In addition, nickel is not only used as a catalyst, but also as a mask to etch the LED mesas. The measurement results show that the as-grown graphene film effectively improves the electrical performance of LEDs. The effects of different growth time on the performance of LEDs are compared as well. The process is simple, efficient and highly repeatable, which directly realizes good, tight contact between graphene and GaN, providing a solution for the integration of graphene and GaN devices.

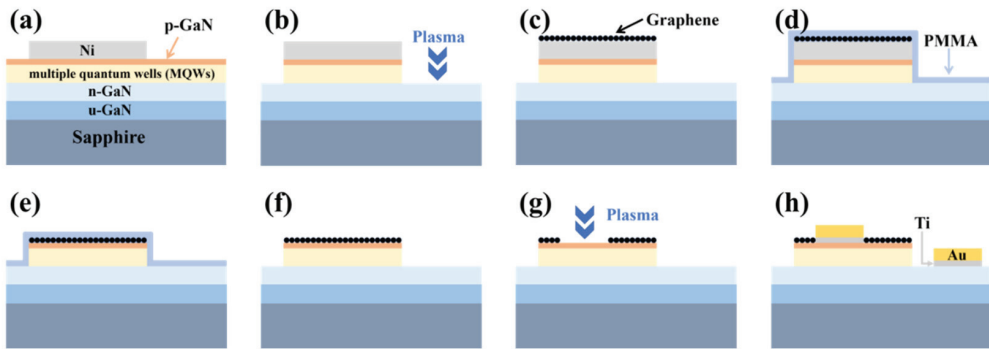
## 2. Materials and Methods

Since lift-off photolithography of metal electrodes after graphene growth may cause some damage to graphene, in order to pursue more stable and excellent electrical performance nickel is selected as the catalyst to grow graphene with more layers, reducing the impact of subsequent processes on the continuity of graphene.

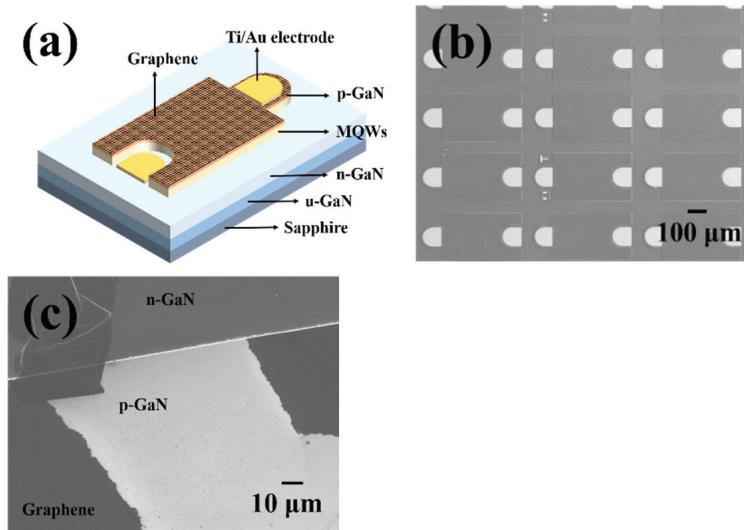
Figure 1 shows a schematic diagram of the process flow of the LEDs in this paper. The epitaxial wafers used were provided by Xiangneng Hualei Optoelectronics Company. First, a 300 nm nickel film was photolithographically sputtered on the epitaxial wafer as the subsequent etching mask and growth catalyst. The  $260 \times 515 \mu\text{m}^2$  LED mesas were etched with inductively coupled plasma (ICP) at an etching ratio of approximately 1:80 for nickel and GaN, as shown in Figure 1b. The samples were subsequently grown in cold-wall plasma-enhanced chemical vapor deposition (PECVD) at  $600 \text{ }^\circ\text{C}$  and 6 mbar, under an atmosphere of  $\text{CH}_4/\text{H}_2/\text{Ar}$  (5/20/960 sccm) and at a plasma power of 40 W. As shown in Figure 1d, after the growth of graphene, PMMA (poly(methyl-methacrylate)) was spin-coated on the sample (3000 rpm for 30 s) and baked at  $150 \text{ }^\circ\text{C}$  for 10 min. It is approximately 150 nm thick. Then the sample was put into the etching solution for more than four hours ( $\text{CuSO}_4:\text{HCl}:\text{H}_2\text{O} = 10 \text{ g}:50 \text{ mL}:50 \text{ mL}$ ). The etching solution can pass through the PMMA and graphene to slowly etch Ni film. Since PMMA is in close contact with graphene and n-GaN, after the metal is etched, PMMA and graphene will fall onto the surface of the sample instead of floating away in the solution. Then PMMA was removed by acetone and isopropyl alcohol (Figure 1f). Due to the weak van der Waals force on the surface of graphene, it is necessary to remove the graphene on the electrode area with oxygen plasma etching to prevent metal electrodes from falling off, as shown in Figure 1g. Finally, 15 nm Ti and 300 nm Au were sputtered as electrodes and annealed in a  $450 \text{ }^\circ\text{C}$  vacuum for five minutes (Figure 1h).

Figure 2a shows the structure of the LEDs. Figure 2b shows the scanning electron microscope (SEM) image of the LED arrays (SE2 mode). An area of intentionally broken graphene has a higher contrast for better observation of graphene film, which is characterized by SEM (in-lens mode), as shown in Figure 2c. Since the in-lens mode has higher resolution, which is more suitable for observing the microscopic morphology, the graphene layer can be clearly seen in Figure 2c. The white boundary line in the image is the edge of the LED mesa, below which is the p-GaN and graphene on the mesa, and above which is the n-GaN beside the mesa. The dark film is graphene, and p-GaN is exposed in the broken area of graphene, corresponding to the white area in the image. It can be clearly seen that the graphene film has been broken and folded in this area, and even some graphene falls on n-GaN.





**Figure 1.** Process flow diagram of growth of graphene and fabrication of LEDs. (a) Sputter Ni film. (b) Etch the mesas. (c) Grow graphene. (d) Spin-coat PMMA. (e) Etch Ni film. (f) Remove the PMMA. (g) Remove some graphene. (h) Sputter metal electrodes.



**Figure 2.** (a) Structure diagram of LEDs. (b) SEM image of LED arrays in SE2 mode. (c) SEM image of graphene on the mesa in in-lens mode.

### 3. Results and Discussion

In order to study the effect of graphene of different qualities on LED performance, LEDs with different graphene growth time were fabricated. Figure 3 shows the Raman characterization of graphene with different growth time after the fabrication of LEDs. The number of graphene layers is usually estimated in terms of the 2D/G ratio and the shape of the peaks [14]. It can be seen that with the increase of growth time, the 2D/G ratio gradually decreases, indicating that the number of graphene layers gradually increases. The graphene is estimated to be about 5–10 layers thick, based on both the Raman spectra [15] and our previous atomic force microscopy (AFM) measurement [12]. In addition, the Raman characterization was performed after the LEDs were fabricated, indicating that the graphene still maintains good quality after the lift-off photolithography of the metal electrodes.

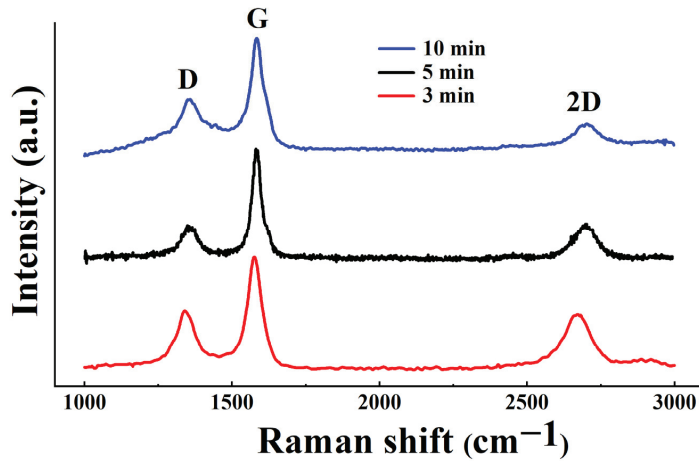


Figure 3. Raman characterization of graphene grown for 3 min, 5 min and 10 min, respectively.

Figure 4 is the energy dispersive spectroscopy (EDS) surface scanning result, inset is the characterized area and the characterized elements are Ni, Ga and Au. Among them, the molecular ratio of Ni is 0.01%, and the weight ratio is 0.02%. This indicates that the Ni film has been substantially etched away.

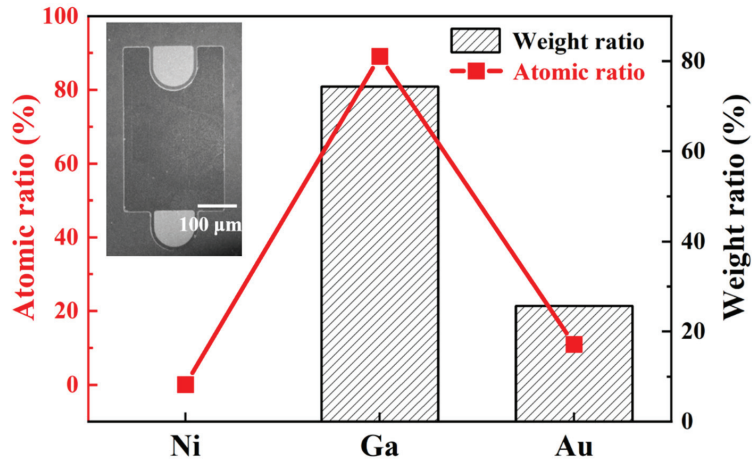
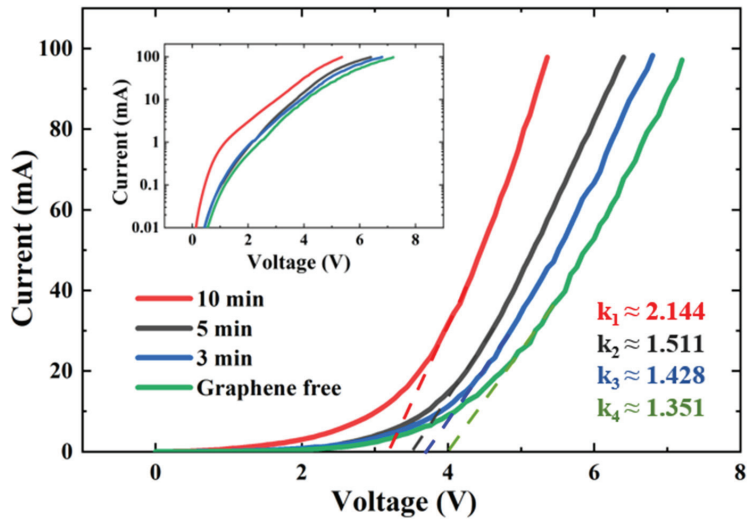


Figure 4. EDS characterization of the LED. Characterized elements are Ni, Ga and Au. The inset is the characterized area.

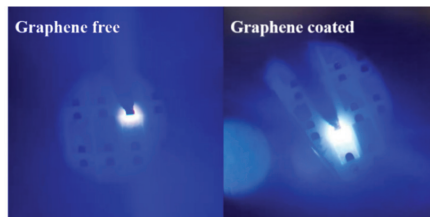
In addition to the fabrication of LEDs with graphene, graphene-free LEDs were also fabricated for comparison using basically the same process, and their current–voltage characteristics are shown in Figure 5. The inset is the current–voltage characteristics in semi-log scale. The dotted auxiliary lines are the reverse extension lines of the nearly linear part of the current–voltage characteristic curves, and their intersections with the abscissa represent the turn-on voltages of LEDs. The turn-on voltages of LEDs with growth time of 10 min, 5 min, 3 min and without graphene are about 3.2 V, 3.5 V, 3.7 V and 4 V, respectively; the operating voltages at 20 mA are about 3.5 V, 4.2 V, 4.4 V and 4.7 V, respectively. The slopes ( $k_1$ – $k_4$ ) of these auxiliary lines, which are mainly related to the LED series resistance, are also shown in Figure 5. Compared with graphene-free LEDs, the current spreading effect of graphene will reduce the series resistance of graphene-coated LEDs. Therefore,

with the increase of growth time, the slope increases and the series resistance decreases. It can be inferred that graphene improves electrical performance of LEDs, and the thicker the graphene the greater the improvement, which may be attributed to its better continuity. From the inset, it is clear that these LEDs have a certain degree of leakage current before reaching their respective turn-on voltage, which may be related to the recombination current in the barrier area. Compared with graphene-free LEDs, the leakage current of LEDs with a growth time of 3 min and 5 min is not much different. However, the LEDs with graphene grown for 10 min have serious leakage current. This may be due to the fact that many carbon atoms are adsorbed on the sidewalls of the mesas because the growth time is too long, even though graphene is not formed because there is no metal catalyst on the sidewalls. Therefore, properly increasing the growth time can effectively improve the electrical performance of LEDs.



**Figure 5.** Current–voltage characteristics of LEDs with and without graphene. The dotted auxiliary lines are the reverse extension lines of the nearly linear part of the current–voltage characteristic curves, and  $k_1$ – $k_4$  represent their slopes. The inset is the current–voltage characteristics in semi-log scale.

Figure 6 is the optical microscope luminescence images of LEDs with and without graphene at 20 mA. Even though thicker graphene theoretically blocks more light [10], the difference in luminescence of LEDs coated with different graphene is still small when observed under an optical microscope, so only a representative graphene-coated LED is shown. It can be seen that the graphene-free LED only emits light near the metal electrodes, while the graphene-coated LED emits light evenly on the entire mesa. This shows that graphene plays a good role in current expansion, which indicates that graphene plays a good role in current spreading.



**Figure 6.** Images of LEDs without and with graphene at 20 mA.

#### 4. Conclusions

In this paper, a method of growing transfer-free graphene on GaN by PECVD is introduced. LEDs with different thickness of graphene are fabricated by controlling the growth time. In the whole process, the Ni film is not only used as the mask for mesa etching but also as the catalyst for graphene growth, which is subsequently removed to achieve direct contact between graphene and GaN. When the growth time is less than ten minutes, the thickness of graphene increases with the growth time. The measurement results show that graphene realizes current spreading and effectively improves the electrical performance of LEDs, although excessive growth time may lead to current leakage of LEDs. This method makes CVD graphene achieve good contact with GaN substrate, avoiding the defects and impurities introduced in the transfer process.

**Author Contributions:** Conceptualization, P.T. and J.S.; methodology, P.T., F.X. and J.S.; investigation, K.L.; data curation, P.T. and Y.M.; writing—original draft preparation, P.T.; writing—review and editing, P.T., Z.D. and J.S.; supervision, W.G. and J.S. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research was funded by the Fujian Provincial Projects (2021HZ0114, 2021J01583, 2021L3004), the Fujian Science & Technology Innovation Laboratory for Optoelectronic Information of China (2021ZZ122, 2020ZZ110), the National Key R&D Program of China (2018YFA0209004) and the Beijing Municipal Commission of Education (KM201810005029).

**Data Availability Statement:** Not applicable.

**Conflicts of Interest:** The authors declare no conflict of interest.

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Article

# Effect of Source Field Plate Cracks on the Electrical Performance of AlGa<sub>N</sub>/Ga<sub>N</sub> HEMT Devices

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**Abstract:** In the current study, the effects of cracks in source field plates (SFPs) on the electrical performance of AlGa<sub>N</sub>/Ga<sub>N</sub> high electron mobility transistors (HEMTs) are investigated systematically using numerical simulation. In detail, the influence of crack width and junction angle in SFPs on device performance is studied. The results indicate that the SFP structure increases the breakdown voltage of a device, but the occurrence of cracks causes premature breakdown, which is confirmed experimentally by the structural analysis of these devices after breakdown. With an increase in crack width, the electrical performance becomes worse. A beveled SFP architecture is proposed by increasing the angle at the SFP junction to reduce the probability of cracking and enhance the reliability of the device. However, with an increase in bevel angle, the modulation effect of the SFP on the channel electric field is gradually weakened. Therefore, it is necessary to balance the relationship between electrical performance and bevel angle according to the actual demands. This work provides potential support for SFP structural optimization design for AlGa<sub>N</sub>/Ga<sub>N</sub> HEMTs.

**Keywords:** AlGa<sub>N</sub>/Ga<sub>N</sub> HEMTs; source field plate cracks; Ga<sub>N</sub> TCAD modeling; electrical performance

**Citation:** Bie, Y.-N.; Du, C.-L.; Cai, X.-L.; Ye, R.; Liu, H.-J.; Zhang, Y.; Duan, X.-Y.; Zhu, J.-J. Effect of Source Field Plate Cracks on the Electrical Performance of AlGa<sub>N</sub>/Ga<sub>N</sub> HEMT Devices. *Crystals* **2022**, *12*, 1195. <https://doi.org/10.3390/cryst12091195>

Academic Editors: Peng Chen and Zhizhong Chen

Received: 29 July 2022

Accepted: 23 August 2022

Published: 25 August 2022

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## 1. Introduction

Compared with silicon, gallium nitride (Ga<sub>N</sub>) has a wider band gap, higher thermal conductivity and higher electron mobility in AlGa<sub>N</sub>/Ga<sub>N</sub> heterostructures. At present, Ga<sub>N</sub>-based power and radio frequency high-electron-mobility transistors (HEMTs) show excellent performance and are widely applied in the field of base station communication, aerospace and radar systems [1–4]. As a core component of the power amplifier (PA) in the radio remote unit of a base station, the failure of an AlGa<sub>N</sub>/Ga<sub>N</sub> HEMT reduces the product yield, work efficiency and service life, further aggravating the failure rate of PAs.

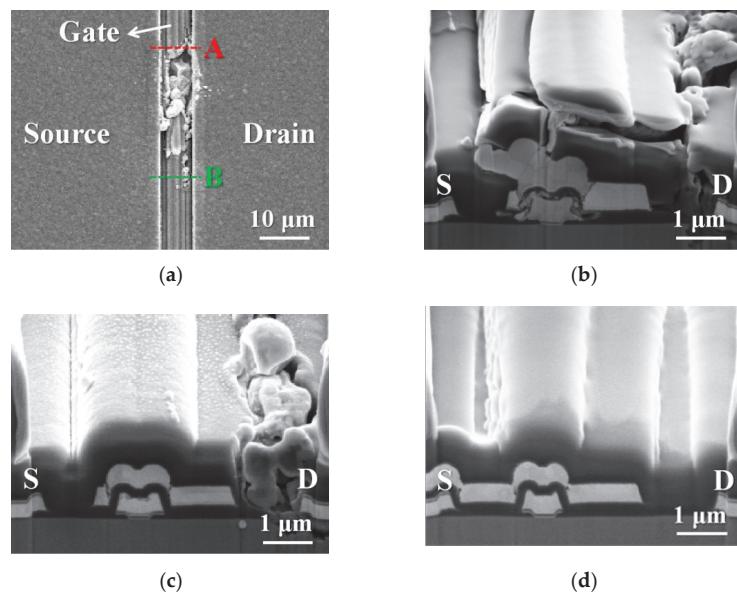
AlGa<sub>N</sub>/Ga<sub>N</sub> HEMTs usually work under high-frequency and high-voltage conditions. On the one hand, low-frequency dispersion is induced by traps and has an impact on high-frequency performance [5–7]. On the other hand, these devices need to withstand extremely high drain voltages. The electric potential lines gather at either the gate or drain of the device and result in an electric field peak. When the electric field peak is higher than the critical breakdown electric field, avalanche ionization occurs and the device breaks down [8,9]. Therefore, it is necessary to optimize the electric field distribution by designing the device structure so as to improve the breakdown voltage ( $V_{br}$ ). The electrical characteristics of AlGa<sub>N</sub>/Ga<sub>N</sub> HEMTs can be enhanced by introducing a field plate structure, which brings in a uniform space charge distribution in a lateral direction and, therefore, increases the  $V_{br}$  [10–15]. In a failure analysis and reliability study of AlGa<sub>N</sub>/Ga<sub>N</sub> HEMTs, cracks are always found at the junctions of the source field plate (SFP). It is reported that these cracks may come from the process of field plate metal deposition on uneven surfaces because of the stresses at these junctions [16–18]. However,

SFP cracks are potentially risky, and their effects on a device's electrical performance are still unclear; therefore, further research is urgently needed.

In this work, firstly, an AlGaIn/GaN HEMT device with an SFP structure is characterized experimentally after its breakdown, and cracks are found at the junctions of the SFP. Secondly, the effects of these SFP cracks on the device's electrical performance are studied systematically based on TCAD simulations. Various device structures with and without an SFP and with differing crack widths are simulated and compared. Finally, a beveled SFP architecture is proposed to provide a feasible solution for avoiding cracks and increasing the reliability of AlGaIn/GaN HEMTs.

## 2. Failure Analysis Experiments

During the failure analysis of a commercial AlGaIn/GaN HEMT device, a large number of focused ion beam (FIB, Thermo Scientific Helios G4 PFIB UXe DualBeam system) characterizations were carried out after breakdown. The images were acquired at 5 kV and 0.17 nA under secondary electron imaging mode. From scanning electron microscope (SEM) surface morphology, the gate metal at the breakdown points was broken or partially damaged, as shown in Figure 1a. FIB cross-section characterization was carried out at position A, near the breakdown point as shown in Figure 1b. The morphology of the gate metal was partially damaged, and there was a crack in the SFP near the drain side. The SFP broke at the crack and was lifted near the source side. Position B, with a better surface morphology below the breakdown point, was characterized as shown in Figure 1c. The SFP was disconnected, and there were cracks at the junctions above the gate cap. Another position, C (not shown in Figure 1a), on the same gate where no breakdown occurred was also characterized. As shown in Figure 1d, the SFP was still connected, but there was also a trend of cracking at the junctions. It is inferred that the cracks were not caused by breakdown but caused by the SFP deposition process, since there was no crack in the secondary passivation layer between the SFP and the gate cap. In the SFP deposition process, the metal is relatively prone to fracture due to stress [16–18]. According to the FIB characterization results, there is a certain correlation between gate breakdown and SFP cracking; however, a further study of the internal mechanism is still needed.

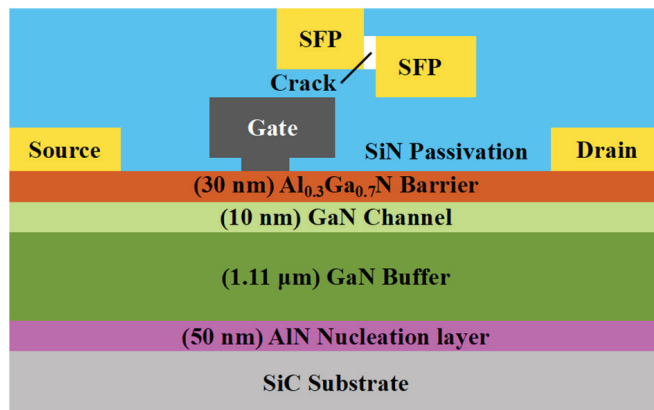


**Figure 1.** (a) SEM surface image of the AlGaIn/GaN HEMT after breakdown; (b–d) SEM cross-section images of different breakdown and non-breakdown points along the same gate as marked in (a).



### 3. Materials and Methods

APSYS (Crosslight, Vancouver, Canada) device simulations were carried out to analyze the detailed electrical characteristics [19]. The simulated AlGaIn/GaN HEMT structure with a T-gate is illustrated in Figure 2. The epitaxial layer structure consisted of an n-doped ( $2 \times 10^{16} \text{ cm}^{-3}$ ) semi-insulating SiC substrate layer, AlN nucleation layer, GaN buffer layer and GaN channel layer. Above these were an unintentionally doped  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}$  barrier layer and a SiN passivation layer. Traps with a maximum concentration of  $1 \times 10^{17} \text{ cm}^{-3}$  and a relative energy level of 0.45 eV were assigned to model Fe doping in the buffer layer [20,21]. Two-dimensional electron gas was generated using interface and polarization statements, and the electron mobility of  $1400 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$  was used in the simulation. In order to simulate the breakdown mechanism, the Chenoweth law for impact ionization with user-definable parameters was used [22]. The  $V_{\text{br}}$  was defined as the drain voltage when the drain-to-source current reached  $1 \text{ mA/mm}$  [10,23].



**Figure 2.** Cross-sectional illustration of the AlGaIn/GaN HEMT with a cracked SFP.

A Schottky contact with a work function of 5.4 eV was used as a gate electrode, and an ohmic contact with a work function of 4.0 eV was used for the source and drain electrodes. For the AlGaIn/GaN HEMT with a cracked SFP, the crack height was set as 200 nm, and the width was varied from 0–50 nm in 10 nm step. In addition, the material within the crack was set as air in the simulation. The SiC substrate and source electrode were grounded. For the breakdown simulation, a gate voltage of  $V_g = -6 \text{ V}$  was applied to imitate the off-state situation. The SFP and source electrode maintained the same potential in the simulation. The other main dimension parameters used are provided in Table 1.

**Table 1.** Dimension parameters for simulation.

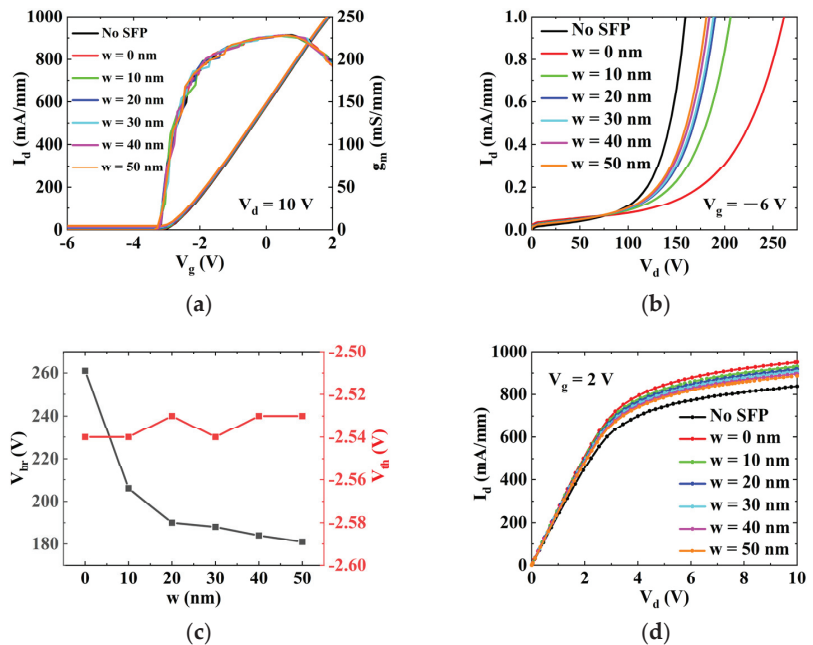
Name	Value	Name	Value
Source-to-gate distance	1.7 $\mu\text{m}$	Gate foot thickness	0.05 $\mu\text{m}$
Gate-to-drain distance	4.5 $\mu\text{m}$	Gate head thickness	0.55 $\mu\text{m}$
Source/drain length	1 $\mu\text{m}$	Source/drain thickness	0.2 $\mu\text{m}$
Gate foot length	0.45 $\mu\text{m}$	SFP length	1.7 $\mu\text{m}$
Gate head length	1.25 $\mu\text{m}$	SFP thickness	0.55 $\mu\text{m}$

### 4. Results and Discussion

Cracks of different shapes often appear at the junctions of a SFPs, and it is necessary to investigate the effect of different crack widths on a device's electrical performance. Therefore, simulations of different AlGaIn/GaN HEMT structures were carried out. When  $w = 0 \text{ nm}$ , it means an HEMT with a conventional SFP but without a crack. For comparison, an HEMT without an SFP was also investigated. The transfer and transconductance



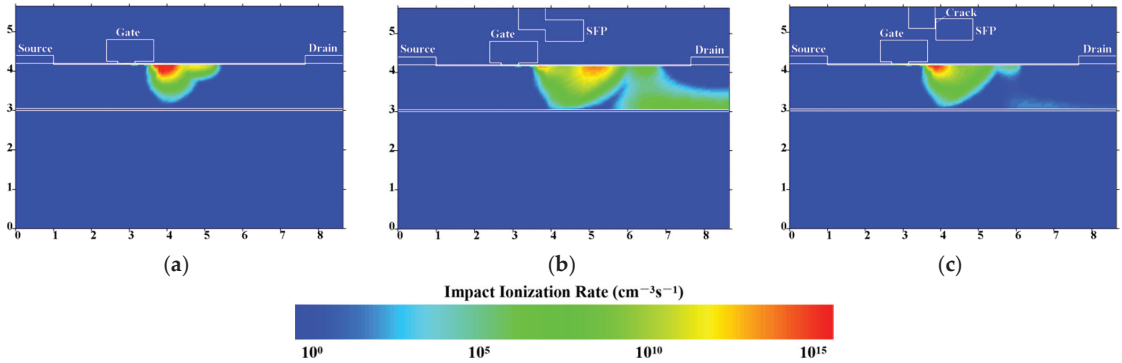
characteristics of these devices are shown in Figure 3a. The drain voltage ( $V_d$ ) was set to 10 V, and the gate voltage ( $V_g$ ) was swept from  $-6$  V to  $2$  V. Then, the threshold voltage ( $V_{th}$ ) was extracted from a linear extrapolation of the transfer characteristics at the point of maximum transconductance. The presence of an SFP and SFP cracks had little effect on the transfer and transconductance properties of the device. The  $V_{th}$  and the maximum transconductance were about  $-2.53$  V and  $227$  mS/mm, respectively. As shown in Figure 3b, the  $V_{br}$  was 160 V at  $V_g = -6$  V for the HEMT without an SFP. For the HEMT with an SFP, when  $w$  increased from 0 nm to 50 nm, the  $V_{br}$  decreased from 261 V to 181 V. This decreasing trend slowed down when  $w$  increased to 20 nm. It was seen that the SFP had a positive effect, improving the  $V_{br}$ . However, once the SFP had a crack, the  $V_{br}$  considerably decreased. Furthermore, the relationship between  $V_{br}$  and  $V_{th}$  depending on crack width is depicted in Figure 3c. Figure 3d shows simulated pulsed I-V characteristics with a  $1 \mu$ s pulse width and a 1 ms pulse period. The quiescent bias point was set as ( $V_{g,q} = -6$  V,  $V_{d,q} = 80$  V). In contrast to the static results, the HEMT with a conventional SFP showed a maximum saturated drain current, while the HEMT without an SFP showed a minimum one. The reason for the discrepancy between the dynamic and static I-V characteristics is that the SFP alleviates the high electric field and restrains the trapping in the buffer [24,25]. The appearance of a crack affected the modulation effect of the SFP on the electric field. As a result, the trapping process increased, and the saturated drain current decreased.



**Figure 3.** (a) Drain current and transconductance versus gate voltage; (b) off-state drain current versus drain voltage; (c) breakdown voltage and threshold voltage versus crack width; (d) pulsed I-V characteristics for AlGaN/GaN HEMTs without SFP and with SFP of different crack widths.

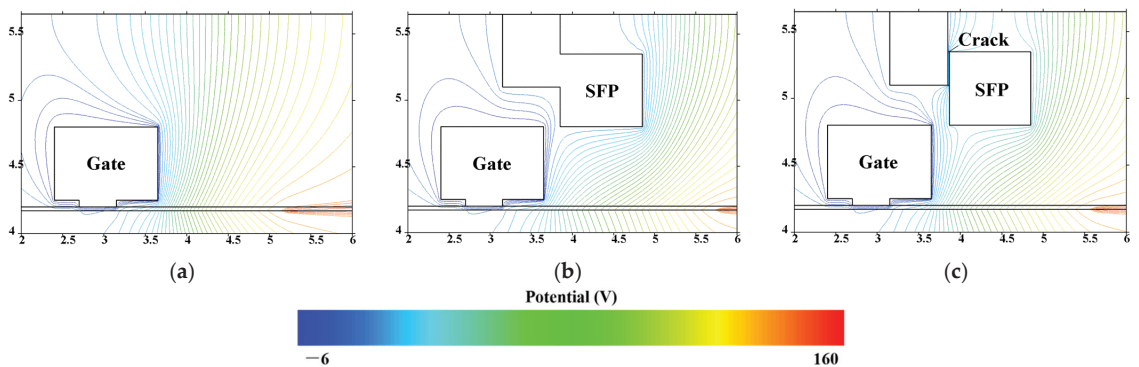
In order to find the weak point where the device is prone to breakdown, the impact ionization rates were simulated at their respective  $V_{br}$  points. Cross-sections of the impact ionization rate distribution for three different AlGaN/GaN HEMT structures are shown in Figure 4. For the HEMT without an SFP and the HEMT with a 20 nm wide cracked SFP, the max impact ionization rate was located at the gate edge of the drain side. However, if there was no crack in the SFP ( $w = 0$  nm), the position of the max impact ionization rate moved to the SFP edge of the drain side, as shown in Figure 4b. High impact ionization rates lead to

enhanced carrier generation and early breakdowns of a device [8,9], and the appearance of an SFP decreases the impact ionization rate and changes the distributions at the same time [13,14].



**Figure 4.** Impact ionization rate contours for AlGaIn/GaN HEMT (a) without an SFP; (b) with a conventional SFP; (c) with a 20 nm wide cracked SFP at their respective  $V_{br}$  points.

The potential distributions for the three different aforementioned AlGaIn/GaN HEMT structures were simulated at  $V_g = -6$  V and  $V_d = 160$  V. The contours for a closeup region, including the gate and SFP, are shown in Figure 5. It was observed that for the HEMT without an SFP, most of the potential lines crowded at the drain side of the gate, as well as in the barrier and buffer layers. Crowded potential lines usually lead to a high electric field and consequently a high impact ionization rate. For the HEMT with a conventional SFP, high potential line density appeared at both the drain side of the gate and the drain side of the SFP, which is attributed to the modulation effect of the SFP [12,26,27]. The potential line densities in the barrier and buffer layers were also lower than those for the HEMT without an SFP. Once the SFP had cracked, some potential lines appeared in the cracked region. The right part of the SFP did not share the same potential as the left part anymore, and its modulation effect finally weakened.



**Figure 5.** Potential contours for AlGaIn/GaN HEMT (a) without an SFP; (b) with a conventional SFP; (c) with a 20 nm wide cracked SFP at  $V_g = -6$  V,  $V_d = 160$  V.

The electric field is also an important parameter which determines the  $V_{br}$  of an HEMT device [28–30]. Therefore, the electric field along the channel before breakdown ( $V_g = -6$  V,  $V_d = 160$  V) is shown in Figure 6. It was found that the electric field peaks all appeared at the gate edge of the drain side. The HEMT without an SFP showed the maximum electric field peak of 1.82 MV/cm. As the  $w$  increased, the electric field peak increased from 1.38 MV/cm to 1.70 MV/cm. It is obvious that the  $V_{br}$  is inversely proportional to the

electric field peak. The field plate plays a major role in the electric field, impact ionization rate distribution and the breakdown of the AlGaIn/GaN HEMT; however, the occurrence of a crack will reduce the electric field peak inhibition by the field plate. Given this, the wider the SFP crack becomes, the poorer the electrical performance.

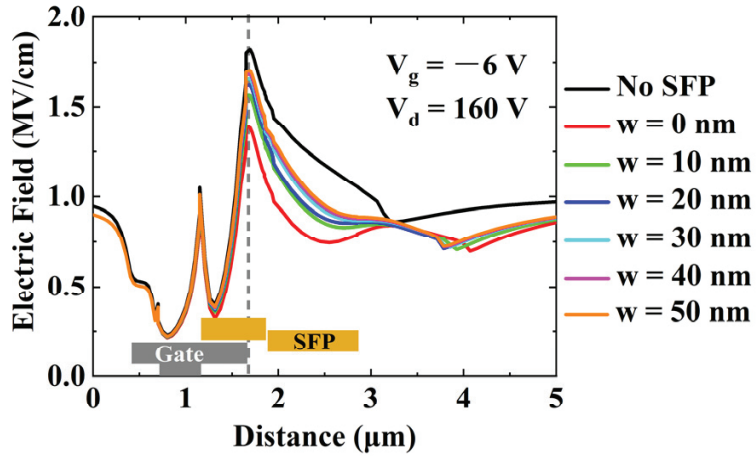
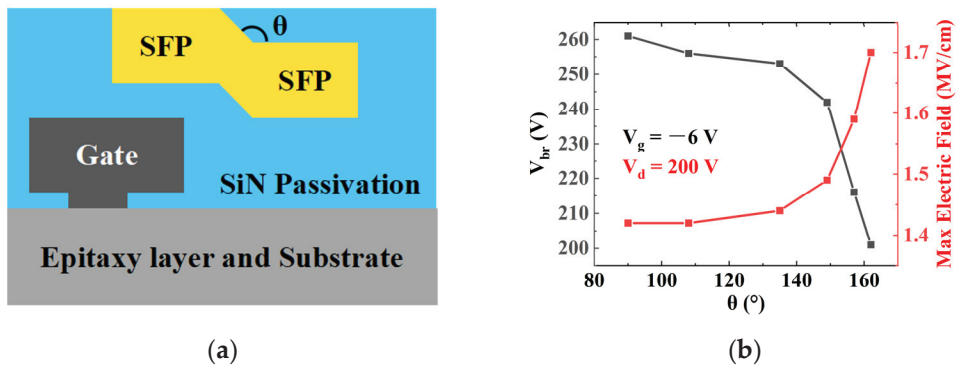


Figure 6. Electric field along the channel for various AlGaIn/GaN HEMTs.

As discussed above, the appearance of SFP cracks degrades the electrical performance of AlGaIn/GaN HEMTs. In the process of SFP metal deposition, cracks form easily at these junctions due to the steep angle and high stresses [16–18]. High stress usually appears at the right-angled corner. When the angle increases, the stress reduces, and, consequently, the cracking tendency decreases [31,32]. Accordingly, we propose a beveled SFP structure (see Figure 7a) since increasing the bevel angle at this junction may relieve the stress and reduce the probability of cracking. A further simulation study investigating whether the rise of junction angle affects the electrical performance of a device was carried out. For convenience, the angle is named  $\theta$  as illustrated in Figure 7a. When  $\theta = 90^\circ$ , it means the HEMT with a conventional SFP of which the junction is a right angle. In the following simulations, the total length of SFP was kept unchanged and  $\theta$  changed from  $90^\circ$  to  $162^\circ$  ( $90^\circ$ ,  $108^\circ$ ,  $135^\circ$ ,  $149^\circ$ ,  $157^\circ$  and  $162^\circ$ ). The same electrical parameter simulations were carried out as in the above study. As an example, a proposed HEMT with an SFP bevel angle of  $108^\circ$  achieved a  $V_{br}$  of 256 V, which is very close to the HEMT with a conventional SFP. The channel electric field and the cross-sectional impact ionization rate distributions also showed similar results. As shown in Figure 7b, when  $\theta$  increased from  $90^\circ$  to  $162^\circ$ , the  $V_{br}$  decreased from 261 V to 201 V. Furthermore, when  $\theta$  was increased to  $135^\circ$ , the rate of decline in  $V_{br}$  increased. Even so, the  $V_{br}$  of 201 V was still higher than that of the HEMT with a 20 nm wide cracked SFP. The channel electric field peak was extracted before breakdown ( $V_g = -6$  V,  $V_d = 200$  V), and it showed an inverse trend compared with the  $V_{br}$ . With an increase in  $\theta$ , the distance from the lower edge of the SFP to the channel becomes longer, so the modulation effect of the SFP on the electric field is weakened [12,33,34]. As a result, the beveled SFP reduces the stress and the risk of cracking, but it also reduces the electrical performance of the device.



**Figure 7.** (a) Cross-sectional illustration of AlGaN/GaN HEMT with a bevel SFP; (b) breakdown voltage and channel electric field peak versus the bevel angle.

## 5. Conclusions

To investigate the effects of cracks in SFPs on a device's electrical performance, Al-GaN/GaN HEMTs with different SFP structures were studied by using simulations. The results show that compared with the HEMT without an SFP, the HEMT with a conventional SFP showed better breakdown and dynamic I-V performances. However, we found that once a crack appeared in the SFP, the device's electrical performance degraded, and the decreasing trend slowed down when the crack width increased to 20 nm. The physical mechanism was investigated from the aspects of impact ionization rate, potential and channel electric field. The SFP structure effectively alleviated the peak electric field at the gate edge of the drain side, but the crack reduced the effect of SFP undesirably. The beveled SFP structure is a good strategy to reduce the risk of cracking; however, this is at the expense of a device's electrical indicators. When the bevel angle increases to  $135^\circ$ , the breakdown voltage begins to drop rapidly. Thus, it is recommended to balance these factors according to actual needs, and a bevel angle of no more than  $135^\circ$  is suggested. Field plate technology is simple and compatible with other electric field optimization technologies. These results can be used for fabricating future HEMT devices with SFPs to achieve a high breakdown voltage and high reliability.

**Author Contributions:** Conceptualization, Y.-N.B., C.-L.D. and X.-L.C.; characterization, C.-L.D.; simulation, Y.-N.B. and C.-L.D.; data curation and analysis, Y.-N.B., C.-L.D., X.-L.C. and R.Y.; writing—original draft preparation, Y.-N.B. and C.-L.D.; writing—review and editing, Y.-N.B., C.-L.D., X.-L.C., R.Y., H.-J.L., Y.Z., X.-Y.D. and J.-J.Z. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research was funded by the Fundamental Research Funds for the Central Universities under Grant QTZX22022.

**Institutional Review Board Statement:** Not applicable.

**Informed Consent Statement:** Not applicable.

**Data Availability Statement:** Not applicable.

**Conflicts of Interest:** The authors declare no conflict of interest.

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## Article

# Numerical Study of Growth Rate and Purge Time in the AlN Pulsed MOCVD Process

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**Abstract:** The relationship between the purge time and the overall growth rate in pulsed injection metal–organic chemical vapor deposition with different V/III ratios is studied by numerical analysis. The transport behavior of TMAI and TMAINH<sub>3</sub> during the process is studied to understand the effect of the adductive reaction. The results show that, as the V/III ratio increases, there is a significant reduction in the average growth rate per cycle, without the addition of a purging H<sub>2</sub> pulse between the III and V pulses, due to stronger adductive reaction. The adductive reaction can be reduced by inserting a purging pulse of pure H<sub>2</sub> between the III and V pulses, but there is a decrease in the overall growth rate due to the longer cycle time. At smaller V/III ratios, the growth rate decreases with increasing purge times, since the gain in reducing the adductive reaction is offset by the detrimental effect of extending the cycle time. The degree of reduction in the adductive reaction is higher for larger V/III ratios. When the benefit of reducing the adductive reaction overcomes the deficiency of the extending cycle time, a remarkable enhancement of the growth rate can be obtained at high V/III ratios by inserting a pure H<sub>2</sub> purge pulse between the III and V pulses. A higher overall growth rate can be achieved at higher V/III ratios by choosing an appropriate purge time.

**Keywords:** MOCVD; nitride; pulsed injection; growth rate

**Citation:** Lin, W.-J.; Chen, J.-C.

Numerical Study of Growth Rate and Purge Time in the AlN Pulsed MOCVD Process. *Crystals* **2022**, *12*, 1101. <https://doi.org/10.3390/cryst12081101>

Academic Editors: Peng Chen and Zhizhong Chen

Received: 18 July 2022

Accepted: 4 August 2022

Published: 5 August 2022

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## 1. Introduction

III-nitride materials are widely used in power devices, high-frequency communications, and UV applications because of their excellent properties. Among the many III-nitride materials, aluminum nitride (AlN) is one of the most important, often used as a buffer layer between the sapphire substrate and other III semiconductor materials, because the lattice mismatch between AlN and sapphire is minor. However, the small migration of Al atoms on the substrate makes it difficult to grow high-quality AlN film [1]. One way to increase the migration of the Al atoms is to increase the temperature of the substrate. However, the high-temperature growth conditions not only make the parasitic reaction more intense, they also induce the problem of thermal expansion. Another way to increase the migration of Al atoms is to apply the pulsed injection method (PI method) during the metal–organic chemical vapor deposition (MOCVD) process. During the pulsed process, the supply of TMAI and NH<sub>3</sub> is carried out separately. The TMAI follows the pyrolysis reaction pathway instead of adducting with NH<sub>3</sub> in the gas phase before being deposited on the surface. It changes the dominant species on the surface from Al-N to Al. The migration of Al atoms increases because the number of N atoms is much lower during the pulsed process [2]. Smoother AlN film can be achieved due to the lateral growth of film caused by the higher Al migration. Demir et al. [3] grew high-quality AlN by pulsed MOCVD (PIMOCVD) at a growth temperature of 1443 K with III and V pulse durations of 4 s and 2 s, respectively.

Many studies have pointed out the need for a hydrogen purge between the TMAI pulse (III pulse) and NH<sub>3</sub> pulse (V pulse) to further suppress the adductive reactions and achieve better surface roughness. Khan et al. [4] fixed the duration of the different pulses to 1 s with a 1 s hydrogen purge time in between. The crystalline quality of the material

grown by the pulsed process at 723 K was as good as the material grown by the steady-flow process at 1273 K. Takeuchi et al. [5] compared the growth rates of AlN film grown by the steady-flow process and pulsed process with a 1 s purge time. In the steady-flow process, the TMAI and NH<sub>3</sub> were supplied at the same time. At a V/III ratio of 20.8, it was found that the growth rate of the pulsed process was 5.56 times that of the steady-flow process.

The effects caused by different TMAI and NH<sub>3</sub> flow rates have also been investigated. Kröncke et al. [6] varied the effective V/III ratio between 200 and 700 and found that increasing the purge time after supplying TMAI could reduce the density of pits. The growth rate of the AlN film for these processes was about 1 µm/h. Rahman et al. [7,8] grew AlN films using NH<sub>3</sub> flow rates ranging from 0.2 to 2.2 slm, with a fixed TMAI flow rate of 15 slm. The durations of the III and V pulses were 4 s and 2 s, respectively, and the growth temperature was 1453 K. The results showed that the best AlN film quality was obtained with 0.6 slm NH<sub>3</sub>. The growth rate of the AlN films was between 0.225 and 0.249 µm/h.

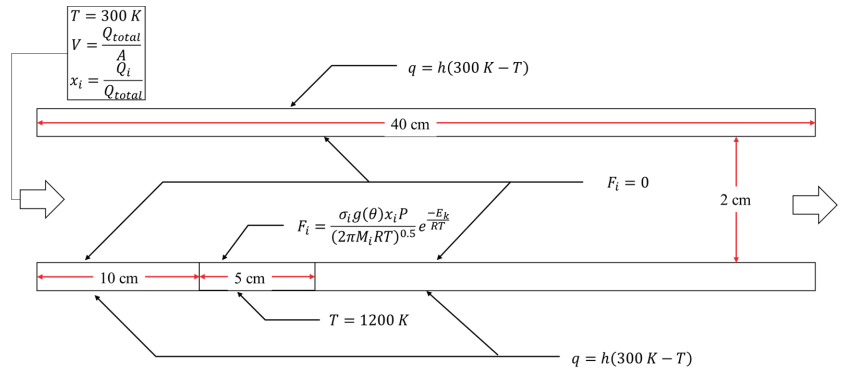
The potential of the pulsed method to improve the quality of AlN has been confirmed in numerous studies. However, there has been great divergence in the growth conditions used in different works. The pulsed process includes more external control parameters than a steady-flow process, making the transport phenomenon during the growth process more complicated. In order to obtain optimal growth conditions, it is important to have an in-depth understanding of its transport phenomena. The transport phenomena during the pulsed process have been investigated numerically in several works. Nakamura et al. [9] performed numerical experiments and observed the generation of AlN particles with different purge times (0, 1, and 2 s) and a constant V/III ratio of about 4000. The results showed the mole concentration of AlN particles to be eliminated with a purge time of 2 s. However, there was a decrease in the overall growth rate per cycle as the purge time increased. Endres et al. [10] also carried out numerical experiments. They showed that for a V/III ratio of 20.8, the optimal purge duration would be 5–6 times the duration of the III and V pulses, resulting in the highest growth rate. Lin and Chen [11] conducted a numerical investigation to explore the physical mechanisms in the evolution of flow motion and heat and mass transfer during the pulse process. They found that the duration of the III and V pulses does not affect the particle generation if the duration time is longer than a critical value (a pulse steady state is reached). The diffusive mass transport of NH<sub>3</sub> in H<sub>2</sub> is greater than that of TMAI in H<sub>2</sub> due to the higher mass diffusion coefficient of NH<sub>3</sub> in H<sub>2</sub>. Therefore, the V pulses easily exceed the III pulses before reaching the substrate when the III/V ratio is 1. More AlN particles occur in the high-temperature region during the H<sub>2</sub> pulse after the III pulse. To reduce the occurrence of AlN particles, the duration of the H<sub>2</sub> pulse after the III pulse should be longer than that after the V pulse. However, the relationship between the purge time and the V/III ratio during the pulsed process and the transport phenomena is still unclear. When the V/III ratio is increased, the purge time should be extended, since more NH<sub>3</sub> will remain in the chamber, leading to stronger parasitic reactions. Furthermore, at a higher V/III, the transient mass transport process becomes more complex, since the main species of the V pulse changes from H<sub>2</sub> to NH<sub>3</sub>.

In this study, the numerical scheme developed in our previous study [11] is extended to first study the transport phenomenon and overall growth rate of the cases without purging and with different V/III ratios. Then, the relationship between the purge time, V/III ratio and overall growth rate is investigated and the maximum overall growth rates for different V/III ratios are investigated.

## 2. Modeling

Figure 1 shows a schematic diagram of the simplified horizontal MOCVD reactor built in our previous study [11] based on the study of Chen et al. [12]. The temperature of the substrate surface was maintained at 1200 K and the operating pressure was 85 Torr. For pulsed processes, the total flow rate for all pulse sequences was fixed at 7 slm to maintain the stability of the flow field. The flow rates of the III and V pulses are denoted by  $Q_{\text{TMAI,p}}$  and  $Q_{\text{NH}_3,p}$ , respectively. The molar flow rate of TMAI for the III pulse was kept

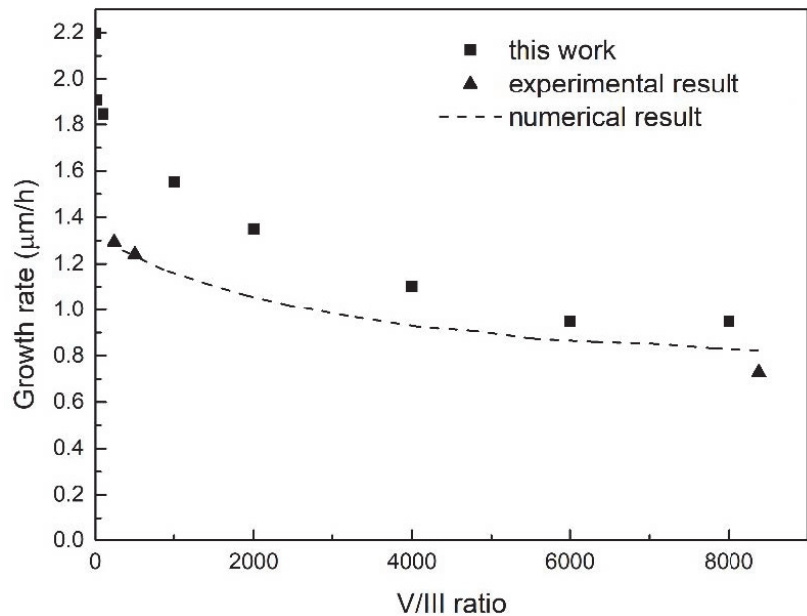
at 30  $\mu\text{mol}/\text{min}$ . The V/III ratio was varied from 1 to 10,000. In the previous study, the concentration of precursors was found to remain stable at 0.15 s after the start of the III or V pulse, which is close to the effective residence time (about 0.13 s). Therefore, in this study, the supply time of the TMAI and  $\text{NH}_3$  was fixed at 0.15 s and the pure hydrogen purge time between III and V pulses was changed from 0 s to 0.1 s. The working fluid in the chamber was considered as an ideal gas. The Reynolds number for the cases investigated in this study was below 400. Compressible laminar flow was applied to describe the flow motion during the process. The equations for the conservation of mass, momentum, heat energy, species, and the detail of material properties are listed in the previous work [10]. The reaction model follows the work performed by Mihopoulos [13]. The commercial software COMSOL was applied to solve the MOCVD processes coupling the fluid dynamics, the heat and mass transfer, and the chemical reactions by the finite element method. The discretization for the momentum and heat equation was linear and that for mass transport and reaction model was quadratic. Due to the rapid chemical reaction near the inlet, the distribution of the width of the element was arranged as arithmetic distribution and the size of the smallest element was 1  $\mu\text{m}$ . The distribution of the height of the elements near the chamber wall also followed arithmetic distribution to calculate the boundary layer effects and the mass flux caused by surface reactions. The backward differentiation formula (BDF) was used to solve the transient behavior and the maximum order for the BDF was 2. To investigate the transport behavior of different species during the process, the maximum time step was limited by 0.001 s. The simulation results obtained in the steady-flow process with this scheme in our previous study [11] are in good agreement with previous results [10,12,13].



**Figure 1.** Schematic diagram and boundary conditions of a simplified horizontal MOCVD reactor.

### 3. Results and Discussion

Before studying the pulsed process, it is necessary to understand the effect of the V/III ratios during the steady-flow process. Figure 2 shows the relationship between the average growth rate along the entire wafer surface and the V/III ratio when the operating pressure is 40 Torr. As the V/III ratio increases, the growth rate decreases due to the higher generation of Al particles caused by higher amounts of  $\text{NH}_3$ . This trend is similar to the numerical and experimental results presented in [14] for a close-coupled showerhead (CCS) reactor during the steady-flow process. However, the growth rate obtained in this study is higher than in the CCS results. This may be due to the difference in growth area between the CCS reactor used in ref. [14] (60.8  $\text{cm}^2$ ) and the channel reactor (25  $\text{cm}^2$ ) used for the present study.

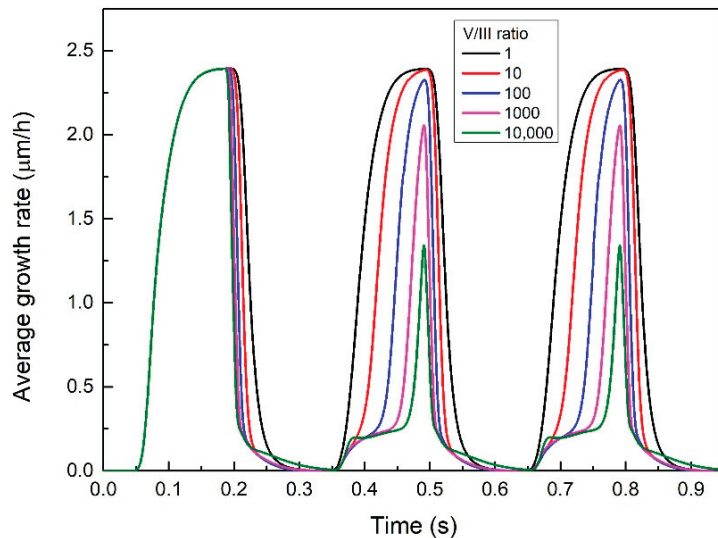


**Figure 2.** Relationship between the average growth rate and the V/III along the entire wafer surface. The square points represent the results obtained in this work and the dashed line and triangles indicate the results from a previous numerical and experimental study [14].

The pulse process considered here first starts with a III pulse, followed by a V pulse, with no purge between the III and V pulses, after which the entire process is cycled repeatedly. Figure 3 shows the average growth rate along the wafer surface during the pulsed process and Figures 4–6 show the mass fraction distributions of TMAI and TMAINH<sub>3</sub> at  $t = 0.18$  s, 0.35 s, and 0.46 s for different V/III ratios. The III pulse reaches the hot substrate surface at approximately  $t = 0.05$  s and the AlN film grows through the pyrolysis reaction [13]. Therefore, there is significant increase in the average growth rate around  $t = 0.05$  s. The V pulse is injected into the chamber at 0.15 s and then the adductive reaction occurs at the rear interface of the III pulse. The adductive reaction between the TMAI and NH<sub>3</sub> leads to the formation of Al particles. Figure 4 shows that at  $t = 0.18$  s, the front interface of TMAINH<sub>3</sub> is still noted to reach the region close to the hot substrate. The movement of the front interface of TMAINH<sub>3</sub> is faster with a higher V/III ratio. Due to the stronger adductive reaction, more TMAINH<sub>3</sub> is produced at a higher V/III ratio (Figure 4b). It affects the substrate at approximately  $t = 0.2$  s. In Figure 3, the beginning of an abrupt drop at around  $t = 0.2$  s can be observed, which occurs earlier and faster with a higher V/III ratio.

The second III pulse starts at 0.3 s and the growth rate increases again at approximately  $t = 0.36$  s (Figure 3). However, as the V/III ratio increases, the magnitude of the maximum growth rate becomes smaller. As can be seen from Figure 5a, for higher V/III ratios, the movement of the front interface of the III pulse is slower because more NH<sub>3</sub> remains in the chamber from the previous cycle which reacts with the TMAI to form TMAINH<sub>3</sub>. The production of TMAINH<sub>3</sub> increases when the V/III ratio is higher (Figure 5b). This results in a greater V/III ratio, and a later and slower increase in the growth rate after  $t = 0.35$  s (Figure 3). Figure 6 shows the mass fraction distributions of TMAI and TMAINH<sub>3</sub> at  $t = 0.46$  s for different V/III ratios, which is 0.01 s after the start of the second V pulse. When the V/III ratio is higher, the rear interface of the III pulse moves faster (Figure 6a), similar to the movement of the rear interface shown in Figure 4a. However, the front interface of the III pulse is affected by the remaining NH<sub>3</sub> in the chamber. The larger

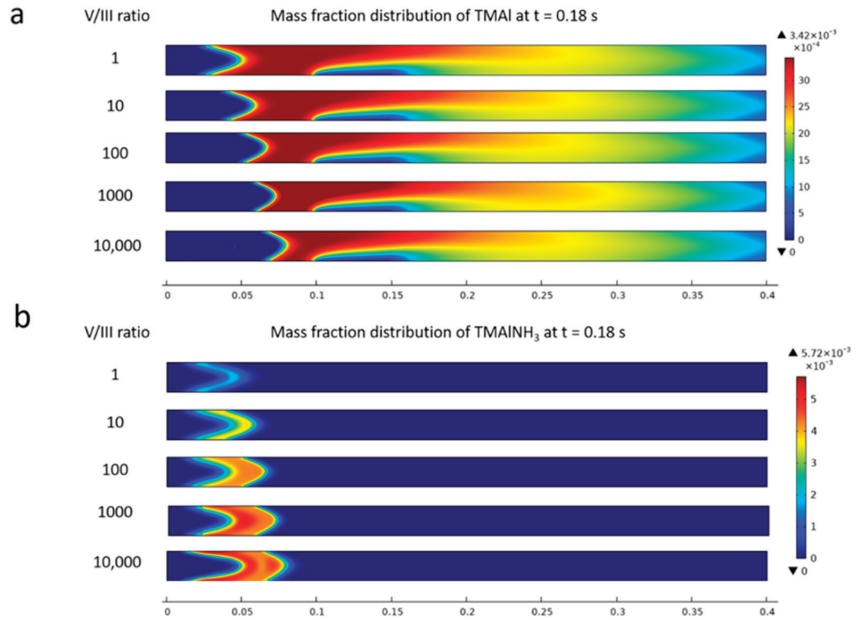
the V/III ratio, the greater the formation of TMAINH<sub>3</sub> near the front and rear interfaces (Figure 6b). This makes the region occupied by the TMAI smaller. Therefore, the maximum value of the average growth rate for the second cycle decreases as the V/III ratio increases (Figure 3). Figure 7 shows the mass fraction distribution of TMAI at  $t = 0.49$  s for different V/III ratios. The movement of the rear interface over the wafer with a V/III ratio equal to 10000 can be seen. This results in a rapid drop in the average growth rate because the rear interface causes a rapid drop in TMAI above the wafer. The phenomena in the third and subsequent cycles are similar to those in the second cycle. It is clear that the decrease in the average growth rate for higher V/III ratios is due to greater TMAINH<sub>3</sub> formation. The insertion of a pure H<sub>2</sub> pulse between the III and V pulses prevents the NH<sub>3</sub> from reacting with the TMAI to form TMAINH<sub>3</sub>.



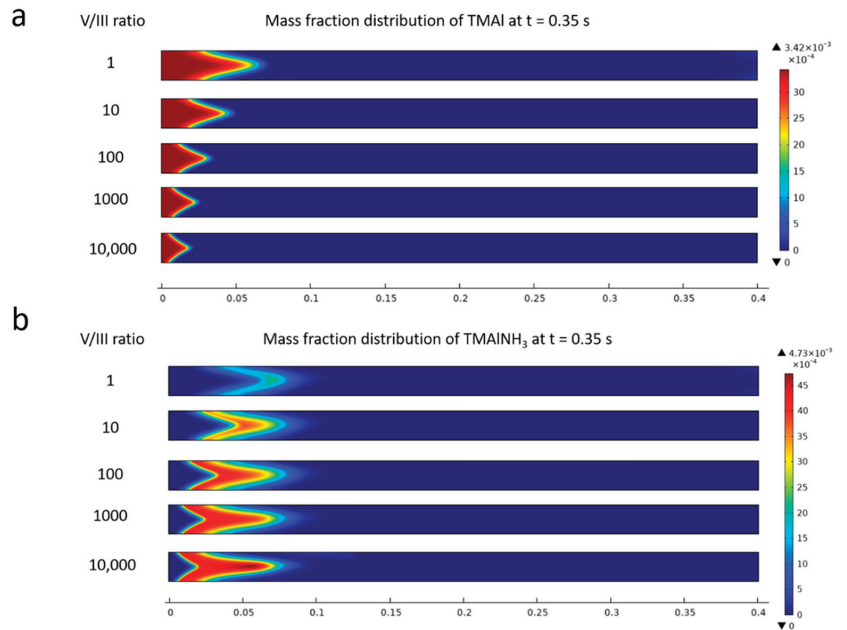
**Figure 3.** Average growth rate along the wafer surface during the pulsed process.

According to our previous results [11], the formation of TMAINH<sub>3</sub> can be minimized by inserting a pure H<sub>2</sub> purge pulse between the III and V pulses. On the other hand, there is a decline in the overall growth rate due to a wider cycle time. As can be seen in Figure 3, the growth rate after the first cycle is significantly affected by changes in the V/III ratios. In practice, the pulsed process time is usually greater than several minutes. Therefore, the differential impact of the first cycle on the overall growth rate will be very small. To investigate the effect of the purge time on the overall growth rate, the average growth rate for the second cycle is calculated. Figure 8 shows the average growth rate throughout the second cycle for different purge times and different V/III ratios. The decrease in the average growth rate as the V/III ratio increases occurs because of the formation of TMAINH<sub>3</sub>. The adductive reaction is weak when the V/III ratio is equal to 1. The benefit of reducing the formation of TMAINH<sub>3</sub> is outweighed by the detrimental effect of the increasing cycle time which causes the average growth rate to decrease with an increase in purge time. When the V/III ratio is equal to 100, there is an increase in the average growth rate as the purge time increases from 0 s to 0.05 s, because the benefit of the reduction in TMAINH<sub>3</sub> outweighs the disadvantage of the increasing cycle time. However, there is a decrease in the average growth rate when the purge time increases from 0.05 s to 0.1 s. In this case, the generation of particles (formation of TMAINH<sub>3</sub>) is very low. The benefit of reducing particle generation is outweighed by the disadvantage of an increase in the cycle time. The maximum growth rate is about 0.75 μm/h. When the V/III ratio is equal to 10,000, the average growth rate increases as the purge time increases. However, the average growth rate may not increase

with longer purge times, because the growth rate at higher V/III ratios does not exceed that obtained at lower V/III ratios. The maximum average growth rate can be expected to be around 0.7  $\mu\text{m}/\text{h}$ .



**Figure 4.** Mass fraction distributions of (a) TMAI and (b) TMAINH<sub>3</sub> at 0.18 s for different V/III ratios.



**Figure 5.** Mass fraction distributions of (a) TMAI and (b) TMAINH<sub>3</sub> at 0.35 s for different V/III ratios.

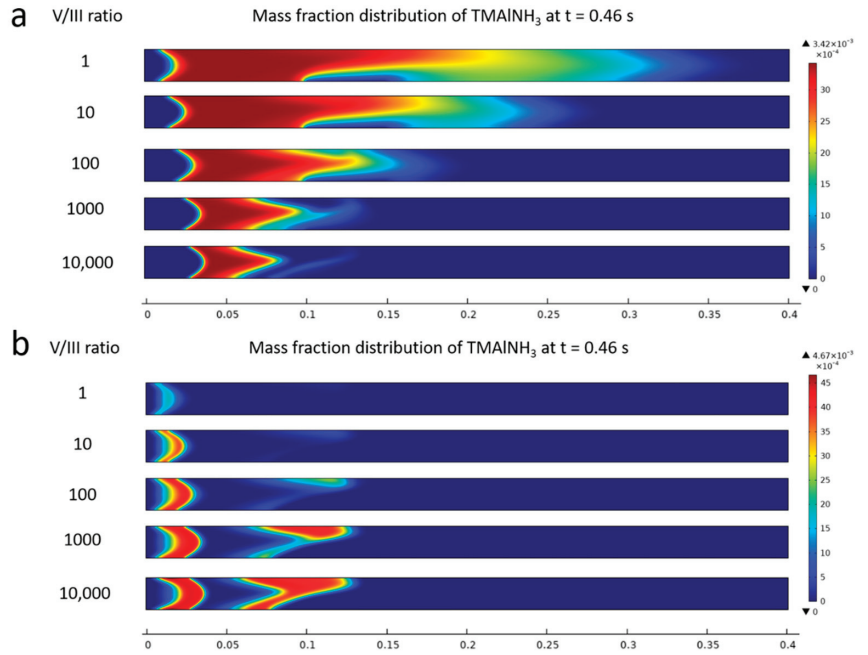


Figure 6. Mass fraction distributions of (a) TMAI and (b) TMAINH<sub>3</sub> at 0.46 s for different V/III ratios.

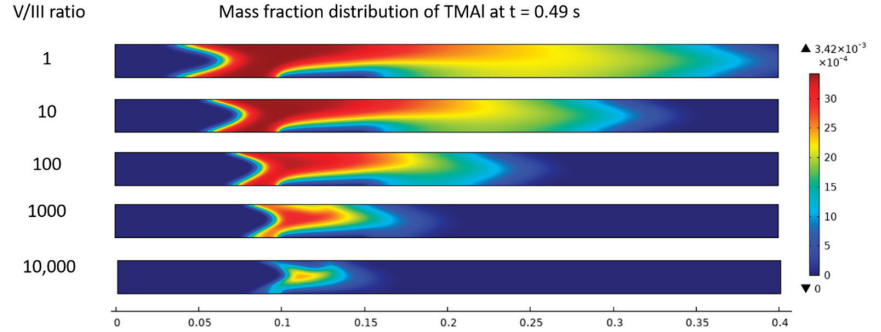


Figure 7. Mass fraction distributions of TMAI at 0.49 s for different V/III ratios.



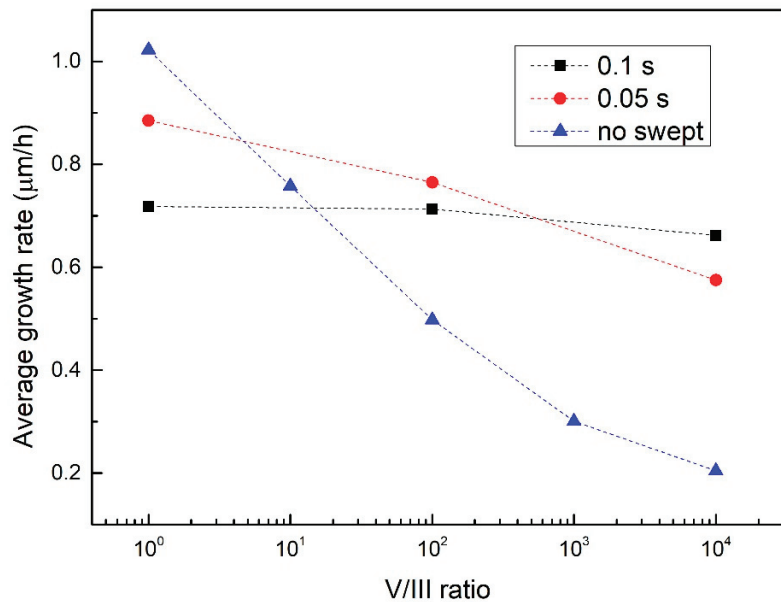


Figure 8. Average growth rate in the second cycle for different purge times and V/III ratios.

#### 4. Conclusions

A numerical analysis is performed to investigate the effects of the V/III ratio on the growth rate during the pulse injection process. The evolution of TMAI and TMAINH<sub>3</sub> during the process is studied in detail. The adductive reaction can be reduced by inserting a pure H<sub>2</sub> purge pulse between III and V pulses, but there may be a decrease in the overall growth due to the longer cycle time. The trade-off between the benefits of reducing particle generation and the disadvantages of increasing the process time can be understood by investigating the relationship between the purge time, the III/V ratio, and the overall growth rate. When the V/III ratio is increased, there is a significant decrease in the average growth rate per cycle, when there is no purge pulse between the III and V pulses due to the stronger adductive reaction (the higher Al particle generation). For smaller V/III ratios, there is a decrease in the growth rate as the purge time increases because the benefit of reducing the adductive reaction is offset by the detrimental effect of the increasing cycle time. This causes the average growth rate to decrease as the purge time increases. The benefit of reducing the adductive reaction is more significant for higher V/III ratios. With increasing purge times, the decline in the growth rate becomes smaller as the V/III ratio increases. Clearly, inserting a pure H<sub>2</sub> purge pulse between the III and V pulses can significantly improve the growth rate when the V/III ratios are high. Higher overall growth rates can be obtained at higher V/III ratios by selecting an appropriate purge time.

**Author Contributions:** W.-J.L., conceptualization, methodology, formal analysis, writing—original draft; J.-C.C., conceptualization, writing—review and editing, supervision. All authors have read and agreed to the published version of the manuscript.

**Funding:** The authors would like to thank the Ministry of Science and Technology, R.O.C, for their support of this study through grant number MOST-106-2221-E-008-052-MY3.

**Institutional Review Board Statement:** Not applicable.

**Informed Consent Statement:** Not applicable.

**Data Availability Statement:** Not applicable.

**Conflicts of Interest:** The authors declare no conflict of interest.

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## Article

# Efficiency Droop and Degradation in AlGaIn-Based UVB Light-Emitting Diodes

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**Citation:** Chang, Y.-T.; Lai, M.-J.; Liu, R.-S.; Wang, S.-C.; Zhang, X.; Zhang, L.-J.; Lin, Y.-H.; Huang, S.-F.; Chen, L.-C.; Lin, R.-M. Efficiency Droop and Degradation in AlGaIn-Based UVB Light-Emitting Diodes. *Crystals* **2022**, *12*, 1082. <https://doi.org/10.3390/cryst12081082>

Academic Editor: Peng Chen

Received: 22 June 2022

Accepted: 11 July 2022

Published: 1 August 2022

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**Abstract:** In this study, we found that the current droop (J-droop) in AlGaIn-based UVB light-emitting diodes was more obvious at higher temperatures, despite both the main and parasitic peaks undergoing monotonic decreases in their intensity upon an increase in the temperature. The slower temperature droop (T-droop) did not occur when the forward current was increased to temperatures greater than 298 K. After an aging time of 6000 h, the emission wavelengths did not undergo any obvious changes, while the intensity of the parasitic peak barely changed. Thus, the degradation in the light output power during long-term operation was not obviously correlated to the existence of the parasitic peak.

**Keywords:** current droop; temperature droop; AlGaIn; ultraviolet-B; light-emitting diodes; external quantum efficiency

## 1. Introduction

AlGaIn-based ultraviolet-B light-emitting diodes (UVB-LEDs) that display emission wavelengths of 280–315 nm have attracted a great deal of attention since the implementation of the Minamata Convention on Mercury and due to the global health crisis arising from the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) [1,2]. This is because there is much potential for using such UVB-LEDs in medical and agricultural applications [3–7]. Although several reports have disclosed that high external quantum efficiencies (EQEs) are possible [8–12], current droop (J-droop) and temperature droop (T-droop) processes, which commonly occur with visible-light LEDs, are also severe problems in AlGaIn-based UVB-LEDs, even for emission wavelengths of less than 280 nm [13–20]. In addition to problems related to efficiency droop, accompanying parasitic peaks are often observed in electroluminescence (EL) spectra plotted on a logarithmic intensity scale [13,14,16,17]. The shapes of the parasitic peaks of AlGaIn-based UVB-LEDs possess a few characteristic features, with a closed-form model having been developed to obtain more insight into their

origin [16]. One emission peak, near 340 nm, which likely originated from an intra-band-gap radiative transition in the last quantum barrier (LQB) next to the electron-blocking layer (EBL), was influenced at high currents by enhanced hole injection upon an increase in the temperature. The other emission peak, near 410 nm, is possibly attributable to a radiative transition on the p-side. In other words, at lower driving currents, significant decreases have occurred in the intensity of both the signals from multiple quantum wells (MQWs) and the parasitic emissions when the temperature is increased to above 300 K [16]. In addition, two main parasitic peaks (310 and 400 nm) have been observed extending the low-energy side of the main peak at 275 nm [17]. The suggested origins of these parasitic peaks are deep-level radiative centers in the active region, or they are associated with other centers located in the p-region. Despite a few recent reports discussing the phenomena of T-droop, J-droop, and current-induced degradation in AlGaIn-based UVB-LEDs [16,21,22], the mechanisms through which the parasitic peaks affect the degradation behavior during aging operation remain unclear—although they have attracted great interest.

In this study, we fabricated AlGaIn-based UVB-LEDs that displayed a main emission peak wavelength of approximately 306 nm and an EL full width at half maximum (FWHM) of approximately 9 nm. We examined the EL characteristics of these UVB-LEDs over a temperature range of 298 to 348 K and a forward current ( $I_f$ ) range from 10 to 130 mA to obtain insight into the behavior of the EL emission and the efficiency droop. Furthermore, we evaluated the impact of the parasitic peaks on the aging lifetimes of these UVB-LEDs, and we suggest a mechanism for the degradation that occurred during the aging operation.

## 2. Materials and Methods

All epitaxial layers were obtained using low-pressure metal–organic chemical vapor deposition (LP-MOCVD). First, a 2.2  $\mu\text{m}$  thick AlN buffer layer was grown on a 2 inch (0001)-oriented sapphire substrate. Next, a strain-relieving interlayer consisting of 30 periods of an AlN/AlGaIn superlattice was grown on the AlN buffer layer. A 1.5  $\mu\text{m}$  thick layer of undoped  $\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}$  was then grown on the interlayer, followed by a 2  $\mu\text{m}$  thick Si-doped  $n\text{-Al}_{0.5}\text{Ga}_{0.5}\text{N}$  layer as the n-contact layer. The active region of the MQWs included five pairs of 2 nm thick  $\text{Al}_{0.35}\text{Ga}_{0.65}\text{N}$  quantum wells (QWs) and 8 nm thick  $\text{Al}_{0.45}\text{Ga}_{0.55}\text{N}$  quantum barriers (QBs), followed by a two-fold Mg-doped  $p\text{-Al}_{0.55}\text{Ga}_{0.45}\text{N}$  (10 nm)/Mg-doped  $p\text{-Al}_{0.4}\text{Ga}_{0.6}\text{N}$  (2 nm) structure as the EBL. Subsequently, a 50 nm thick Mg-doped  $p\text{-AlGaIn}$  layer, with the Al content decreasing from 30% to 0%, was grown on the EBL. Finally, a 20 nm thick Mg-doped  $p\text{-GaIn}$  layer was deposited, serving as the p-contact layer. After the epitaxial layers had been grown, the sample was annealed in situ (700  $^\circ\text{C}$ , 15 min) under a  $\text{N}_2$  ambient to activate the Mg dopants. UVB-LED chips having dimensions of  $550 \times 550 \mu\text{m}^2$  were fabricated using standard flip-chip processing technologies [23].

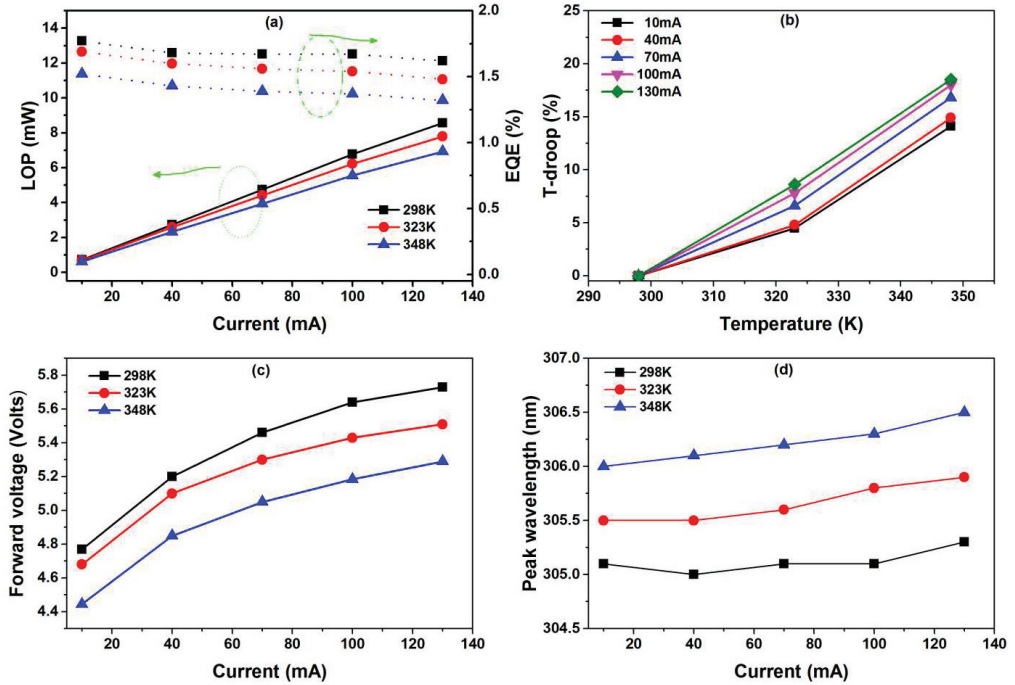
The prepared UVB-LED chips were flip-bonded onto AlN-based direct plating copper ceramic (AlN-DPC) lead frames (LFs) using the eutectic method, then attached to a quartz glass as the hermetic cover. The packaged samples were soldered onto an Al core printed circuit board (MCPCB). The light output power (LOP), current–voltage characteristics, and EL spectra of the samples were measured using an ATA-5000 LED photoelectric measurement system (Everfine) equipped with a 30 cm diameter integrating sphere. During measurement, the temperature of the heat-sink enclosing the samples was controlled (at 298, 323, or 348 K) while the values of  $I_f$  varied from 10 to 130 mA. Aging tests were performed over 6000 h at a value of  $I_f$  of 40 mA at room temperature (RT) to investigate the UVB-LED characteristics.

## 3. Results and Discussion

Figure 1a reveals the dependence of the EQEs and LOPs of the fabricated UVB-LED on the three tested temperatures and the various forward currents. The LOP increased monotonically when the forward current was increased to 130 mA, reaching maximum values of 8.6, 7.8, and 6.9 mW at 298, 323, and 348 K, respectively. The maximum EQEs at 298, 323, and 348 K (1.77, 1.69, and 1.52%, respectively) occurred when the value of

$I_f$  was 10 mA; at 130 mA, they decreased to 1.62, 1.48, and 1.32%, respectively. After applying Equation (1), we obtained J-droops of 8.47, 12.42, and 13.16% at 298, 323, and 348 K, respectively.

$$J - \text{droop} (\%) = \frac{\text{Peak EQE @10mA} - \text{Peak EQE @forward current}}{\text{Peak EQE @10mA}} \times 100\% \quad (1)$$



**Figure 1.** (a) EQEs (dotted lines) and LOPs (solid lines) of the AlGaN-based UVB-LED plotted with respect to the forward current, measured at three different temperatures. (b) T-droop plotted with respect to temperature, measured at various forward currents. (c) Forward voltage and (d) peak wavelength plotted with respect to forward current, measured at the three temperatures.

For a given value of  $I_f$ , the EQEs decreased monotonically upon an increase in the temperature, and then decreased further upon an increase in the value of  $I_f$ . These findings suggested that the efficiency droop was probably related to a mechanism of enhanced non-radiative recombination, with carrier leakage or Auger recombination being exacerbated [16–21]. Figure 1b presents the T-droops with respect to temperature, which was quantified as follows:

$$T - \text{droop} (\%) = \frac{\text{Peak EQE @298K} - \text{Peak EQE @T}}{\text{Peak EQE @298K}} \times 100\% \quad (2)$$

Interestingly, after applying Equation (2), the T-droops measured at 10, 40, 70, 100, and 130 mA were 4.52, 4.76, 6.59, 7.78, and 8.64%, respectively, when the value of  $T$  was 323 K; at 348 K, they increased to 14.12, 14.88, 16.77, 17.96, and 18.52%, respectively. We observed monotonically increasing T-droops upon an increase in the temperature from 298 to 348 K, with higher T-droops occurring at higher values of  $I_f$  at a constant temperature. This behavior is not consistent with a previous finding that the T-droop decreased upon an increase in the current from 0.5 to 100 mA at a temperature of 340 K [20]. We suggest that

the mechanism of T-droop in this study originated from Auger recombination, with carrier leakage becoming dominant when the temperature reached 348 K.

Figure 1c,d displays the effects of the forward voltage ( $V_f$ ) and peak wavelength on the forward currents of the fabricated UVB-LED at the three tested temperatures. The forward voltages decreased and the peak wavelengths increased upon an increase in the temperature at the same forward current due to shrinkage of the band gap; the peak wavelength underwent a slight blue-shift ( $<0.5$  nm) upon an increase in the current from 10 to 40 mA, when the temperature was 298 or 323 K. This result implies the absence of a band-filling effect or coulomb screening of the quantum confinement Stark effect (QCSE) in the MQWs of the fabricated UVB-LED. When the temperature was 348 K, the peak wavelength underwent a slight red-shift when the current was increased from 10 to 130 mA due to the effect of self-heating. Thus, suppression of the temperature-dependent recombination mechanism in the MQWs of the fabricated UVB-LED presumably occurred at temperatures of less than 348 K.

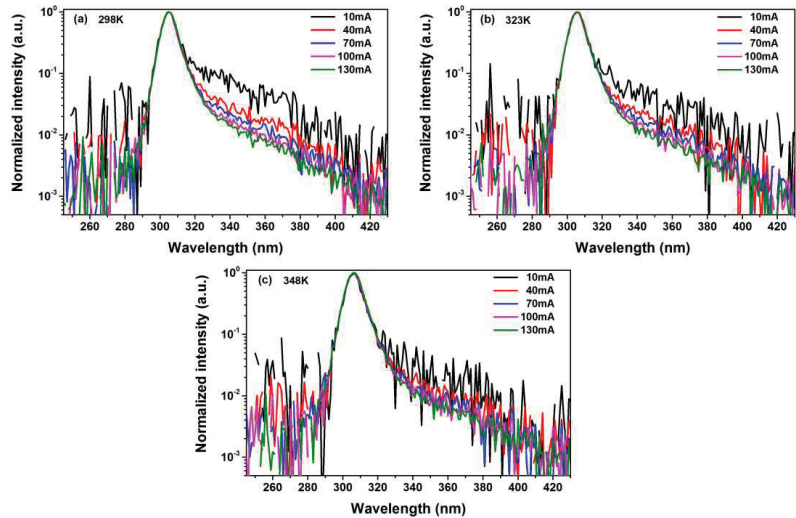
Figure 2a–c presents the normalized EL emission spectra plotted on a logarithmic scale, measured at 298, 323, and 348 K, respectively, for forward currents ( $I_f$ ) supplied in the range from 10 to 130 mA. Each EL emission spectrum featured a main peak wavelength near 306 nm, with a parasitic peak appearing in the range from 330 to 370 nm. The relative intensities of the parasitic peaks decreased when the value of  $I_f$  and the temperature increased. Figure 3a–d displays the spectral distributions and the peak intensities of the EL recorded at various forward currents and temperatures of 298, 323, and 348 K. At a constant temperature, the intensity ratios between the parasitic and main peaks decreased when the value of  $I_f$  increased. However, at a constant value of  $I_f$ , the intensity ratios of the parasitic and main peaks decreased upon an increase in the temperature (Figure 3d). This behavior is different from that expected when considering the previously suggested hypothesis that the parasitic peak emission is related to a defect-assisted emission in the MQW active region [13]. In addition, Wu et al. reported that the band-edge emission in the EL spectra surged, while the increases in the intensities of two parasitic peaks stalled upon an increase in the value of  $I_f$  at various temperatures [17]. They obtained maximum EQEs of 1.19 and 0.61% at temperatures of 20 and 300 K, respectively; when the current increased from 1 to 7 mA, these values decreased to approximately 0.82 and 0.53%, respectively [17]. In other words, the decrease in the EQE at a temperature of 20 K (ca. 31%) was more pronounced than that at 300 K (ca. 13.1%). In contrast, in this study, we found that the J-droop was more obvious at higher temperatures (Figure 1a). This finding is similar to that for the InGaN-based blue LED [18], despite both the main and parasitic peaks undergoing monotonic decreases in intensity upon an increase in the temperature (Figure 3b,c).

Figure 4 provides the normalized intensities of the peak wavelengths recorded at temperatures of 298, 323, and 348 K with forward currents applied in a range from 10 to 130 mA. In a previous study, Santi et al. observed a parasitic peak near 340 nm for their UVB-LED and attributed its origin to radiative transitions through deep levels in the QB next to the EBL and not inside the QWs [16].

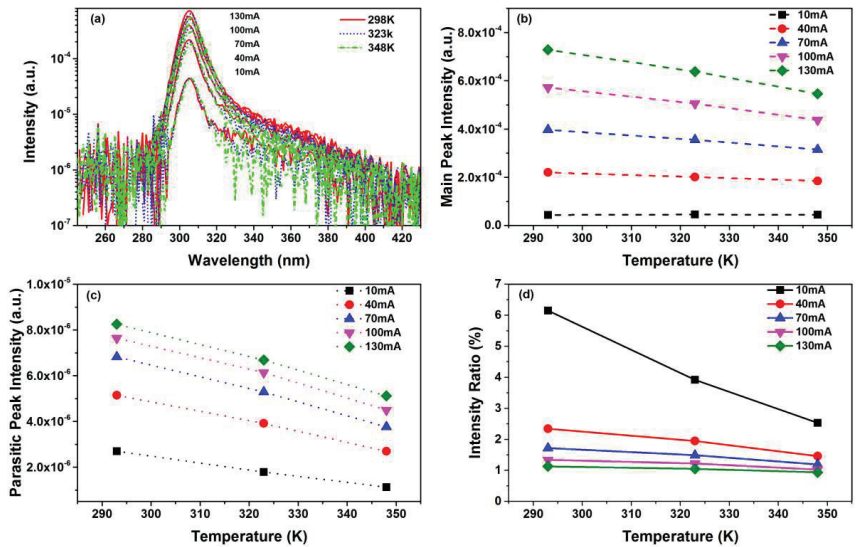
However, their paper reveals that a slower T-droop occurred when the temperature was greater than 300 K upon an increase in the value of  $I_f$  [16]. Nevertheless, in the present study, we did not observe a similar T-droop phenomenon when the temperature was 348 K. Furthermore, we found that the normalized intensities of the peak wavelengths underwent a steeper decline upon an increase in the temperature when increasing the value of  $I_f$ . According to the dependence of the emission intensity on temperature, Figure 4 indicates that at a higher forward current, the AlGaN-based UVB-LED exhibited weaker temperature stability. This trend is dramatically different from that reported previously [19]. Figure 5 presents the relative LOP measured over time for the UVB-LED operated at 40 mA (current density: ca. 28.5 A/cm<sup>2</sup>) and RT, as well as a photograph of the UVB-LED during operation. A rapid degradation in the LOP, to 79.7% of its initial value, occurred in the first 500 h of the aging operation; it then decreased more slowly to 70.6% of its initial value when the aging time reaching 6000 h (the inset in Figure 5 displays the LOP plotted with respect to a



logarithmic time scale). Such behavior has been observed many times previously [21–28]. This performance is close to the specifications of commercial solid-state lighting products and the estimated 70% lifetime (L70) is comparable with values reported by Ruschel et al. for a 310 nm UVB-LED operated at a current density of 33.5 A/cm<sup>2</sup> [21]. Figure 6a–c presents the time-dependence of the forward voltage, the EL peak wavelength, and the EL FWHM, respectively, which were all measured during aging tests performed with an  $I_f$  value of 40 mA. The forward voltage decreased dramatically at the onset of operation but remained stable during operation between 500 and 6000 h.



**Figure 2.** Normalized EL emission spectra of the AlGaIn-based UVB-LED, recorded at various forward currents (a) 298, (b) 323, (c) 348 K.



**Figure 3.** EL spectral data recorded at various forward currents and temperatures of 298, 323, and 348 K. (a) Spectral distributions, (b) main peak intensities, (c) parasitic peak intensities, and (d) peak intensity ratios.

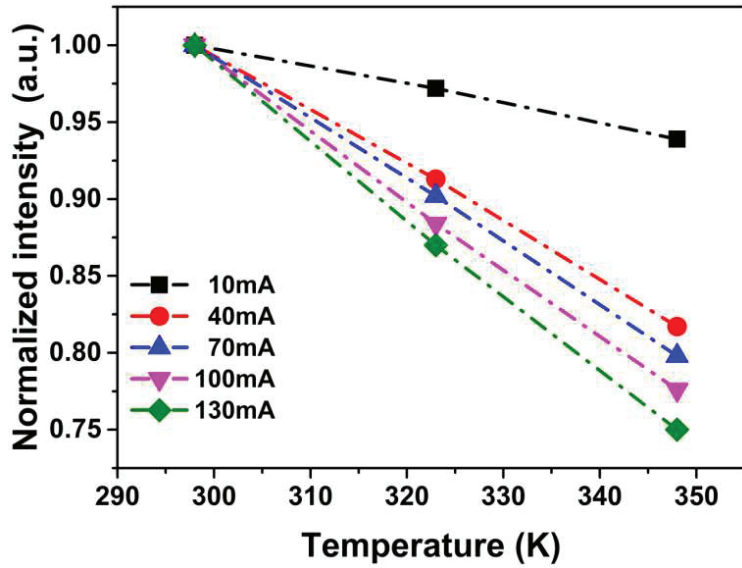


Figure 4. Normalized QW intensities of the peak wavelengths of the AlGaIn-based UVB-LED measured at temperatures of 298, 323, and 348 K while applying forward currents from 10 to 130 mA at a step of 30 mA.

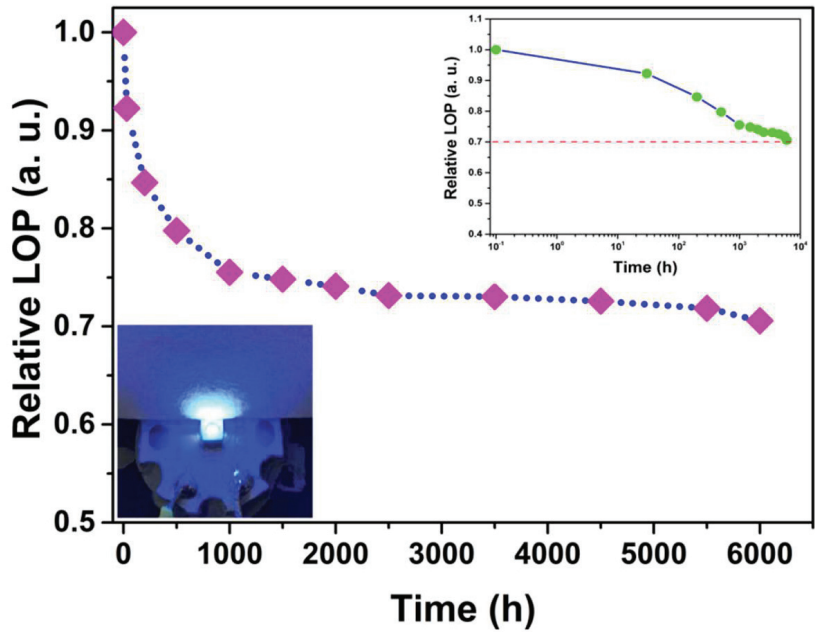
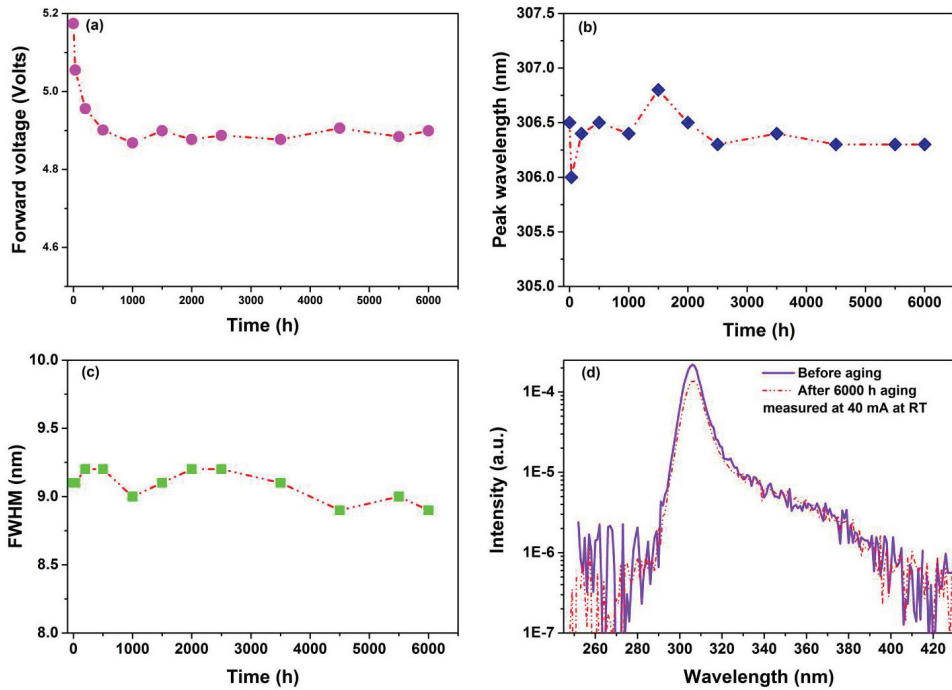


Figure 5. Relative LOP of the AlGaIn-based UVB-LED, measured during aging tests performed at 40 mA. Insets: (left) photograph of the UVB-LED during operation; (right) LOP plotted on a logarithmic time scale.



**Figure 6.** (a) Forward voltages, (b) EL peak wavelengths, and (c) EL FWHMs of the AlGaIn-based UVB-LED measured at a value of  $I_f$  of 40 mA during the aging tests. (d) EL emission spectra of the AlGaIn-based UVB-LED measured at a value of  $I_f$  of 40 mA before and after performing the aging tests.

Interestingly, while the LOPs and forward voltages decreased simultaneously when the aging time was increased to 6000 h, no significant changes occurred in the peak wavelengths or the FWHMs. This behavior suggested that the crystal quality of the MQWs did not undergo serious deterioration over time. Moreover, Figure 6d displays the EL emission spectra measured at a value of  $I_f$  of 40 mA before and after aging for 6000 h. Although the emission wavelengths of both the main and parasitic peaks did not undergo any obvious changes before and after aging, the intensity of the main peak decreased to 63.6% of its initial value, whereas the intensity of the parasitic peak barely changed. The behavior of the parasitic peak in this case was different from that reported by Trivellini et al. during the degradation of a 280-nm UVC-LED [13]. Thus, further investigations will be necessary to determine whether the mechanism responsible for the parasitic peak observed in our EL spectra involved radiative recombination in the EBL or p-layer through electron leakage. In addition, the degradation of the LOP during long-term operation was not obviously correlated with the existence of the parasitic peak. Therefore, we infer that the rapid decrease in the LOP and the decrease in the value of  $V_f$  that occurred simultaneously at the onset of the current stress were due to intrinsic defects in the MQWs and extrinsic defects dynamically induced by the current stress; those defects were occupied by injection carriers, resulting in a decrease in the width of the space-charge region. Because the number of defects in the MQWs gradually became saturated, the rate of degradation decreased during further operation. Previous reports have suggested that decreases in LOPs arise as a result of the diffusion of dopants [24,26–28]. We will investigate this phenomenon in future studies.

#### 4. Conclusions

We found that the J-droop in an AlGaIn-based UVB-LED was more obvious at higher temperatures, despite both the main and parasitic peaks undergoing monotonic decreases in their intensity upon increases in the temperature. A higher T-droop occurred upon increases in both the value of  $I_f$  and the temperature. Although the emission wavelengths did not undergo obvious changes after 6000 h of aging, the intensity of the main peak decreased to 63.6% of its initial value, whereas the intensity of the parasitic peak barely changed. This result suggested that the mechanism responsible for the origin of the parasitic emission peak did not also lead to serious deterioration in the crystal quality; furthermore, the degradation of the LOP during long-term operation was not obviously correlated with the existence of the parasitic peak. At the onset of current stress, the intrinsic defects in the MQWs and the extrinsic defects dynamically induced by the current stress (occupied by injection carriers) resulted in a decrease in the width of the space-charge region. Moreover, the decelerating rate of degradation during further operation was due to the gradual saturation of the number of defects in the MQWs.

**Author Contributions:** Conceptualization, M.-J.L. and Y.-T.C.; methodology, M.-J.L., Y.-T.C. and R.-S.L.; formal analysis, M.-J.L. and Y.-T.C.; investigation, M.-J.L., R.-S.L. and R.-M.L.; data curation, L.-J.Z., Y.-H.L. and M.-J.L.; writing—original draft preparation, M.-J.L. and Y.-T.C.; writing—review and editing, S.-F.H., S.-C.W., X.Z., L.-C.C. and R.-M.L.; visualization, X.Z., L.-C.C. and R.-M.L.; supervision, L.-C.C. and R.-M.L.; project administration, M.-J.L., L.-C.C., S.-F.H. and R.-M.L.; funding acquisition, Y.-T.C., S.-C.W., S.-F.H. and R.-M.L. All authors have read and agreed to the published version of the manuscript.

**Funding:** Jimei University Research Project (contract no. Z91956/4412), National Natural Science Foundation of China (grant no. 62005026), Natural Science Foundation of Jiangsu Province (grant no. BK20191027), and Suzhou Science and Technology Project (grant no. SZS2020313), Ministry of Science and Technology (MOST) of Taiwan (contract MOST 109-2221-E-182-060), Chang Gung Memorial Hospital (grant BMRP 591).

**Institutional Review Board Statement:** Not applicable.

**Informed Consent Statement:** Not applicable.

**Data Availability Statement:** Not applicable.

**Acknowledgments:** We thank Keh-Yung Cheng, Liann-Be Chang, and Chieh-Hsiung Kuan for the helpful discussions.

**Conflicts of Interest:** The authors declare no conflict of interest.

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# The Sensing Mechanism of InAlN/GaN HEMT

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**Abstract:** The sensing mechanism of InAlN/GaN high electron mobility transistors (HEMTs) is investigated systematically by numerical simulation and theoretical analysis. In detail, the influence of additional surface charge on device performance and the dependence of surface sensing properties on InAlN barrier thickness are studied. The results indicate that the saturation output drain current  $I_{dsat}$  and two-dimensional electron gas (2DEG) concentration increase with the increase of positive surface charge density, which decrease with the increase of negative surface charge. The influence of negative surface charge on device performance is more remarkable than that of positive surface charge. Additionally, the modulation ability of surface charge on device performance increases with the decrease of InAlN barrier thickness. The modulation of surface charge on device performance and the influence of barrier thickness on surface sensing sensitivity are mainly attributed to the variation of the energy band structure, surface potential and 2DEG concentration in the HEMT heterostructure. This work provides important support for structural optimization design of GaN-based HEMT sensors.

**Keywords:** surface charge; InAlN/GaN; HEMT; surface sensitivity

**Citation:** Liu, Y.; He, X.; Dong, Y.; Fu, S.; Liu, Y.; Chen, D. The Sensing Mechanism of InAlN/GaN HEMT. *Crystals* **2022**, *12*, 401. <https://doi.org/10.3390/cryst12030401>

Academic Editors: Peng Chen, Zhizhong Chen and Cheljong Choi

Received: 16 January 2022

Accepted: 13 March 2022

Published: 16 March 2022

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## 1. Introduction

Due to the superior properties such as wide bandgap, high breakdown electric field, high saturation drift velocity and high thermal conductivity, GaN-based high electron mobility transistors (HEMTs) exhibit important applications in the fields of high temperature, high frequency and high power devices [1–4]. Meanwhile, two dimensional electron gas (2DEG) with a sheet concentration of as much as  $10^{13} \text{ cm}^{-2}$  is formed because of the polarization discontinuity at AlGaIn (or InAlN) /GaN heterointerface. The 2DEG density strongly depends on surface states of GaN-based heterostructure. Any changes of surface state will result in changes of energy band structure and surface potential of the heterostructure. Moreover, 2DEG responds quite sensitively to any changes of the free surface charge situation. To a first approximation, for each positive or negative ion adsorbed at the free surface, accordingly, one electron is gained or lost in the 2DEG. Since the mobilities of adsorbed ions at the free surface and electrons in the 2DEG differ by many orders of magnitude, changes in the surface charge will be visible as changes in the 2DEG conductivity, however, they will be amplified by the mobility ratio. This is the basic mechanism which makes GaN-based HEMT attractive for sensor applications [5–7]. Recently, there are tremendous reports about AlGaIn/GaN HEMT sensors for detecting gas, liquid, chemical and biomaterial, which can be used in the fields of environmental monitoring, food safety analysis and biomedicine [8–12]. In the past few years, researchers mainly focused on surface modification of AlGaIn/GaN HEMTs for the detection of various target substances. For different targets to be tested, the best obtained result is different. For example, the highest sensing sensitivities for a pH sensor [13] and a  $\text{Hg}^{2+}$  ion sensor [14] are 167.71 mV/pH and 0.3  $\mu\text{A/ppb}$ , respectively. Besides, there are a few studies about

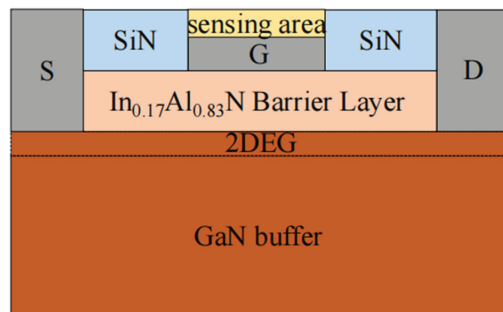


the methods to improve the sensing performance by optimizing HEMT device structure such as gateless structure [15,16], gate-recessed structure [17,18] and extended-gate structure [19,20]. For gateless HEMT, the sensing distance between the surface sensing area and the 2DEG channel is scaled compared to the conventional GaN-based HEMT, which makes sensing sensitivity enhanced. Due to the progress of controlling ability from the gate-recessed region, the sensing performance of the gate-recessed HEMT sensors obviously enhanced compared with the planar gate HEMT. For extended-gate HEMT, by extending the gate area and separating the sensing area from the channel of the HEMT, the device has a larger sensing area. Therefore, all of the sensing sensitivity, stability and detection limit of the HEMT sensors are improved.

In fact, to further improve the sensing performance of GaN-based HEMTs effectively, it is necessary to investigate the sensing mechanism comprehensively. Until now, there are few reports about the sensing mechanism of GaN-based HEMT. Besides, owing to the relatively mature epitaxial and manufacturing technology, the heterostructure mainly used for HEMT sensors in the past few years is AlGaIn/GaN. Compared with conventional AlGaIn/GaN heterostructure, the lattice-matched  $\text{In}_{0.17}\text{Al}_{0.83}\text{N}/\text{GaN}$  heterostructure, has higher carrier concentration and better 2DEG confinement [21,22]. In fact, lattice-matched  $\text{In}_{0.17}\text{Al}_{0.83}\text{N}/\text{GaN}$  heterostructure is more suitable for HEMT sensors. However, there are only a few reports about InAlN/GaN HEMT sensors [23,24]. In this work, the modulation law of surface charge on the device performance and the effect of InAlN barrier layer thickness on the sensing performance of InAlN/GaN HEMT are studied systematically, which is considered to provide a broad-version route map for designing InAlN based HEMT sensors.

## 2. Device Structure and Theoretical Models

The InAlN/GaN HEMT device structure used in this study is shown in Figure 1. The HEMT heterostructure on sapphire substrate consists of a 2- $\mu\text{m}$ -thick GaN buffer layer and a thin  $\text{In}_{0.17}\text{Al}_{0.83}\text{N}$  barrier layer. A SiN passivation layer was applied between the gate sensing area and ohmic contacts (source and drain electrodes). To be close to the real experiment, the n-type doping densities in both GaN buffer layer and InAlN barrier layer used in this work were set to be  $1 \times 10^{16} \text{ cm}^{-3}$ , due to the fact that the unintentionally doping InAlN/GaN heterostructures grown in the experiment exhibit n-type doping with a concentration of  $1 \times 10^{16} \text{ cm}^{-3}$ . The distance between the source and drain electrodes is 3  $\mu\text{m}$ . The length of the sensing area for gate region is 1.5  $\mu\text{m}$ .



**Figure 1.** Schematic diagram of the InAlN/GaN HEMT.

To obtain the  $I_{\text{dsat}}$ , 2DEG concentration and the energy band profile of the HEMT with varying surface charge, the Schrödinger equation, Poisson's equation and the carrier continuity equation are solved self-consistently [25,26]. The equations can be expressed as follows, respectively.

Schrödinger equation:

$$\left[ \frac{\hbar^2}{2m^*} \frac{d^2}{dz^2} + V(z) \right] \psi(z) = E\psi(z) \quad (1)$$

where  $\hbar$  is the Planck's constant,  $m^*$  is the effective mass of the electron,  $V(z)$  is the potential energy of the electron,  $E$  is the energy of the electron and  $\psi$  is the wave function. Poisson's equation:

$$\frac{d}{dz} \left( \epsilon \frac{d}{dz} \right) \phi(z) = -q [N_d^+(z) - n(z)] \quad (2)$$

where  $\epsilon$  is the dielectric constant,  $\phi(z)$  is the electrostatic potential,  $q$  is the charge,  $N_d^+$  is the dissociative donor concentration and  $n$  is the electron concentration. Since the contribution of the acceptor charge as well as the holes on the total charge are very small, the acceptor charge and holes are neglected in the calculation.

Carrier continuity equation:

$$\frac{\partial n}{\partial t} = \frac{1}{q} \text{div} J_n + G_n - R_n \quad (3)$$

where  $J_n$  is the electron current density,  $G_n$  is the electron production rate and  $R_n$  is the electron recombination rate.

The self-consistent procedure is that the potential  $V$  is obtained using Poisson's equation from an initial guess of the mobile charge concentration, and then inserted into the Schrödinger equation, which is solved to obtain the energy levels and wavefunctions of the systems. The new electron charge density is then calculated by applying Fermi statistics

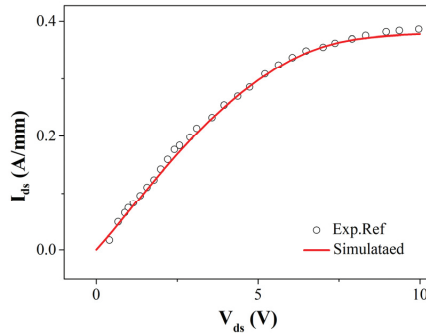
$$n_{2D}(z) = \frac{m^* K_B T}{\pi \hbar^2} \sum_i |\psi_i(z)|^2 \ln \left[ 1 + e^{(E_F - E_i)/m^* K_B T} \right] \quad (4)$$

where  $E_F$  is Fermi level,  $E_i$  is energy of the  $i$ th quantized level,  $T$  is temperature and  $K_B$  is Boltzmann's constant.

The calculated density is then plugged into Poisson's equation and the iteration repeated until convergence is achieved.

The polarization model, Shockley–Read–Hall recombination model and Albrecht model incorporated for concentration dependent low field mobility were incorporated in the simulations study through Silvaco TCAD [27]. We applied a fixed temperature of 300 K due to the neglecting self-heating effect when the device is operated at low biases. The electron transport was also included based on a drift-diffusion model [28,29]. In the simulation, we set the value of saturation velocity and the parameters of electron and hole recombination lifetimes ( $\tau_{n0}$  and  $\tau_{p0}$ ) in SRH recombination model. Besides, we adopted the parameters for GaN, InN, and AlN that Braga et al. [30] have reported such as energy band structure, spontaneous polarization, mobilities and saturation velocities. Linear interpolations are adopted to compute parameter values as a function of mole fraction in InAlN.

To verify the validity of the simulation results in this work, we compare the simulation results with previous experimental report. As shown in Figure 2, simulated DC current of InAlN/GaN HEMT without additional surface charge is basically matched to the experimental results of the same structure [31,32].

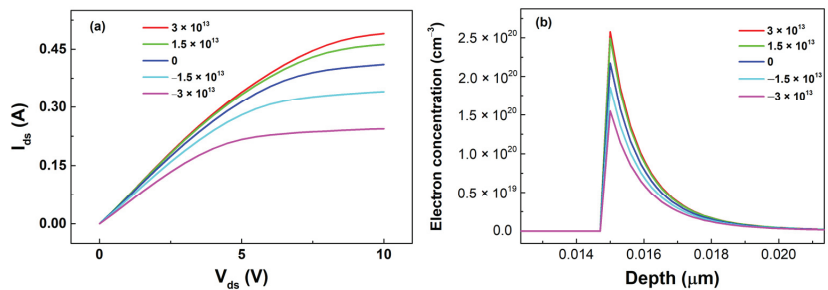


**Figure 2.** Output characteristics of InAlN/GaN HEMT from simulation and experimental results.

### 3. Results and Discussion

#### 3.1. Influence of Surface Charge on Device Performance of InAlN/GaN HEMTs

Figure 3 shows the output characteristics and carrier concentration distributions of the InAlN/GaN HEMT with different surface charge density. As shown in Figure 3a, the saturation drain current  $I_{dsat}$  increases with the increase of positive surface charge density and decreases with the increase of negative surface charge. The influence of negative surface charge on device performance is more significant than that of positive charge. In fact, the effect of surface charge on the  $I_{dsat}$  mainly resulted from the changes of 2DEG concentration. The carrier concentration distributions of the HEMT under gate region with different surface charge density are shown in Figure 3b. Corresponding to the change of  $I_{dsat}$ , the 2DEG concentration increases with the increase of positive surface charge, which decreases with the increase of negative surface charge.



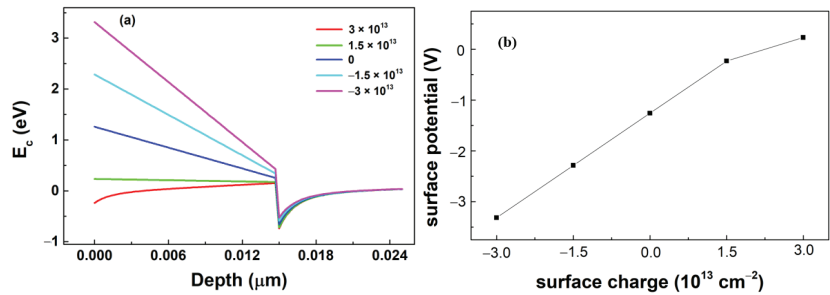
**Figure 3.** (a) The output characteristics and (b) carrier concentration distributions of the HEMT with different surface charge density at  $V_g = 0$  V.

The intrinsic physical reason for the changes of  $I_{dsat}$  and 2DEG concentration with surface charge can be mainly attributed to the effect of the energy band structure and surface potential of the InAlN/GaN HEMT heterostructure. The conduction band diagram of the HEMT under gate region with different surface charge density is shown in Figure 3a. The corresponding surface potential representing energy difference between the conduction band edge of surface and Fermi level  $E_F$  is shown in Figure 3b. Considering the energy band diagram of the HEMT as sketched in Figure 3, the sheet charge density  $N_s$  can be written as [33]

$$N_s = \sigma_{pol,interface} - \left[ \frac{\epsilon_{barrier}}{d_{barrier} \cdot q} (\Phi_s + (E_F - \Delta E_c)) \right] \quad (5)$$

where  $d_{barrier}$  is the barrier thickness,  $q$  is the elementary charge,  $\Phi_s$  is the surface potential,  $E_F$  is the Fermi level at the interface relative to the bottom of the GaN conduction band and  $\Delta E_c$  is the conduction band offset between InAlN barrier layer and GaN buffer.

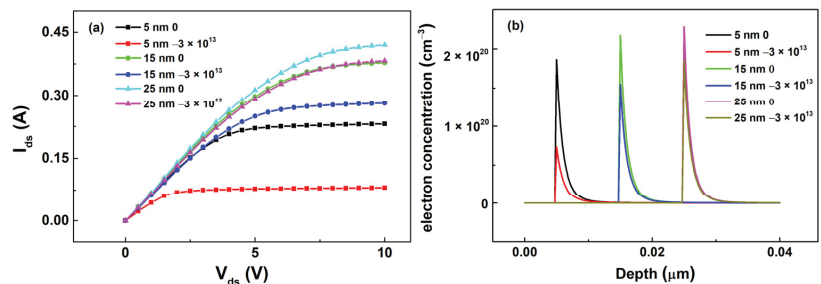
As shown in Figure 4, the surface potential of InAlN/GaN HEMT heterostructure under gate region increases slightly with positive surface charge. Correspondingly, the depth of triangular quantum potential well at InAlN/GaN interface becomes deeper, which enhanced the 2DEG confinement. So, the 2DEG concentration and  $I_{dsat}$  increase with the increase of positive surface charge density. As the negative surface charge density increases, the surface potential decreases and the depth of the triangular potential well becomes shallower, which weakens the confinement of the 2DEG at InAlN/GaN interface. So, the 2DEG concentration and  $I_{dsat}$  will decrease. In fact, the simulated sensing rule in this work is consistent with a previous experiment report that the output current of HEMT device decreases gradually as the pH value increases [11]. For HEMT pH sensor, the drain current decreased with increased pH value, because the adsorbed negative charges on HEMT sensing area increases with pH value.



**Figure 4.** (a) The conduction band diagram and (b) surface potential of the HEMT under the gate region with different surface charge density.

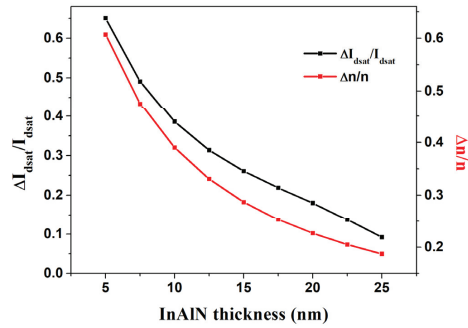
### 3.2. The Effect of InAlN Barrier Thickness on the Sensing Performance of InAlN/GaN HEMT Device

To further study the surface sensing properties of HEMT, the effect of the InAlN barrier thickness on the surface sensing performance of InAlN/GaN HEMT devices is investigated by comparing the device performance before and after adding the same density of surface charges ( $\sigma_s = -3 \times 10^{13} \text{ cm}^{-2}$ ). The InAlN barrier thicknesses ranged from 5 to 25 nm. Figure 5 shows the output characteristics and 2DEG concentration distributions of HEMT for varying InAlN thickness with and without additional surface charge. As shown in Figure 5, with the increase of barrier layer thickness, the  $I_{dsat}$  and 2DEG concentration increase when the additional surface charge is zero, which can be deduced from the energy band diagram [34,35]. Correspondingly, the energy drop in the barrier layer increases, leading to a deeper triangular quantum well at the hetero-interface. In further, the confinement of the quantum well on 2DEG is enhanced. Consequently, the 2DEG concentration and drain current also increase with the increase of barrier layer thickness.



**Figure 5.** (a) The output characteristics and (b) carrier concentration distributions of HEMT with surface charge on the structure at different InAlN barrier layer thicknesses.

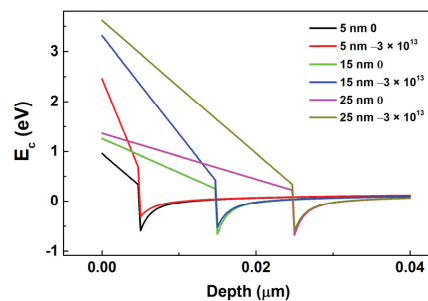
Additionally, from Figure 5 we can get the variation quantity of the saturation current  $\Delta I_{\text{dsat}}$  and 2DEG concentration  $\Delta n$  before and after adding the same density surface charges for various InAlN thicknesses. The change rates of the  $\Delta I_{\text{dsat}}/I_{\text{dsat}}$  and the  $\Delta n/n$  are shown in Figure 6. In contrast to the variation of the  $I_{\text{dsat}}$  and 2DEG concentration, the  $\Delta I_{\text{dsat}}/I_{\text{dsat}}$ ,  $\Delta I_{\text{dsat}}/I_{\text{dsat}}$ ,  $\Delta n$  and  $\Delta n/n$  decrease gradually with the increase of InAlN thickness for HEMT. The change rates of the  $\Delta I_{\text{dsat}}/I_{\text{dsat}}$  are approximately in the range of 0.1–0.65.



**Figure 6.** The change rates of the saturation drain current and the 2DEG concentration of the HEMT with different InAlN barrier thicknesses.

From the above results, it can be confirmed that the influence of surface charge on device performance increases with the decrease of the InAlN barrier thickness, which means that the modulation ability of surface charge on device performance will be increased by decreasing the InAlN thickness. So, we can conclude that the surface sensing sensitivity can be enhanced by thinning the barrier layer thickness in a certain range, when GaN-based HEMT is used as sensor.

The intrinsic physical mechanism for the above phenomenon and results is still resulted from the changes of the energy band structure and surface potential of the InAlN/GaN HEMT heterostructure. Figure 7 shows the energy band diagram of the HEMT under the gate region with and without additional surface charge for various InAlN barrier thicknesses. It can be seen from the diagram that with the increase of InAlN barrier thickness, the depth difference of the triangular potential well before and after additional surface charge decreases due to the enlarged distance between the sensing area and the 2DEG channel. Therefore, the influence of the same density surface charge on the interface potential well increases with the decrease of InAlN barrier thickness, which in turn affects the output characteristics and 2DEG concentration of the HEMT. So, the modulation ability of surface charge on device  $I_{\text{dsat}}$  and the 2DEG concentration increase with the decrease of InAlN thickness, which means that the sensing sensitivity of GaN-based HEMT sensor can be improved by thinning the barrier layer.



**Figure 7.** The conduction band diagram of HEMT for different InAlN barrier layer thicknesses with and without additional surface charge density.

#### 4. Conclusions

In this work, the sensing mechanism of InAlN/GaN HEMT and the dependence of the sensing sensitivity on the InAlN barrier layer thickness were studied by solving the Schrodinger equation, Poisson's equation and the carrier continuity equation self-consistently. The results exhibit that both the  $I_{\text{dsat}}$  and 2DEG concentration increase with the increase of positive surface charge, which decrease with the increasing negative charge. The influence of negative surface charge on device performance is more significant than that of positive surface charge. This can be attributed to the change of the energy band structure and surface potential of HEMT with varying surface charge density. Moreover, the  $I_{\text{dsat}}$  and 2DEG concentration increase with the increase of InAlN barrier thickness, while the modulation ability of surface charge on device performance will decrease due to the enlarged distance between the sensing area and 2DEG channel. This means that the sensing sensitivity will decrease. So, when GaN-based HEMT is used as surface ion sensors, the barrier layer thickness should be as thin as possible.

**Author Contributions:** Conceptualization, Y.L. (Yanli Liu) and D.C.; formal analysis, X.H. and Y.D.; investigation, S.F. and Y.L. (Yuhui Liu); writing—original draft preparation, Y.L. (Yanli Liu); writing—review and editing, D.C. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research was funded by the National Nature Science Foundation of China, grant number 61804089; Shandong Provincial Science and Technology Support Program of Youth Innovation Team in College, grant numbers 2019KJN041 and 2020KJN005; Basic Research Project of the Basic Research Business of the Provincial University in Heilongjiang Province, grant number 2021-KYYWF-0036; and the PhD Start-up Fund of Shandong Technology and Business University, grant number (BS201608).

**Institutional Review Board Statement:** Not applicable.

**Informed Consent Statement:** Not applicable.

**Data Availability Statement:** Not applicable.

**Conflicts of Interest:** The authors declare no conflict of interest.

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Review

# Recent Progress on AlGa<sub>N</sub> Based Deep Ultraviolet Light-Emitting Diodes below 250 nm

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**Abstract:** AlGa<sub>N</sub> based deep ultraviolet (DUV) light-emitting diodes (LEDs), especially with a wavelength below 250 nm, have great application potential in the fields of sterilization and disinfection, gas sensing, and other aspects. However, with the decrease of emission wavelength, performance collapse occurs and the external quantum efficiencies (EQE) of sub-250 nm LEDs are usually below 1% for a long time. Low efficiencies are resulted from problem accumulation of all aspects, including n/p-type doping and contacts, carrier confinements and transports, light extraction, etc. To achieve high EQE of sub-250 nm LEDs, problems and solutions need to be discussed. In this paper, the research progress, development bottlenecks, and corresponding solutions of sub-250 nm LEDs are summarized and discussed in detail.

**Keywords:** UVC-LED; AlGa<sub>N</sub>; doping; carrier confinement; light extraction

**Citation:** Zhang, C.; Jiang, K.; Sun, X.; Li, D. Recent Progress on AlGa<sub>N</sub> Based Deep Ultraviolet Light-Emitting Diodes below 250 nm. *Crystals* **2022**, *12*, 1812. <https://doi.org/10.3390/cryst12121812>

Academic Editors: Peng Chen, Zhizhong Chen and Shin-Tson Wu

Received: 21 November 2022

Accepted: 9 December 2022

Published: 13 December 2022

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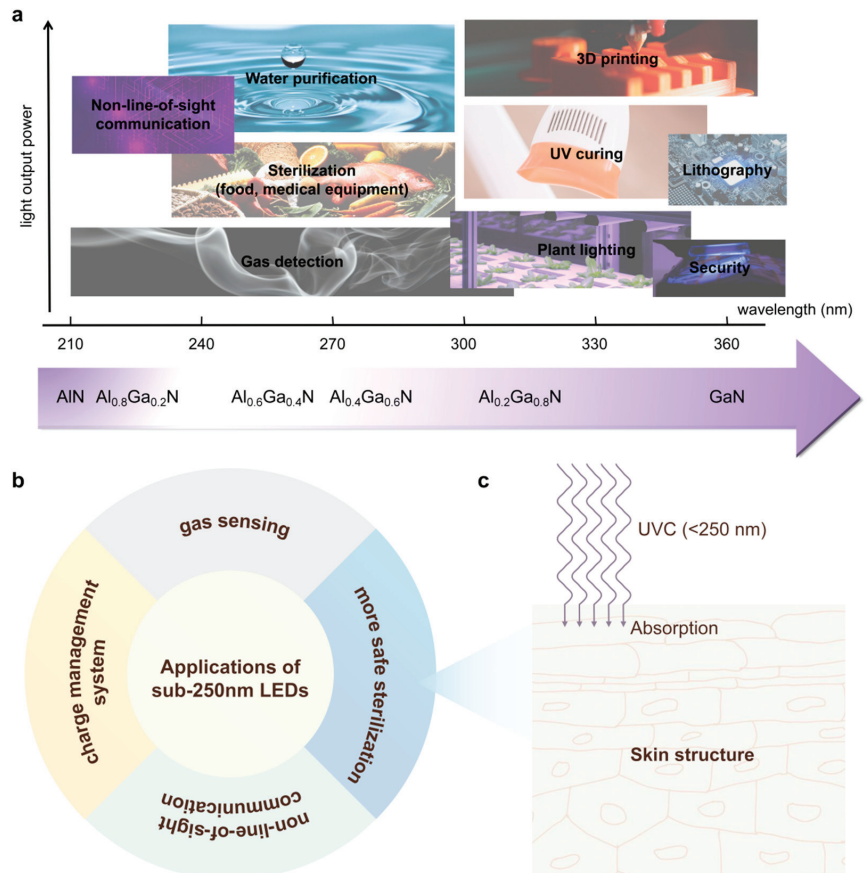
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## 1. Introduction

The ultraviolet (UV) spectrum can be divided into UVA (315–400 nm), UVB (280–315 nm), UVC (200–280 nm), and VUV (10–200 nm) of which the far-UVC band is from 200 to 250 nm. Mercury lamp is currently the most important UV light source on the market. However, the toxicity of mercury makes it urgent to find alternative UV light sources. AlGa<sub>N</sub> based LEDs have many advantages, including the light weight, small size, long lifetime, low power consumption, easy integration, fast switching, and tunable emission wavelength from 365 to 210 nm through adjusting the alloy composition. These characteristics make AlGa<sub>N</sub> based LED the unique and most potential light source in the UV range. Some applications of AlGa<sub>N</sub> based UV LEDs are summarized in Figure 1a. In addition to the ordinary applications, such as medical treatment, gas sensing, non-line-of-sight communication, and charge management system [1–6], as shown in Figure 1b, AlGa<sub>N</sub> based sub-250 nm LED is more suitable for safe and highly efficient sterilization due to its high radiation energy and strong absorption by the stratum corneum that does not contain cell nuclei [7], as shown in Figure 1c. Recent research proved that at the biocidal doses for multi-resistant pathogens at 40 to 60 mJ/cm<sup>2</sup> irradiation of 222 and 233 nm irradiation, no relevant DNA damage and radical formation occurred in the skin [8,9].

However, AlGa<sub>N</sub> based sub-250 nm LEDs are faced with many bottlenecks at present. It has been reported that the EQE drops from 0.6% to 0.00013% when the emission wavelength decreases from 264 to 220 nm [10]. Additionally, when the emission wavelength decreases from 239 to 217 nm, the EQE drops by more than three orders of magnitude [11]. There are many reasons for the sharp drop in quantum efficiency in this wave band, most of which are the effects brought about by the increase of Al composition. Generally, to achieve an emission below 250 nm, the Al composition of quantum well must be higher than 62%. Inevitably, the other function layers, such as the buffer layer, n-type electron

injection layer, quantum barrier layers, electron block layer, and p-type hole injection layer, must provide even higher Al composition, usually higher than 70% [12]. The super-high Al composition introduces many more serious problems than UVA-, UVB-, and above-250 nm UVC-LEDs. This paper first summarizes the development status of sub-250 nm LEDs and then introduces the problems that limit the efficiency improvement from the aspects of n/p-type doping, carrier confinement and transport, and light extraction and solutions that have been provided nowadays.



**Figure 1.** Partial applications of AlGaIn-based LEDs of (a) UV band and (b) below 250 nm. Images are partially from internet. (c) Schematic of sterilization on the skin by high UVC below 250 nm.

## 2. Advances in DUV-LEDs below 250 nm

On the whole, the performance level of sub-250 nm LEDs is much lower than that of the above-250 nm LED. The internal quantum efficiency (IQE), EQE, wall-plug efficiency (WPE), and light out-put power (LOP) have all dropped significantly. Up to now, the maximum EQE of 275 nm LED is 20.3% [13], the maximum EQE of 265 nm LED is 10% [14], while the majority of reported EQEs of sub-250 nm LEDs are below 1%. In 2006, Taniyasu et al. [15] obtained both n- and p-type AlN, and developed p-AlN/undoped AlN/n-AlN pin LED structure with n-AlN/AlGaIn and p-AlN/AlGaIn superlattices as the electron and hole lateral conduction layers, realizing emission at 210 nm. This is the first report of successful realization of AlGaIn based 210 nm emission, confirming the possibility of full band coverage of AlGaIn based LEDs. However, the device performance is extremely

low, with the operation voltage of 45 V at 20 mA, LOP and EQE of 0.02  $\mu$ W and  $10^{-6}\%$  at 40 mA, respectively. In 2009, Hirayama et al. [16] fabricated an LED on a multilayer AlN buffer layer. They used a thin quantum well of 1.3–2 nm to suppress the polarization field in the well. At 100 mA, the peak wavelength located at 227 nm and the LOP and EQE were 0.15 mW and 0.2%, respectively. Next year, they [17] further improved the LED efficiency by introducing multi-quantum-barrier (MQB) electron blocking layers (EBL), providing an important scheme for preventing electron leakage of sub-250 nm LEDs. They achieved an LOP of 4.8 mW at 135 mA under CW operation for the 250 nm LED, corresponding to an EQE of 1.18%, which is still the highest EQE reported for 250 nm and sub-250 nm LEDs.

Recent years, the performance of sub-250 nm LEDs has been further improved. In 2020, Lobo-Ploch et al. [18] optimized the growth and fabrication processes including using epitaxially laterally overgrown (ELOG) sapphire substrates and vanadium-based low resistance n-contacts. They fabricated a 233 nm LED with an EQE of 0.36% at 100 mA. Recently, Jo et al. [19] demonstrated a 228 nm LED on sapphire substrates with an LOP of 1.4 mW at 150 mA by modifying the multiple quantum well (MQW) and spacer layer structures.

The method of using non-polar plane have also been explored [20]. Although the light extraction efficiency (LEE) was estimated to be 25 times higher than that on the polar plane, the EL intensity was approximately 70 times lower than that on the polar plane, which probably resulted from the higher defect density. New design concepts may break through the transparency and conductivity problem of sub-250 nm LEDs. Liu D. et al. [21] demonstrated a 229 nm LED adopting a p-type Si nanomembrane as both a p-contact and a hole injection layer. LOP was measured to be 0.16 mW under 100 mA current and EQE was calculated to be 0.03%. Next year, they demonstrated a 226 nm LED with a p-Si nanomembrane and achieved an EQE of 0.2% [22], which was the highest value among LEDs with emission wavelength below 230 nm in the CW mode.

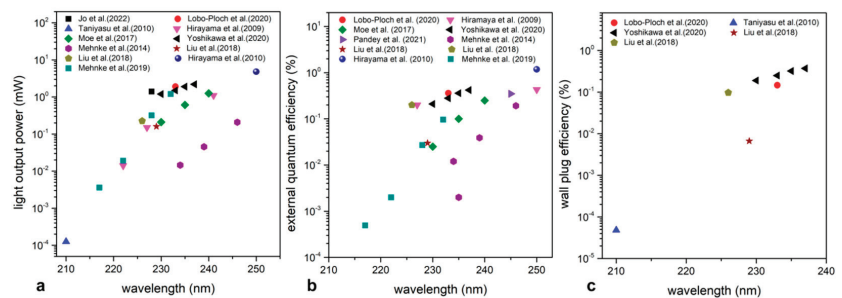
Strong quantum-confinement GaN/AlN heterostructures can produce optical emission far above the bulk bandgap of GaN (3.4 eV), and offer another path to achieve DUV emission below 250 nm. Furthermore, it has been reported that delta-QW design could resolve the band-mixing issue and ensure large transverse electric (TE) spontaneous radiation rate [23]. S.M. Islam et al. [24] demonstrated that ultrathin (1–2 monolayers) GaN dots/disks embedded in an AlN matrix can achieve controllable emission in the 219–235 nm range, showing the shortest wavelength emission of 219 nm with an IQE of 40% from binary GaN active regions till date.

AlGaIn based far-UVC LEDs grown by homogeneous epitaxy were also reported due to development of AlN single-crystal substrate. Toshio Nishida et al. [25] fabricated UV LED structures on AlN substrates as early as 2004, and compared the performance with LEDs on sapphire substrates. They found that the saturation injection current of LEDs on AlN substrate was two times higher than that of LEDs on sapphire substrate. This work confirmed the huge potential of bulk AlN substrates for UV-LEDs. In 2020, Yoshikawa et al. [26] reported the fabrication of 230–237 nm LEDs on AlN substrates. Thanks to the high-quality single crystal AlN substrate, the 233 nm LED exhibited EQE of 0.25% at 233 nm. Compared to sapphire and AlN substrates, Si substrate has several advantages [27], including low cost, good electrical and thermal conduction, and easy integration to Si-based electronics, etc. However, to obtain DUV LEDs on Si substrate has some problems that AlGaIn epilayers grown on Si possess poor material quality owing to the large lattice and thermal mismatches between AlGaIn and Si. The nanowire technology may solve the problem [28]. In 2015, S. Zhao et al. [29] achieved the first 210 nm emitting AlN nanowire LEDs with a turn on voltage of approximately 6 V by utilizing N-polar AlGaIn nanowires directly grown on Si substrate. The IQE of the N-polar AlN nanowires LED can reach 80%.

Another important aspect of an LED are the reliability and lifetime. Lifetime in the order of 10,000 h for the long-wavelength UV LED (UVA and UVB) have been commercialized [30], while the lifetime for the long-wavelength UVC LED (>250 nm) is still limited to thousands of hours [31,32] although Ruschel et al. [31] demonstrated a 265 nm UVC LED with L70 lifetime more than 10,000 h. Meneghini et al. [33] pointed out that the

stress induced nonradiative recombination increase and point defects in or around the active region might cause output power degradation. However, at present, there are few studies on the reliability and lifetime of sub-250 nm LEDs. The reported record lifetime of sub-250 nm LEDs was created by Yoshikawa et al. [26], which was expected to exceed 3600 h. The authors speculated that the possible reason for the long lifetime was the lower oxygen content in the novel structure. Glaab et al. [34], in detail, analyzed two possible degradation mechanisms of sub-250 nm LEDs. The first mechanism may be the activation of initially H-passivated defect complexes in or around the quantum well active region by hot carriers from Auger recombination, which may be responsible for the rapid decrease of LOP during the initial 50 to 100 h. The second mechanism may be the carrier injection efficiency reduction triggered by hot carriers from Auger recombination, which may be responsible for the LOP degradation after working more than 50 h.

The EQE, LOP and WPE of 250 nm and sub-250 nm LEDs are summarized in Figure 2a–c, respectively. Up to now, the research on AlGaIn based sub-250 nm LED is still relatively few, compared to other UV wave bands. There are even no reports that demonstrated a WPE over 1%, implying a long way to realize large-scale commercial application. However, as it can be seen, the performance of recently reported sub-250 nm LEDs have increased by more than one magnitude over those reported several years ago, indicating the future of the commercialization of AlGaIn based sub-250 nm LED is expectable.

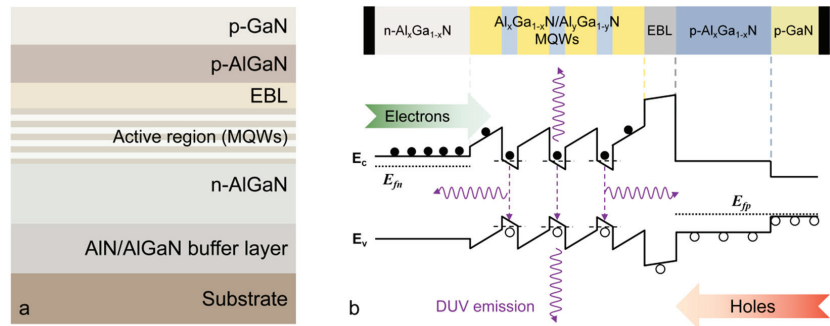


**Figure 2.** Summary of the reported (a) EQE, (b) LOP, and (c) WPE of 250 nm and sub-250 nm LEDs in dependence of emission wavelength in recent literature [11,16–22,26,35–37].

### 3. Key Issues and Challenges

To analyze the key issues and challenges limiting the performance of AlGaIn-based sub-250 nm LEDs, it is usually necessary to discuss from the two aspects of material growth and device physics. Generally, the technology roadmap of AlGaIn-based sub-250 nm LEDs follows the ordinary UVC LEDs, which means the typical device structure and fabrication process of a sub-250 nm LED are basically identical to an UVC one. Figure 3a is a schematic diagram of the basic structure of an AlGaIn-based UV LED. Typically, the epitaxial structure from bottom to top includes (1) substrate, generally sapphire or single crystal AlN, (2) AlN or AlGaIn buffer layer, to reduce defects density and relax stress during growth, (3) n-AlGaIn layer, to form n-type ohmic contact and provide electrons to active region for recombination, (4) active region, the main light emission region and usually made up of 3–5 periods of undoped  $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_y\text{Ga}_{1-y}\text{N}$  quantum wells ( $x < y$ ), (5) EBL, with a wider bandgap than all other function layers to suppress the electrons to overflow to p-side, (6) p-AlGaIn, to inject holes into active region for recombination, and (7) p-GaN cap layer, to form a p-type ohmic contact. From the perspective of materials, the bottom buffer layer quality that basically determines the upper epi-layer quality and the n/p doping efficiency that determine the carrier injection efficiency will significantly influence the device performance. Figure 3b is the schematic energy band structure of an AlGaIn-based UV LED. The electrons and holes transport to the active region and recombine to each other to emit UV photons. If the carriers cannot effectively transport to the active region and be confined, the radiative recombination must be very weak. To say the least, even

though the carrier recombination generates a large number of photons, the photons cannot be effectively extracted, and the device performance will be very low, too.



**Figure 3.** Schematic diagram for (a) epitaxial structure and (b) energy band structure of a typical AlGaIn-based UV LED, which are suitable for sub-250 nm LEDs, too.

Quantitatively, if we choose the WPE as the key parameter to assess the performance of an LED, the relationship between the device performance and the main parameters can be expressed as the following Formula (1):

$$\text{WPE} = \frac{I_{\text{OP}}}{I \cdot V} = \text{EQE} \cdot \text{EE} = \text{IQE} \cdot \text{LEE} \cdot \text{EE} = \text{RRE} \cdot \text{CIE} \cdot \text{LEE} \cdot \text{EE} \quad (1)$$

where  $I$  and  $V$  are the operation current and voltage,  $\text{EE}$  is the electrical efficiency,  $\text{RRE}$  is the radiative recombination efficiency,  $\text{CIE}$  is the carrier injection efficiency, respectively. The ABC model [38] is often used to estimate the  $\text{RRE}$  by the following Formula (2):

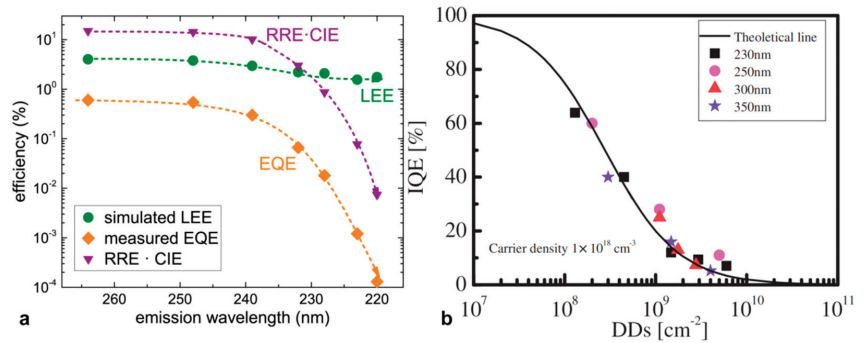
$$\text{RRE} = \frac{Bn^2}{An + Bn^2 + Cn^3} \quad (2)$$

where the coefficients  $A$ ,  $B$ , and  $C$  represent the SRH non-radiative recombination coefficient (Shockley-Read-Hall, SRH), radiative recombination coefficient, and Auger recombination coefficient, and  $n$  is the carrier concentration, respectively. Apparently, the material crystal quality and carrier distribution will influence the performance through  $\text{RRE}$ , the doping efficiency and contact quality can mainly determine the performance through  $\text{EE}$  and  $\text{CIE}$ , and furthermore the  $\text{LEE}$  will directly determine the device performance. Consequently, the key issues and challenges including material crystal quality,  $n/p$ -type doping, carrier transport and confinement, and light extraction will be discussed in this part.

### 3.1. Material Crystal Quality

Guttmann et al. [10] have studied the reasons for the decrease of  $\text{EQE}$  at 264–220 nm. As shown in Figure 4a, with the wavelength decreasing, the trend of  $\text{EQE}$  is consistent with the trend of  $\text{IQE}$ , implying to improve the  $\text{IQE}$  becomes even more urgent for short wavelength range. As can be seen from the ABC model,  $\text{IQE}$  and non-radiative recombination process are inseparable. Due to the mismatch of lattice constants and thermal expansion coefficients between the AlGaIn epilayer and substrates, dislocation density is generally high. Ban et al. [39] explored the relationship between  $\text{IQE}$  and dislocation densities (DDs) in the  $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_y\text{Ga}_{1-y}\text{N}$  active region with different Al compositions, and found that under the condition of the same dislocation density and injected carrier density, the active region has the same  $\text{IQE}$  regardless of the emission wavelength. The functional relationship between  $\text{IQE}$  and DDs is depicted in Figure 4b. It can be seen from the figure that the dislocation density needs to be less than  $10^7 \text{ cm}^{-2}$  to achieve an  $\text{IQE}$  of over 95%.





**Figure 4.** (a) Measured on-wafer EQE, simulated on-wafer LEE and corresponding product of RRE and CIE as a function of the emission wavelength [10]. (b) IQE as the function of DD at a weak excitation with the carrier density of  $1 \times 10^{18} \text{ cm}^{-3}$  [39].

Before growing the LED structure, an AlN buffer layer is first grown on the sapphire substrate. The AlN buffer layer quality largely determines the quality of the upper LED structure. At the present stage, several technologies are commonly used to reduce dislocation density in the AlN/Sapphire template.

1. Two-step growth method [40–43]. It is used to alleviate the mismatch between AlN and sapphire substrate and improve the AlN quality. The first step is to form AlN crystal islands under high V/III ratio and low temperature. The second step is to grow AlN buffer layer with low threading dislocation density (TDD) and smooth surface through enhanced Al atom surface migration and lateral growth. The mechanism for reducing TDD is the transition from 3D to 2D growth mode that facilitates dislocation bending and annihilation along the growth direction. Hasan et al. [40] recently reported 4  $\mu\text{m}$ -thick AlN layers with total dislocation density of  $1.1 \times 10^9 \text{ cm}^{-2}$ . Two-step growth exists the issue that the crystal islands may change their crystal orientation under the actions of airflow and rotation, etc., and thus generate threading screw dislocations. Three-step growth based on two-step growth was proposed [42]. The additional growth step is inserting a morphology control layer between the buffer layer and the step-flow-growth layer by adjusting the ammonia gas flow rate to a certain value. The twist angle of island could be controlled and the threading edge dislocation lines are more likely to form a loop and annihilate. The edge dislocation can drop to the order of  $10^7 \text{ cm}^{-2}$ ;
2. Epitaxial lateral overgrowth (ELOG) method [44–50]. To be specific, the low DD is caused by filtration related to patterns on sapphire substrate and annihilation related to the formation of a loop structure during growth [47]. Nakano et al. [49] first demonstrated the ELOG-AlN layers on trencched-patterned sapphire substrates and achieved a dislocation density of  $6.7 \times 10^8 \text{ cm}^{-2}$ . To further enhanced the coalescence of ELOG-AlN, Imura et al. [48] grew ELOG-AlN layers on patterned AlN templates grown on sapphire substrates and achieved a TDD value of less than  $10^7 \text{ cm}^{-2}$ . Recently, Liu et al. [50] proposed a preset strain modulation method on nano-patterned AlN templates by introducing HTA pretreatment. The XRC FWHM values of the (0002) and (10 $\bar{1}$ 2) reflections were significantly dropped from 190 and 311 arcsec to 140 and 228 arcsec, respectively. At present, ELOG combined with HTA is believed to be the most effective approach for the growth of AlN layers in terms of crystal quality, cost and stability;
3. High-temperature annealing (HTA) of sputtered AlN on Sapphire [51–56]. Miyake et al. [55] first investigated the annealing of an AlN layer grown on a sapphire substrate and achieved a TDD of  $4.7 \times 10^8 \text{ cm}^{-2}$ . Annealing at temperatures above 1500  $^\circ\text{C}$  is effective in improving the quality of AlN layers. Due to the evolution mechanism

of strains induced by HTA, it possesses high repeatability and stability and exhibits great potential in realizing mass production. The mechanism for reducing TDD after HTA was discussed in detail by Ben et al. [52]. Under TH, adjacent dislocations with different Burgers Vectors are more likely to form voids, which provide the inner surface for dislocations to terminate. The TDD below  $10^7 \text{ cm}^{-2}$  can be achieved through this method;

4. Migration-enhanced epitaxy (MEE) method [57–61]. MEE is achieved by alternative supply of the TMAI and  $\text{NH}_3$  sources. The Al atom migration can be enhanced and the gas phase reaction can be prevented in the meantime. When  $\text{NH}_3$  is not supplied, there are few N atoms on the epitaxial surface and the migration of Al atoms can be enhanced. Based on this route,  $\text{NH}_3$  pulsed-flow method and modified MEE were proposed [58–60]. Hirayama et al. [58] fabricated a high-quality AlN buffer by  $\text{NH}_3$  pulse-flow growth technique for the first time. The  $\text{NH}_3$  pulse-flow growth is realized by firstly injecting continuous TMAI flow during the  $\text{NH}_3$  pulse-flow sequence, secondly introducing continuous-flow mode to reduce the surface roughness, and then repeating the pulse- and continuous-flow modes. Li et al. [56] recently realized growing AlN layers under a relatively fast growth rate of  $0.98 \mu\text{m}/\text{h}$  and achieved flat surface morphology (RMS = 0.5 nm) by  $\text{NH}_3$ -pulse flow mode with a small duty ratio of  $\text{NH}_3$ . A modified MEE is characterized by a combination of simultaneous source supply and conventional MEE, consisting of three different growth sequences including simultaneous, alternating supply and a combination of the two. Banal et al. [61] utilized the modified MEE to control the initial nucleation and achieved the XRC FWHM values of  $\sim 45$  and  $\sim 250$  arcsec for the (0002) and (10 $\bar{1}$ 2) planes;
5. Interlayer method [62–68]. The inserting layers work by stress management and dislocation filter. Common insertion layers include medium-temperature (MT) interlayer [62–65], superlattices [66,67], graphene [68], etc. The introduction of a MT interlayer could lead to the formation of high-density self-organized nano-voids, which can alleviate tensile stress and reduce TDD due to promoting dislocation termination and bending at macrosteps at the same time. He et al. [64] recently successfully fabricated a  $5.6 \mu\text{m}$ -thick AlN film by employing a MT interlayer ( $930^\circ\text{C}$ ). The tensile stress in the AlN film had a reduction of 64% through this method and the TDD showed an extremely low value of  $4.7 \times 10^7 \text{ cm}^{-2}$ . Wang et al. [66] grew high quality thick AlGaIn on sapphire by inserting ten periods AlN (8 nm)/ $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$  superlattices (SLs), and the TDD was reduced by two orders of magnitude.

For substrate selection, AlN single-crystal substrate is an ideal substrate for AlN and Al-rich AlGaIn growth with low extended defect density and low non-radiative recombination centers [69–71]. The DD of AlGaIn grown on AlN single crystal can be lower than  $10^3 \text{ cm}^{-2}$ , which provides a significant progress for the application of ultrawide-bandgap AlGaIn. However, with the development of ELOG and HTA technologies, the AlN template DD grown on sapphire substrate has reached very low magnitude of  $10^8 \text{ cm}^{-2}$  [48], allowing the better performance of sub-250 nm LEDs grown on cost-effective sapphire substrate. Although, at present, the DD of LEDs grown on sapphire substrates is four orders of magnitude larger than that of LEDs grown on single-crystal AlN, the EQE of sub-250 nm LEDs grown on sapphire are similar to those grown on single-crystal AlN [18].

### 3.2. n-AlGaIn with High Al Composition

The contact resistivity and sheet resistivity of the n-AlGaIn layer, which influence the electron injection efficiency, are depended on the Si doping efficiency. The ionization energy ( $E_a$ ) of Si is approximately 15 meV when Al composition is smaller than 80% [72], therefore the free electron concentration can achieve the order of  $10^{19} \text{ cm}^{-3}$  and the contact resistance and sheet resistance are within acceptable ranges. However, when the Al content is higher than 80% which is essential for sub-250 nm LED, Si doping faces severe difficulties. First, the Si  $E_a$  sharply increases with Al composition and can reached to 250 meV in



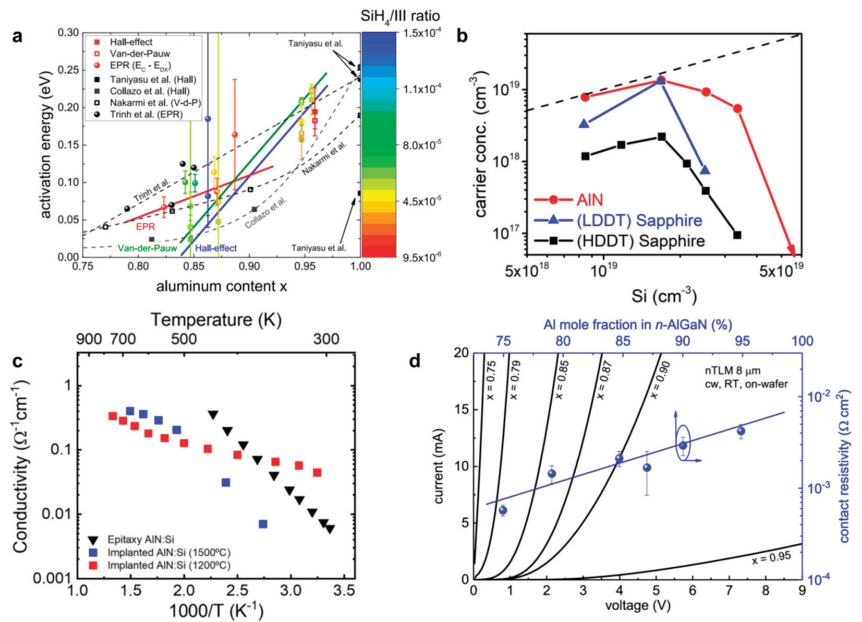
AlN [72,73], as shown in Figure 5a. In principle,  $E_n$  can be reduced by increasing the doping concentration to form impurity bands, yet self-compensation effect will reduce the free electron concentration when the Si doping concentration exceeds the critical doping dose, and the conductivity of the film will drop drastically, which is called a “knee behavior” [74], as shown in Figure 5b. Furthermore, it has been reported that the rapid decrease in conductivity also correlates with the transformation of Si from shallow donor to DX center [74]. The name of DX center derives from the fact that it is originally thought to be a deep donor (D) level associated with an unknown impurity (X) [75]. It is a highly localized center of negative charge related to two donor atoms, whose generation can be described by a chemical-like Equation (3)



where  $d^0$  and  $d^+$  represent neutral and ionized substituted shallow donor atoms, respectively. The DX centers are thought to resulting from the breaking and displacement of covalent bonds of Si atoms and nearest neighbor metal atoms in wurtzite crystals.

Low self-compensation can be achieved via  $V_{Al}$ -nSi<sub>Al</sub> complexes by defect quasi-Fermi level control (dQFL), chemical potential control (CPC), and the optimization of growth conditions including reactor pressure and temperature, etc. [76–78]. Non-equilibrium process such as Si implantation can inhibit the formation of DX centers, providing higher free carrier concentrations. In 2020, Breckenridge et al. [79] implanted Si into homoepitaxial AlN and performed a low thermal budget damage recovery and activation process, achieving an n-AlN with conductivity of  $0.05 \Omega^{-1}\cdot\text{cm}^{-1}$  at room temperature, as shown in Figure 5c. Later, in 2021, Breckenridge et al. [76] further realized Si-implanted n-AlN with higher conductivity ( $>1 \Omega^{-1}\cdot\text{cm}^{-1}$ ) and carrier concentration ( $5 \times 10^{18} \text{ cm}^{-3}$ ) on low TDD AlN substrate, maintaining the Si dopant in a shallow state via a non-equilibrium annealing process and dQFL control method.

For the purpose of enhancing the WPE, the contact resistivity of the n-electrode must be reduced. However, the n-type ohmic contact with high Al composition faces with physical limitations that the electron affinity of AlGa<sub>x</sub>N decreases from 3.18 eV for GaN to 1.01 eV for AlN [80], giving rise to the Schottky barrier increase at the metal semiconductor (MS) interface with Al content. Figure 5d summarized the electrical characteristics of n-contacts by carefully optimizing the annealing conditions on n-AlGa<sub>x</sub>N with Al content from 0.75 to 0.95 [81]. At present, suitable low work function metals have not been found. However, vanadium can form thermal stable nitrides with low work functions and is considered as an alternative metal to Ti. When Al mole fraction is greater than 0.6, the common Ti/Al-based n-electrode should be replaced by V/Al-based contacts [82]. Moe et al. [35] adopted Ti/Al/Ni/Au on n-Al<sub>0.87</sub>Ga<sub>0.13</sub>N as the n-electrode and fabricated an LED with emission wavelength of 233 nm. The device had an operation voltage of 10.4 V at 100 mA. Sulmoni et al. [80] used V/Al-based n-type contacts on n-Al<sub>0.87</sub>Ga<sub>0.13</sub>N and fabricated an LED. The operation voltage was 9.9 V at 100 mA. In addition, Nagata et al. [83] reported that a thin SiN<sub>x</sub> interlayer can reduce the n-type contact resistivity by more than one order of magnitude in the Al mole fraction range from 0.62 to 0.87.



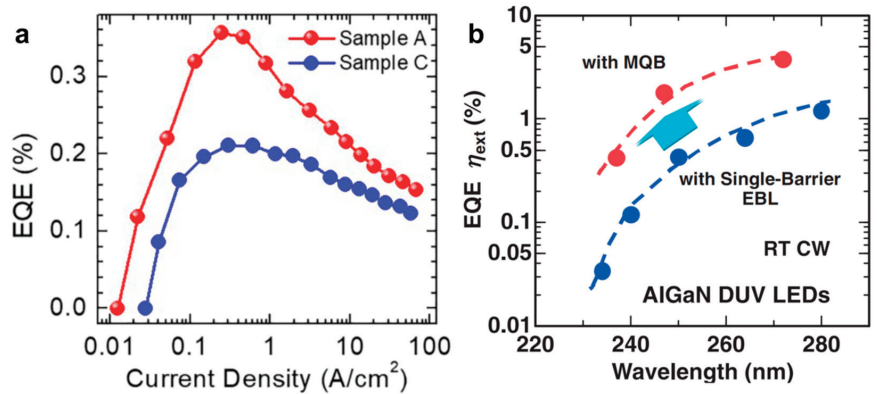
**Figure 5.** (a) The dependence of Si  $E_a$  on Al composition [73]. (b) The conductivity of n-AlGaN on different substrate with increasing Si doping concentration [74]. (c) Temperature dependent conductivity for the epitaxially doped AlN film, the Si-implanted AlN film on sapphire, and the Si-implanted AlN film on AlN substrate [79]. (d) IV curves and contact resistivity for n-contacts on n-AlGaN as a function of Al mole fraction [81].

### 3.3. Carrier Confinement and Transport

Driven by the external electric field, electrons and holes transport through the device by means of tunnelling or diffusion. Insufficient hole injection and electron leakage are the common problems during carrier transport in III-nitride based LEDs. In the review by Li et al. [84], methods of improving hole injection were explained and summarized in detail. The reason why electrons have difficulties in being restricted to the active region is that, the p-type layers cannot provide sufficient holes, and the hole mobility is low due to its large effective mass, resulting in asymmetric electron and hole injection [63]. To make matters worse, when emission wavelengths is smaller than 250 nm, the Al compositions of quantum wells and barriers become higher and higher, and the conduction band offset from the active region to the EBL becomes smaller and smaller. The severe electron leakage makes the electron injection efficiency quite low (<20%) [85]. Electron leakage has become one of the most severe problems for the sub-250 nm LEDs. A. Pandey et al. [36] measured the EQE of 245 nm LEDs with different EBL designs, and observed severe efficiency droop at 0.25 A/cm<sup>2</sup>, as shown in Figure 6a. Their studies suggested that the observed efficiency droop is largely due to an electrical effect instead of an optical phenomenon.

An effective solution for the severe electron overflow is to introduce a MQB EBL, which can cause multiple reflection effects and increase the effective barrier height. In 1986, Iga et al. [86] theoretically compared the MQB and the traditional single barrier EBL, and the results showed that the thickness modulated MQB EBL increased the effective electron barrier height by two times. In a report by Hirayama et al. [17] in 2010, MQB was introduced into UVC LEDs as the EBL. The EQE and LOP of the 250 nm-LED with MQB EBL reached 1.18% and 4.8 mW, respectively, which was 2.7 times increased compared to that with single barrier EBL. Figure 6b summarizes the wavelength dependent EQE with MQB and single barrier EBLs, proving the significant enhancement of carrier confinement by using MQB

EBL. The influences of EBL thickness and doping on the hole injection and electron blocking effect in sub-250 nm LEDs was also explored. It was shown that EBL without doping could greatly suppress the parasitic emission peaks generated by the surface Mg-related deep level transition, and thickening the EBL could increase the radiative recombination [64]. Other methods to improve hole injection and electron confinement by optimizing EBL have been extensively studied such as wideband gap interlayer and Al composition-graded EBL [87,88]. Concerning that it was still difficult to achieve high quality AlGa<sub>N</sub> epitaxial layer and high Mg doping concentration with high Al content, Kuo et al. [89] adopted Al<sub>0.55</sub>Ga<sub>0.45</sub>N/Al<sub>0.75</sub>Ga<sub>0.25</sub>N SLs EBL to replace Al<sub>0.85</sub>Ga<sub>0.15</sub>N single barrier EBL. The WPE and LOP were almost the same.

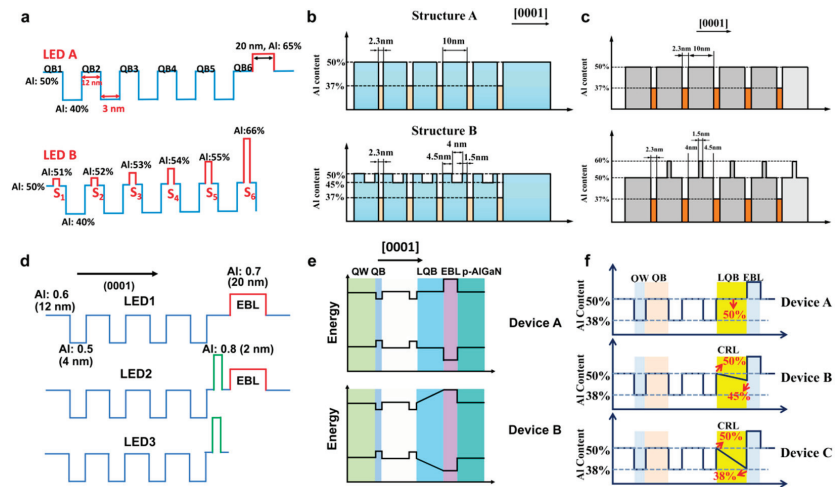


**Figure 6.** (a) Current density dependent EQE under CW bias. Sample A includes an EBL graded from an Al composition of ~95% to ~75%. Sample C is identical to Sample A, except that its EBL is a uniform Al<sub>0.75</sub>Ga<sub>0.25</sub>N:Mg layer with the same thickness [36]. (b) The EQE of DUV LEDs with different wavelength with an MQB and a single barrier EBL [85].

To optimize the quantum barrier (QB) in the active region is also important to improve the carrier confinement and transport efficiency. Velpula et al. [90] inserted a thin AlGa<sub>N</sub> layer with higher Al content into each QB in the active region, as shown in Figure 7a, and the electron leakage was reduced by approximately 11 times and LOP was increased by approximately 225% at 60 mA compared to the reference LED structure. Lang et al. [91] applied an asymmetric concave QB by inserting an AlGa<sub>N</sub> layer with lower Al content into the QB, forming a concave region on the energy band, as shown in Figure 7b. This structure can enhance the electron capture ability of QWs, accelerate the hole transport under polarization induced field, and enhance the hole vertical transport. The maximum EQE was 2.32 times higher than that of the reference one. The QB band modulation can also be achieved by inserting a thin layer with high Al content [92], as shown in Figure 7c. By the energy band modulation effect of the delta-AlGa<sub>N</sub> layer, holes can be accelerated and cross the high barriers with very large kinetic energy, thus enhancing the hole injection into the active region. The maximum EQE is 1.6 times higher than that of the reference one.

There are also many optimizations within the last quantum barrier (LQB) near the EBL, such as the insertion of a thin undoped AlGa<sub>N</sub> strip layer in the middle of the LQB and Al composition-graded LQB [93–95]. Figure 7d–f exhibits schematic conduction band diagrams of different optimizations within the LQB. It is worth mentioning that composition-graded LQB has two kinds of variations, namely increasing and decreasing [94,95], and specific choice need to be optimized according to the material and structure. In addition, although EBL can suppress electron leakage, the hole injection efficiency is still greatly affected due to the formation of positive polarization surface charge between the LQB and EBL [93,96]. To solve this problem, EBL-free structure was also proposed. Simulation analysis by Shi et al. [97] showed that utilizing Al composition-graded AlGa<sub>N</sub> insertion layer and EBL-free

structure could effectively block electrons and improve hole injection efficiency. The IQE was increased by 64.3% compared to the reference device with EBL.



**Figure 7.** Conduction band diagrams of the active region of the DUV LED (a) without (LED A) and with (LED B) inserting thin layers in the QBs [90], (b) without (structure A) and with (structure B) asymmetrical concave QBs [91], (c) without (upper) and with (lower) delta-accelerating QBs [92], (d) without strip-in-a-barrier structure but EBL (LED 1), with strip-in-a-barrier structure and EBL (LED 2), with strip-in-a-barrier structure but EBL (LED 3) [93], (e) constant Al content (Device A) and gradually increasing Al content (Device B) LQB, [94] and (f) constant Al content (Device A) and gradually decreasing Al content (Device B and C) LQB [95].

Although these energy band and carrier velocity modulation methods within EBL and active region are mainly applied in above-250 nm LEDs, we believe they also have great application potential in sub-250 nm LEDs.

### 3.4. p-AlGa<sub>N</sub> with High Al Composition

It is observed that the Mg doping efficiency in AlGa<sub>N</sub> decreases dramatically with increasing Al mole fraction [98,99]. To achieve high-efficiency p-doped AlGa<sub>N</sub> has become one of the key issues limiting the development of sub-250 nm LEDs. The low p-doping efficiency of AlGa<sub>N</sub> is mainly caused by three reasons.

1. The solubility of Mg in GaN and AlN is low. The solubility of Mg replacing Ga or Al atoms in AlGa<sub>N</sub> is limited by the positive formation enthalpies. The influence of formation enthalpies on the solubility of Mg can be expressed as the following Equation (4)

$$C_{Mg} = N \cdot \exp\left(-\frac{\Delta H_f}{kT}\right) \quad (4)$$

where  $C_{Mg}$  is the solubility of Mg atoms,  $N$  is the number of lattice points which can be occupied by the doping atoms,  $\Delta H_f$  is enthalpy change,  $k$  is the Boltzmann constant, and  $T$  is the temperature. As shown in Figure 8a [100], as the Al content in Al<sub>x</sub>Ga<sub>1-x</sub>N increases, both the Mg<sub>Al</sub> and Mg<sub>Ga</sub> formation enthalpies monotonically increase, indicating limited Mg solubility;

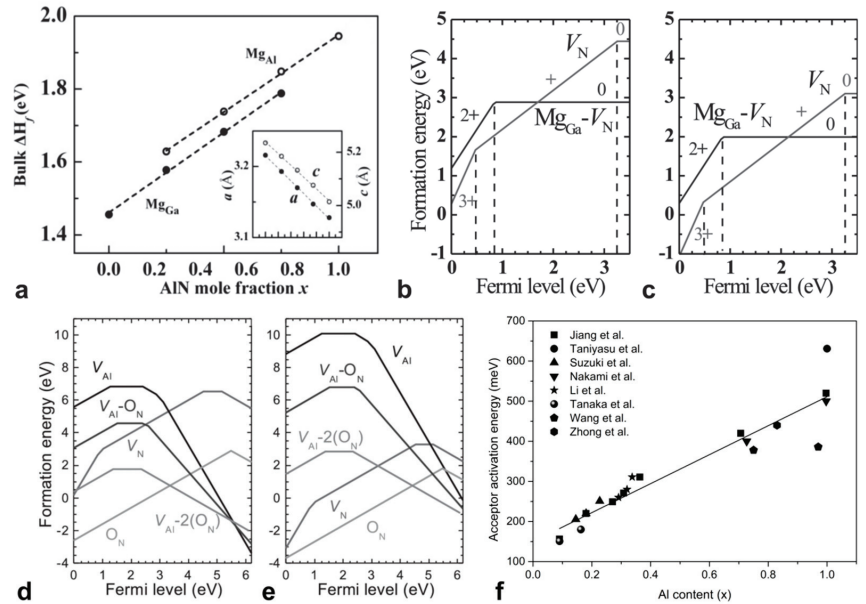
2. Self-compensation of intrinsic defects [101]. Figure 8b–e show the formation energies as a function of Fermi level for different defects in GaN and AlN [102,103]. The compensation of  $V_N$  is an important mechanism resulting in hole concentration decreasing.  $V_N$  can provide one, two, or three electrons, and only the charge states of  $V_N^+$  and  $V_N^{3+}$  are stable. Since  $V_N^{3+}$  has smaller formation energy than  $V_N^+$ ,  $V_N^{3+}$

is believed to be the main compensating defects in Mg-doped AlGa<sub>N</sub> alloys [104]. Stampfl et al. [101] found that  $V_N$  was more easily formed in AlN than in GaN. The compensation of natural defects requires to be controlled especially in Al-rich AlGa<sub>N</sub> alloys;

- The acceptor  $E_a$  is very high and gradually increase with Al content, as shown in Figure 8f [105,106]. Mg is generally used as the p-type dopant in AlGa<sub>N</sub> epilayer. The  $E_a$  of Mg in p-GaN films is in the range from 120 to 200 meV, generating a hole concentration of  $10^{17}$ – $10^{18}$  cm<sup>-3</sup> [107]. However, when the Al content changes from 0 to 100%, the  $E_a$  of Mg increases from 160 meV to over 500 meV [99,105]. The hole concentration (p) in wide-bandgap semiconductors can be estimated by the following Formula (5) [108]

$$p = \sqrt{\frac{1}{g} N_A \cdot N_V} \cdot \exp\left(-\frac{E_a}{2kT}\right) \quad (5)$$

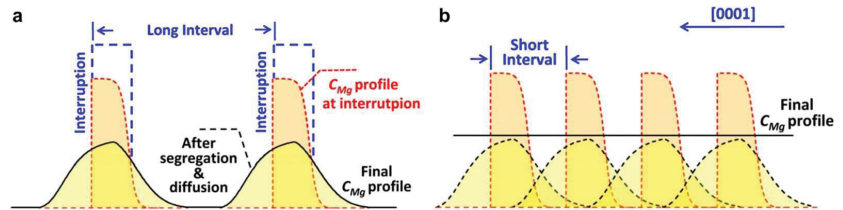
where  $g$  is the acceptor degeneracy ( $g = 2$ ),  $N_A$  is the acceptor concentration, and  $N_V$  is the effective state density near the valence band maximum (VBM). It can be seen that the increase of Mg acceptor  $E_a$  makes the hole concentration exponentially decrease, leading to the decrease of conductivity.



**Figure 8.** (a) Formation enthalpies of  $Mg_{Ga}/Mg_{Al}$  in the bulk AlGa<sub>N</sub> as a function of Al content under N-rich condition [100]. Formation energies as a function of Fermi level for the  $V_N$  and the  $Mg_{Ga}-V_N$  complex in GaN, under (b) N-rich and (c) Ga-rich conditions [102]. Formation energies as a function of Fermi level for the  $V_N$ ,  $V_{Al}$ ,  $O_N$ ,  $V_{Al}-O_N$  and  $V_{Al}-2(O_N)$  in AlN, under (d) N-rich and (e) Al-rich conditions [103]. (f) The activation energy of Mg in  $Al_xGa_{1-x}N$  in dependence of Al mole fraction  $x$ , data extracted from [105,106].

The surface during epitaxy plays an important role in determining the solubility of the dopant. Tersoff [109] pointed that the elastic interaction of the dopants with the surface relieved the stress caused by atomic size mismatch and lowered the impurity energy owing to the coupling of the impurity stress to the spatially surface stress, thus the solubility of dopants could be significantly improved. Zheng et al. [100] proposed a modified surface engineering technique (MSE) by periodic interruptions under an ultimate V/III ratio condition to enhance Mg effective incorporation without affecting the growth of AlGa<sub>N</sub> films. Schematic diagram

of the Mg incorporation behavior in the AlGa<sub>N</sub> is shown in Figure 9. For Al<sub>0.99</sub>Ga<sub>0.01</sub>N, the final doping concentration of Mg can reach  $5 \times 10^{19} \text{ cm}^{-3}$ .



**Figure 9.** Schematic diagram of the Mg incorporation behavior in the AlGa<sub>N</sub> grown by the MSE technique. (a) When the interruption interval is long, only some peaks distribute locally at the interruptions after Mg segregation and diffusion. (b) After optimizing the interruption interval, a high and uniform Mg distribution over the entire AlGa<sub>N</sub> epilayer was achieved [100].

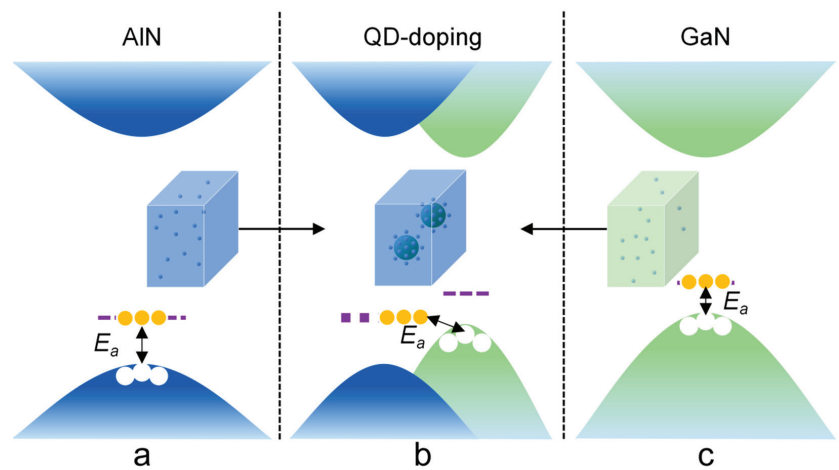
Self-compensation by  $V_N$  complexes can be suppressed by elevating V/III ratio during growth [71,99,104] and defect quasi Fermi level (dQFL) method [110]. Nakarmi et al. [104] increased the V/III ratio up to 5000 in the growth of the p-type Al<sub>0.7</sub>Ga<sub>0.3</sub>N with a Mg concentration of  $10^{20} \text{ cm}^{-3}$  and significantly suppressed the related transition, while T. Kinoshita et al. [99] increased the V/III ratio to 1800 with a Mg concentration of  $10^{19} \text{ cm}^{-3}$  and achieved a low resistivity of  $47 \Omega \cdot \text{cm}$  for Al<sub>0.7</sub>Ga<sub>0.3</sub>N. The discrepancy of the V/III ratio might result from larger formation energy of  $V_N^{3+}$  and higher crystalline quality under lower Mg concentration [99]. dQFL method utilizes illumination during growth to increase the formation energy of the compensating point defects. A. Klump et al. [110] observed the reduction of  $V_N$ -related emission for the dQFL-process samples, and validated the effectiveness of dQFL control process in point defect management for Mg-doped III-nitride films.

To reduce the acceptor  $E_a$  for AlGa<sub>N</sub> with high Al composition, several methods were developed in recent two decades. Under the condition of heavy doping ( $>2 \times 10^{19} \text{ cm}^{-3}$ ), the hole concentration provided by the impurity band is two orders of magnitude larger than the valence band transport, exhibiting very low acceptor  $E_a$ . In addition to forming impurity band, the Mg acceptor  $E_a$  can be reduced by Mg pulse or  $\delta$ -doping [111–118].  $\delta$ -doping had been proved to effectively increase the hole concentration without causing a crystal quality droop [119]. The polarization-induced doping [120–122] and superlattice doping [123–125] are two common-used methods to reduce the apparent acceptor  $E_a$ . Under biaxial strain, AlGa<sub>N</sub> layers will generate huge polarization induced electric field ( $10^5$ – $10^7 \text{ V/cm}$ ), making the valence and conduction bands tilt, thereby the acceptors ionization probability gets larger. Under polarization-induced electric field, free holes will be swept to the interface, generating two-dimensional hole gas (2DHG) near the interface, and simultaneously generating a depletion layer. If the thickness of the depletion layer is too thick, the vertical transport of holes will be hindered. Thus, the thickness of the thin layer should be limited to 0.6–10 nm [126]. To avoid the free carrier accumulation at the interface, three-dimensional polarization doping was adopted by means of gradually changing Al content, which could generate three-dimensional hole gas (3DHG) [122,127]. SLs doping can reduce the  $E_a$  via modulating the band structure based on spontaneous and piezoelectric fields. Kazuaki Ebata et al. [128] achieved high hole concentrations on the order of  $10^{18} \text{ cm}^{-3}$  and small  $E_a$  of 40–67 meV by adopting AlN/Al<sub>0.75</sub>Ga<sub>0.25</sub>N SLs with an average Al composition of 0.8. As one kind of SLs doping methods, short-period superlattice (SPSL) is very effective to improve p-doping efficiency [123,129]. Schubert et al. [107] made a theoretical analysis and found that for SPSL ( $<100 \text{ \AA}$ ) doping, the free carrier concentration could increase by more than ten times when the magnitude of the valence band modulation and the Mg  $E_a$  were equal. Wang et al. [130] proposed a desorption-tailoring method and remarkably reduced the Mg  $E_a$  to 17.5 meV in p-AlGa<sub>N</sub> SLs with an average Al composition of 51%. The desorption process, achieved by interrupting the supply of the precursors, was the



reverse process of absorption of atoms to the surface. Specified SLs can be grown by adjusting the desorption time and matching the desorption time and epitaxy time. Based on the reduction of activation energy and enhancement of Mg surface-incorporation, the hole concentration in SLs reached  $8.1 \times 10^{18} \text{ cm}^{-3}$  at room temperature.

Recently, K. Jiang et al. [106] proposed a new method to improve the doping efficiency called “quantum engineering of non-equilibrium p-doping” in which the key points were, firstly, embedding relatively narrow bandgap quantum structure into wide bandgap matrix to produce a new band edge, and secondly, enriching the Mg dopants near the interfaces to improve ionization, as shown in Figure 10. The Mg  $E_a$  of AlGaN with Al content of 50~70% was reduced to below 50 meV, and the hole concentration reached higher than  $10^{18} \text{ cm}^{-3}$  at room temperature.



**Figure 10.** The VBM modulation mode to lower the acceptor  $E_a$ . Acceptors are randomly doped in (a) AlN and (c) GaN. Both have high  $E_a$  in this condition. (b) GaN QDs are embedded in the AlN matrix and acceptors are doped in the AlN matrix and concentrate near the interface [106].

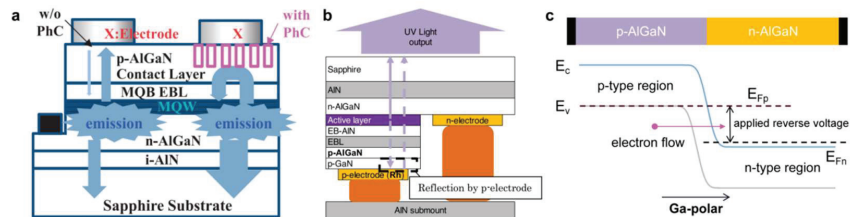
Although the Mg acceptor  $E_a$  in AlGaN with high Al content can be reduced to even lower than that in GaN by various designs, the resistivity is still relatively higher due to significantly reduced hole mobility. Maybe, to increase the hole mobility is the next breakthrough of p-type doping for Al-rich AlGaN.

### 3.5. Light Extraction

According to the current researches, the low LEE may be the most serious problem hindering the UV LED performance, especially for sub-250 nm LEDs. The two main factors restricting the LEE are: (a) the balance between increasing transparency and decreasing driving voltage; (b) the transformation of emission light polarization from TE to transverse magnetic (TM) mode. For instance, to realize 240 nm transparency, the Al content larger than 80% is required within the LED structure. When the emission wavelength is 222 nm, Al mole fraction should be as high as 0.95 to ensure totally transparent, which greatly increases the operation voltage. Hence, a careful trade-off between reducing the optical absorption and increasing the conductivity is needed to achieve relatively high WPE. Furthermore, when the emission wavelength reduces to below 250 nm, the increase of Al mole fraction leads to the rearrangement of valence bands. The main polarization mode of the emission light shifts from TE, which mainly propagates along the (0001) direction that usually vertical to the device surface, to TM mode, which mainly propagates laterally in the c-plane that usually parallel to the device surface [10,131,132]. It was reported that the optical extraction efficiency of TM mode is less than 1/10 that of TE mode [133].



Self light absorption is a severe problem for all UV LEDs and schemes for boost transparency in other UV wavebands can also be applied to sub-250 nm LEDs. The reduction of light absorption can be achieved by using a transparent p-AlGa<sub>N</sub> contact layer [15,134,135], a highly reflective electrode structure, photonic crystal (PhC) and other reflection structures [13,136–138], etc. Mg-doped Al<sub>x</sub>Ga<sub>1-x</sub>N/Al<sub>y</sub>Ga<sub>1-y</sub>N SPSL can provide transparent p-type contacts, yet the turn-on voltage is still high due to the high vertical resistivity and low mobility of the free carriers [15]. Muhin et al. [134] investigated the vertical conductivity of Al<sub>0.71</sub>Ga<sub>0.29</sub>N/Al<sub>0.65</sub>Ga<sub>0.35</sub>N:Mg SPSLs and observed that its value was strongly affected by temperature and electric field, to be specific, the vertical conductivity could increase by almost two orders of magnitude when the electric field varied from 0.05 to 0.98 MV·cm<sup>-1</sup>, or the temperature increased from room temperature to 100 °C. Guttman et al. [135] showed that the average Al mole fraction should be high enough to be transparent for emission wavelength, and a five-fold increase of the on-wafer EQE could be achieved combined with reflective In p-contacts. Kashima et al. [138] improved the EQE of 283 nm LED from 4.8% to 10% by introducing high-reflectance PhC and reflective Ni/Mg p-electrodes on the surface of the contact layer as shown in Figure 11a. Takano et al. [13] reported a 275 nm LED with an EQE of 20.3% by combining various ways to improve the LEE, including the adoption of transparent AlGa<sub>N</sub>:Mg contact layer and Rh mirror electrode. When reflective p-electrodes were used, EQE could be significantly improved by optimizing the thickness of p-type layers [139]. As shown in Figure 11b, there are two light paths: directly from the active region toward the sapphire (solid arrow) and reflected by the p-electrode toward the sapphire (dashed arrow). When the total optical thickness of the p-type layers changes, the optical path difference between the two paths changes, creating interference and significantly affecting the LOP.

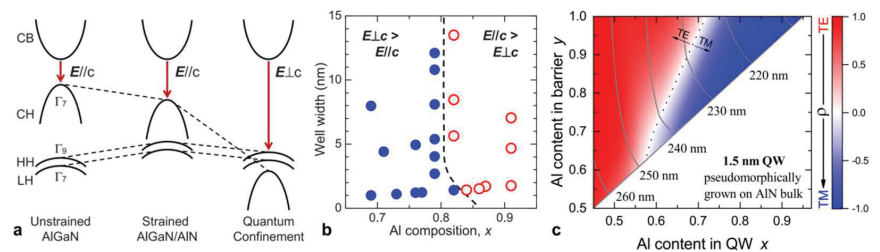


**Figure 11.** Schematic structure of (a) the LEDs with and without a PhC on the p-AlGa<sub>N</sub> contact layer [138] and (b) the flip-chip LED with two light paths [139]. (c) Schematic diagram of homogeneous tunnel junction structure and its corresponding energy band as well as carrier transport.

Since the DUV transparent AlGa<sub>N</sub>:Mg contact layer will lead to the low efficiency of hole injection, it is feasible to utilize the polarization field and tunnel junction. As shown in Figure 11c, the tunnel junction is a p-n junction working at reverse bias, which can achieve high reverse current through interband tunnelling at low reverse bias. In early works, the formation of an effective tunnel junction usually required degenerate p- and n-doping to achieve very narrow depletion regions, so that the carriers could easily tunnel from valence band on one side to conduction band on the other side. Whereas, degenerate p-type doping was almost impossible to achieve in high Al content AlGa<sub>N</sub>, researchers proposed a tunnel junction based on heterointerface polarization charges, which could eliminate the need for heavy doping [140]. Recently, Mehnke et al. [141] fabricated a tunnel heterojunction LED with an emission wavelength of 232 nm. The LOP and EQE reached to 1.73 mW and 0.35% at 100 mA under pulsed operation, respectively. However, the operation voltage (26 V at 10 mA) was still high compared to the reference traditional LED (6.8 V at 10 mA). The doping of the tunnel junction interface should be optimized to reduce the resistance and operation voltage.

Under the crystal field and spin-orbit coupling, the valence band for wurtzite Al-GaN materials contains heavy hole (HH), light hole (LH), and crystal field splitting hole

(CH) sub-bands. The emitting light polarization is determined by the valence sub-band distribution. The topmost CH and HH sub-bands will lead to TM- and TE-dominated emission, respectively. The critical Al mole fraction triggering the transition from TE mode to TM mode depends on the strain state and quantum confinement [142], as shown in Figure 12a. Under compressive strain, the HH and LH sub-bands will be lifted up, while the CH subband will be pulled down, resulting TE mode enhancement. Enhancing the quantum confinement will greatly pull down the CH sub-band due to its light effective mass, even resulting in the intersection to LH and HH and also promoting the TE mode. The QW width and barrier height can affect the quantum confinement, thus controlling the polarization mode. Figure 12b shows that when the QW is relatively thick (>3 nm), the critical Al mole fraction is independent of the QW width. When the QW is relatively thin (<3 nm), the thinner the QW gets, the higher the critical Al mole fraction gets [142]. Figure 12c displays the calculated degree of polarization (DOP,  $\frac{I_{TE}-I_{TM}}{I_{TE}+I_{TM}}$ ) by  $k\cdot p$  theory of an AlGaIn QW with different well and barrier Al contents pseudomorphically grown on AlN bulk substrate with thickness of 1.5 nm [143]. As it can be seen, for a certain well Al content, increasing the barrier Al content can improve the DOP, for a certain barrier Al content, decreasing the well Al content can improve the DOP, and for a certain emission wavelength such as 230 nm, it is necessary to simultaneously increase the barrier Al content and decrease the well Al content.



**Figure 12.** (a) Schematic energy band structures for unstrained AlGaIn, strained AlGaIn on AlN, and AlGaIn/AlN QW near the  $\Gamma$  point with high Al content. CB denotes the conduction band. (b) Emission polarization mode as function of Al composition and well width [142]. (c) DOP of the emission from an AlGaIn-based QW with 1.5 nm thickness pseudomorphically grown on AlN bulk calculated by  $k\cdot p$  theory [143].

Experimentally, when the QW is under strain free or compressive strain states, the TE emission and quantum efficiency will be greatly improved [144–146]. ELOG for reducing TDD can also enhance TE mode emission due to the differences in thermal expansion coefficients. In 2021, Zhang et al. [147] successfully modulated the strain state of AlN template by adopting multiple alternation cycles of low- and high-temperature growth. Hence, the in-plane compressive strain of the QWs had increased. The DOP was enhanced from 41.5% to 61.9%. When the GaN quantum well width is reduced to a few atom monolayers (MLs), strong quantum confinement will appear, which can increase the effective transition energy of GaN by several eV. Some groups [23,24,148,149] have carried out related studies on AlN-delta-GaN QW LEDs and achieved lower wavelength emission. The advantage of this method is that in addition to increasing TE emission, the spontaneous emission rate is also significantly increased by suppressing the QCSE. At present, researches on AlN-delta-GaN QW LEDs are still in the early stage, further and deeper researches need to be carried out and its feasibility requires to be confirmed.

#### 4. Conclusions and Prospect

Nowadays, the technology roadmap of AlGaIn based sub-250 nm LEDs is basically similar to the conventional DUV LEDs. The performance collapse mainly results from the problem accumulation with Al composition increasing of each layer in the device structure.

First of all, improving the material crystal quality is the key issue to promote the sub-250 nm LED performance. Before the AlN single-crystal substrate fabrication and homogeneous epitaxy technologies mature, the AlN/Sapphire template is still the best choice. HTA is a promising method, which can provide cost-effective, stable, high-quality, and compressive strain AlN/Sapphire, benefiting the IQE and LEE.

The contact and sheet resistivity of the n-AlGaIn layer contribute part of the driving voltage. When Al mole fraction is larger than 0.8, shallow donor Si gradually changes into a deeper donor, and finally becomes a stable charge capture center, leading to a significant increase in resistivity. Controlling the formation of DX centers is a critical technical challenge for high Al composition AlGaIn. Optimization of n-layers, including modulating growth conditions and searching for suitable contact metals, need to be further explored. For carrier confinement and transport, although a large number of energy band engineering studies have been carried out to enhance carrier confinement, electron overflow is still one of the most severe problems in sub-250 nm LEDs due to the physic limitations. The MQB EBL is a promising method to increase the effective electron barrier.

Resulting from the increase  $E_a$  of Mg dopants in AlGaIn, p-AlGaIn layers cannot offer sufficient free carriers and enough high conductance. Different methods, such as  $\delta$ -doping, quantum engineering doping, polarization induced doping, and superlattice doping, etc., have been proposed to improve the doping efficiency, while it is still facing daunting challenges. In addition, how to increase the hole mobility may be the next problem to be solved. Serious light absorption and emission mode transition problem greatly reduces the LEE in this wavelength range. Adopting tunnel junction may be a quite hopeful method to achieve fully transparent LED.

**Author Contributions:** Conceptualization, K.J., X.S. and D.L.; methodology, K.J. and C.Z.; writing—original draft preparation, C.Z.; writing—review and editing, K.J.; project administration, K.J., X.S. and D.L.; funding acquisition, K.J., X.S. and D.L. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research was funded by National Key R&D Program of China (grant number 2022YFB3605103); National Natural Science Foundation of China (grant numbers 62004196, U22A2084, 62121005, and 61827813); Youth Innovation Promotion Association of Chinese Academy of Sciences; and Youth Talent Promotion Project of the Chinese Institute of Electronics (grant number 2020QNRC001).

**Data Availability Statement:** Not applicable.

**Conflicts of Interest:** The authors declare no conflict of interest.

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Review

# Reliability, Applications and Challenges of GaN HEMT Technology for Modern Power Devices: A Review

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**Abstract:** A new generation of high-efficiency power devices is being developed using wide bandgap (WBG) semiconductors, like GaN and SiC, which are emerging as attractive alternatives to silicon. The recent interest in GaN has been piqued by its excellent material characteristics, including its high critical electric field, high saturation velocity, high electron mobility, and outstanding thermal stability. Therefore, the superior performance is represented by GaN-based high electron mobility transistor (HEMT) devices. They can perform at higher currents, voltages, temperatures, and frequencies, making them suitable devices for the next generation of high-efficiency power converter applications, including electric vehicles, phone chargers, renewable energy, and data centers. Thus, this review article will provide a basic overview of the various technological and scientific elements of the current GaN HEMTs technology. First, the present advancements in the GaN market and its primary application areas are briefly summarized. After that, the GaN is compared with other devices, and the GaN HEMT device's operational material properties with different heterostructures are discussed. Then, the normally-off GaN HEMT technology with their different types are considered, especially on the recessed gate metal insulator semiconductor high electron mobility transistor (MISHEMT) and p-GaN. Hereafter, this review also discusses the reliability concerns of the GaN HEMT which are caused by trap effects like a drain, gate lag, and current collapse with numerous types of degradation. Eventually, the breakdown voltage of the GaN HEMT with some challenges has been studied.

**Keywords:** GaN HEMT; normally off; reliability; challenges; power devices; semiconductor devices; wide bandgap

**Citation:** Islam, N.; Mohamed, M.F.P.; Khan, M.F.A.J.; Falina, S.; Kawarada, H.; Syamsul, M. Reliability, Applications and Challenges of GaN HEMT Technology for Modern Power Devices: A Review. *Crystals* **2022**, *12*, 1581. <https://doi.org/10.3390/cryst12111581>

Academic Editors: Peng Chen, Zhizhong Chen and Dmitri Donetski

Received: 29 September 2022

Accepted: 2 November 2022

Published: 7 November 2022

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## 1. Introduction

Electrical power has been a fundamental driver of humanity's progress and is indispensable in our daily life. Power electronics are critical components of electrical power usage because they control, convert, and manage electric currents, voltages, or powers. They are extensively utilized in consumer items, energy harvesting, and usage, such as switching power supplies, power converters, power inverters, motor drives, etc. Figure 1 shows the different fields of operation of power devices with the required voltage and current ratings [1,2]. As depicted in Figure 2, a typical power electronic system includes a power source, a filtering mechanism, a power conditioner, a load, and a control circuit. A power conditioner is composed of a series of semiconductor devices working in a switched mode, in which the devices are turned between the "OFF" and "ON" states under the direction of the gate driver [1]. When turned "off", an ideal switch should have no leakage

current and a full voltage drop across it. If switched “on”, it should have a zero voltage drop across it (Figure 3). In actuality, the power devices exhibit a resistance during the on-state ( $R_{ON}$ ) and a leakage current during the off-state. Under the common biasing conditions, the voltage across it is restricted by the off-state drain to source the breakdown voltage ( $BV_{DSS}$ ). Thus, to maximize the energy efficiency and minimize conversion losses, the most crucial properties of power devices to accomplish are a low  $R_{ON}$  and a high  $BV_{DSS}$ .

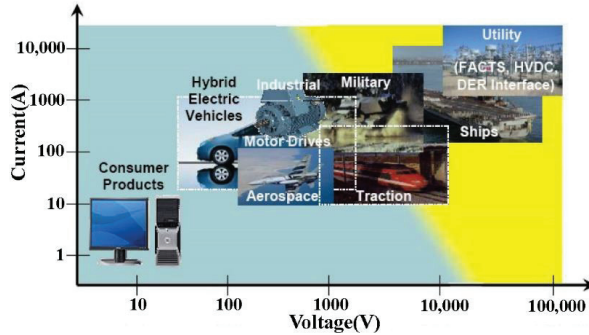


Figure 1. Applications of power electronics in power management and control. Reproduced with permission [2]. Copyright 2019, the author(s). Published by Elsevier.

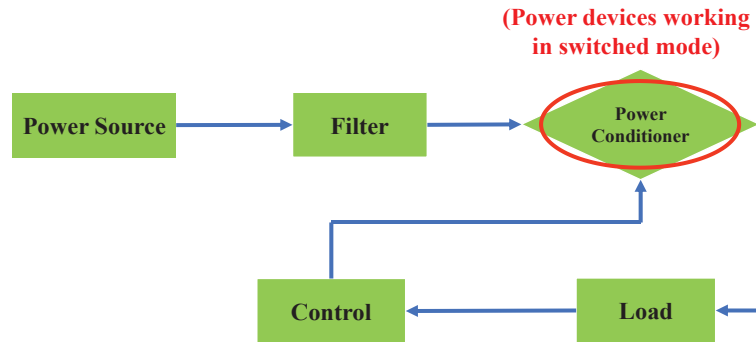


Figure 2. Components of a power electronic system and power semiconductor devices in power conditioners.

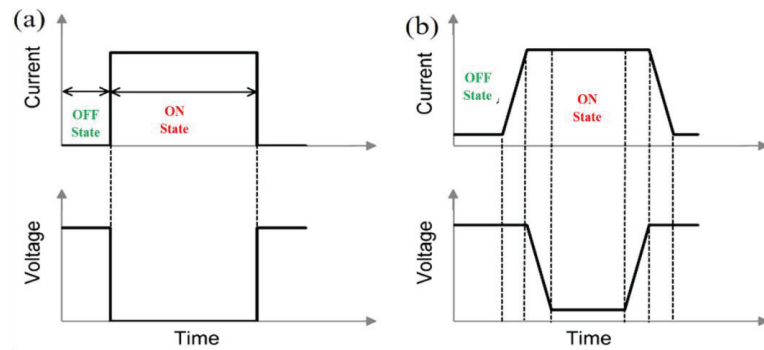


Figure 3. The current and voltage across (a) an ideal power switching device and (b) a power switching device.

Moreover, Gallium Nitride (GaN) has risen as an attractive material for fabricating semiconductor devices over the last decade. Its excellent performance characteristics, like its wide band gap, high electron mobility, high breakdown field, low noise, high saturation velocity, and low thermal impedance, are essential for modern power device technology [3].

This review article will provide a basic overview of the various technological and scientific elements of the current GaN HEMT technology, where we summarize the recent and future potential market strategy of GaN HEMT power devices. Additionally, the previous and present data of the most extensively used commercially device, the normally-off GaN HEMT, are amalgamated, focusing explicitly on the insulator's role in the recessed MISHEMT region and the metal on the p-GaN performances, which makes this review article more comprehensive compared to other review articles. Moreover, this review also discusses the reliability concerns of the GaN HEMT which are caused by trap effects like a drain, gate lag, and current collapse with numerous types of degradation.

### *1.1. Market Strategy of GaN HEMT Power Devices*

GaN-based devices are being reported in various market-driven sectors, including RF power devices, photonics, high-frequency communications, control, and high-power conversion, which assists commerce's and corporations in meeting the constantly expanding need for more outstanding metrics. The inherent robustness of the device enables it to compete effectively in the current markets for tiny, rugged, and highly dependable electronics, such as in vehicle, military, and space applications. GaN engineering appears promising for achieving the critical performance requirements and the possibility of sustained economic benefits upon its maturity.

Figures 4 and 5 show that according to Yole Développement (Yole), the power GaN market will double by 2020, surpassing the USD one billion mark in 2026. As an additional validation of this remarkable GaN market development, Yole projects that the telecom and datacom and automotive sectors will contribute to the total growth in the mid- to long-term, owing to GaNs rise in fast chargers. In the consumer market, GaN had a good year in 2020, owing to the technology adoption by various businesses, including Xiaomi, Lenovo, Samsung, Realme, Dell, LG, and other Chinese aftermarket firms. Yole anticipates that the GaN consumer power supply industry will be the primary driver, growing from USD 29 million in 2020 to about USD 672 million in 2026 at a compound annual growth rate (CAGR) of 69%. In the telecom and datacom sectors, where more efficient, smaller power supplies must comply with the stricter energy consumption standards, data centers and telecom operators are already interested in GaN devices.

Following Eltek, Delta, and BelPower's recent small volume adoption of the GaN-based power supply, it was predicted that there would be a more significant market for GaN in 2020, with a market value of USD 9.1 million and a CAGR of 71% from 2020 to 2026, reaching more than USD 223 million in 2026. The automotive and mobility markets are also paying close attention to GaN because of significant incentives for vehicle electrification and a need to increase the driving range via A system efficiency improvement. AEC-qualified manufacturers include EPC, Transphorm, GaN Systems, and Texas Instruments. STMicroelectronics, a major IDM, also pursues GaN for EVs via partnerships and acquisitions. In 2022, GaN will likely infiltrate at limited levels, primarily via OEM and Tier-1 samples. Yole anticipates that the automobile and mobility industry will exceed a value of USD 155 million in 2026 [4].

## 2020–2026 power GaN market forecast split by application

(Source: GaN Power 2021: Epitaxy, Devices, Applications and Technology Trends report, Yole Développement, 2021)

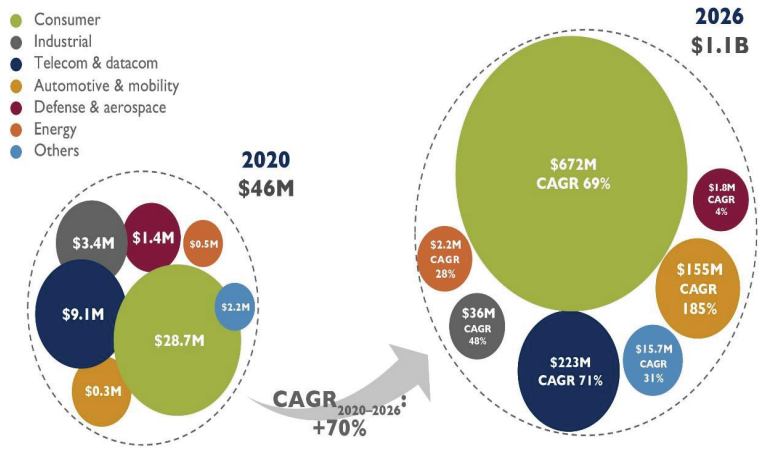


Figure 4. GaN power market forecast split by application prediction by Yole. Reproduced with permission [4]. Copyright 2021, published by Yole Développement.

## Roadmap for GaN power devices

(Source: GaN Power 2021: Epitaxy, Devices, Applications and Technology Trends report, Yole Développement, 2021)

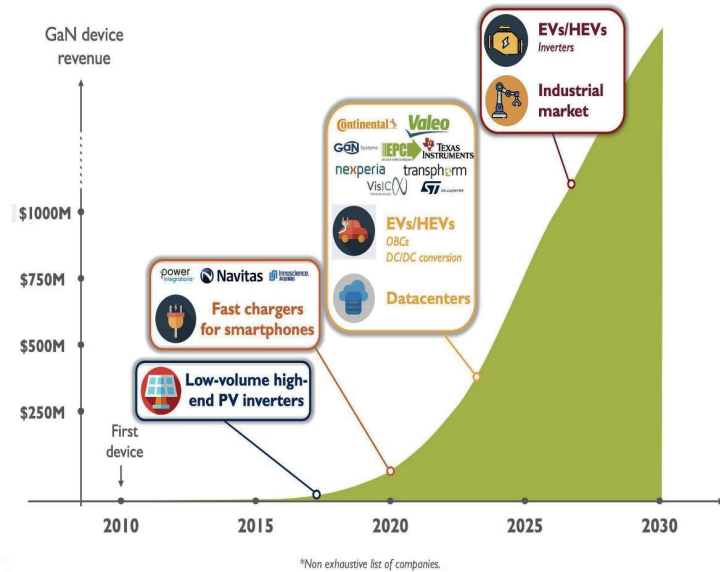
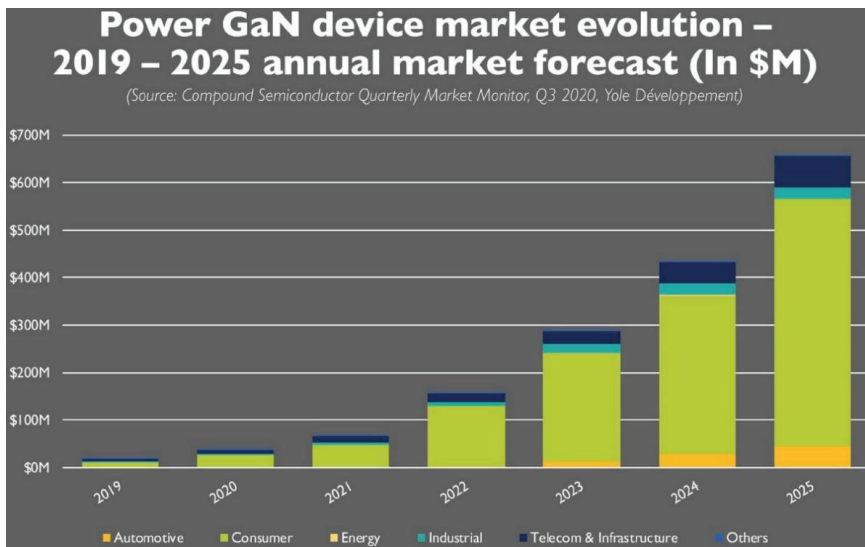


Figure 5. Roadmap for GaN power devices prediction by Yole. Reproduced with permission [4]. Copyright 2021, published by Yole Développement.



While GaN continues to gain traction in the general consumer market, telecom, datacom, automotive, and mobility businesses will benefit from the “economy of scale impact” and price erosion. Indeed, Yole anticipates that a GaN adoption will increase in these areas, where reliability and affordability are critical, beginning in 2023–2024. In the long run, after GaN has shown its durability and high current capability at a lower price, it may be able to reach the more difficult EV/HEV inverter market and the conservative industrial industry, creating an extraordinary high-volume potential for GaN. Indeed, Nexperia and VisIC are developing GaN-based xEV inverter systems to compete with SiC and Si. Furthermore, as various industry experts previously said, GaN is more suitable for low-to-medium voltage applications (200–600 V), including a sizable share of the consumer electronic market (e.g., phone chargers, audio amplifiers, and computer power supplies). GaN is the most excellent contender to replace conventional Si devices in this voltage range. The 600–900 V voltage range is strategically important since it includes converters for electric cars (EVs), hybrid EVs, and inverters for sustainable energy (e.g., photovoltaic). GaN devices are projected to compete or coexist alongside SiC devices in this voltage range. Recent industry analyst studies [5] show that the GaN power device market is expected to grow dramatically, surpassing a value of USD 700 million in 2025, as illustrated in Figure 6.



**Figure 6.** GaN Power device market size prediction by Yole. Reproduced with permission [5]. Copyright 2020, published by Yole Développement.

### 1.2. Market Strategy of GaN HEMT RF Devices

The gallium nitride (GaN) radio-frequency (RF) device market is rising at a compound annual growth rate (CAGR) of 18% from a USD 891 million value in 2020 to a more than USD 2.4 billion value by 2026, forecasts the market analyst firm Yole Développement [6]. It has been forecasted that the market will be dominated by defense and 5G telecom infrastructure applications, representing 49% and 41% of the entire market by 2026, respectively. In particular, the GaN-based macro/micro-cell sector will represent more than 95% of the GaN telecom infrastructure market in 2026, as reflected in Figure 7.

In the RF GaN industry, everything started with GaN-on-SiC (gallium nitride on silicon carbide) technology. Launched more than 20 years ago, GaN-on-SiC is now a serious rival to silicon LDMOS and gallium arsenide (GaAs) in RF power applications. Dominated by GaN-on-SiC technology, a vertical supply chain integration has been preferred in defense and 5G telecom applications. Therefore, GaN-on-SiC technology is still preferred in terms

of its high-power density and thermal conductivity. In addition to its deep penetration in the military radar, GaN-on-SiC has also been the choice of telecom OEMs such as Huawei, Nokia, and Samsung for 5G massive MIMO infrastructures. Due to their high bandwidth and efficiency, GaN-on-SiC devices continuously take a share from LDMOS of the 5G market and are starting to benefit from the 6" wafer platform transition. In this context, the GaN-on-SiC device market is growing at a 17% CAGR from USD 342 million in 2020 to USD 2.222 billion in 2026. However, as a key challenger, GaN-on-Si is still in the game, promising cost-efficient and scalable solutions. The recent entry of foundries and synergy with the emerging power electronics GaN-on-Si industry can also help GaN-on-Si RF to gain momentum in the longer term, says Yole. Driven by handsets but also defense and 5G telecom infrastructure applications, the GaN-on-Si device market is growing at a CAGR of 86% from less than USD 5 million in 2020 to USD 173 million in 2026 [6], as illustrated in Figure 8.

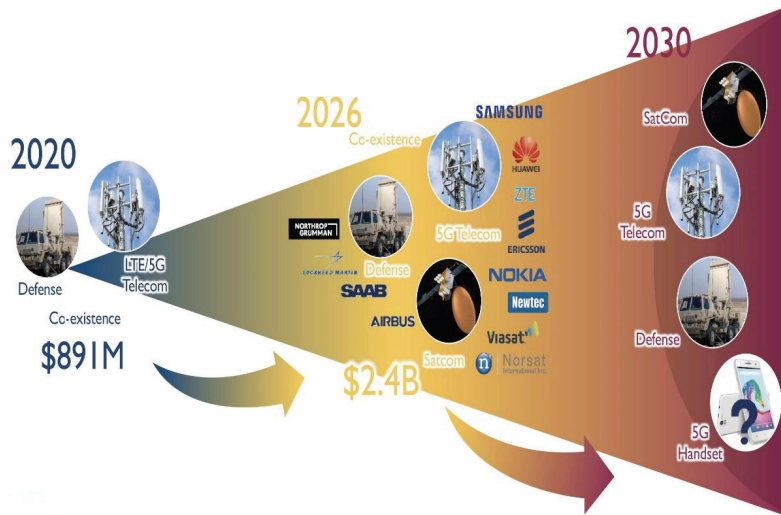


Figure 7. GaN Power RF market evaluation by Yole. Reproduced with permission [6]. Copyright 2021, published by Yole Développement.

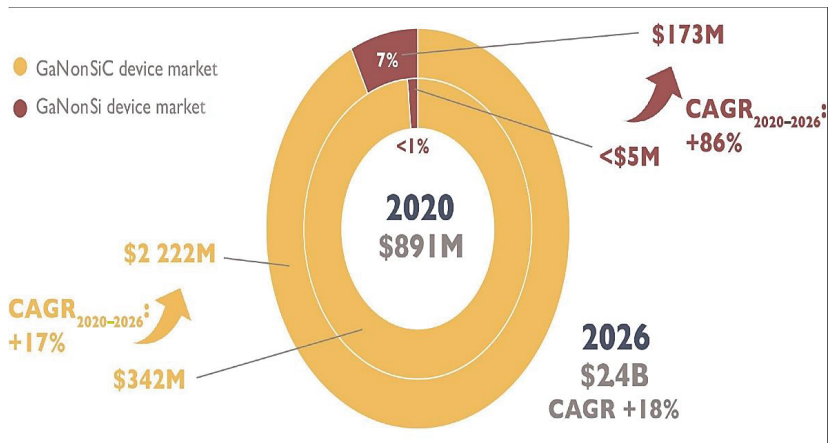
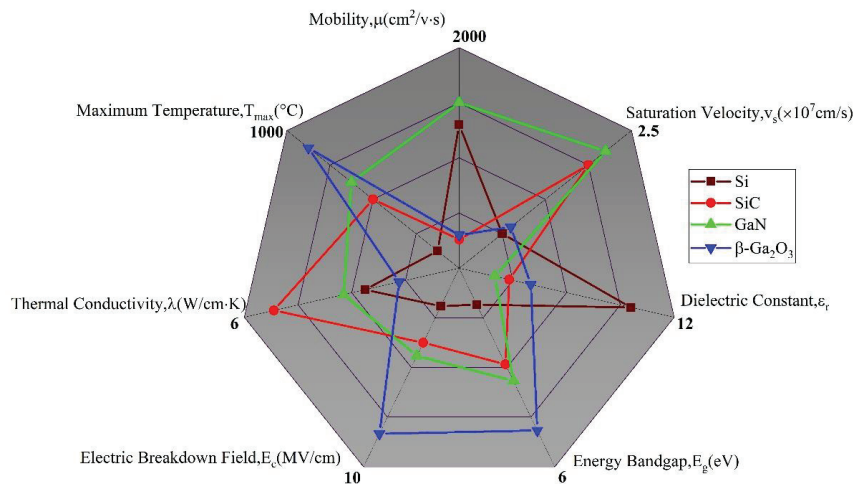


Figure 8. GaN RF application breakdown by substrate markets as compiled in 2021 by Yole. Reproduced with permission [6]. Copyright 2021, published by Yole Développement.

## 2. Wide Bandgap Semiconductors for Power Devices

Due to the many constraints of silicon-based power devices and the rising interest in increasing performances, new semiconductor materials for next-generation power electronic devices are being developed. Because of their better electrical properties, wide bandgap (WBG) semiconductors like GaN,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, and SiC have emerged as market leaders in power electronic applications. Since the material's small bandgap is responsible for many of the constraints for Si-based devices, wide bandgap power devices have a better performance with a larger blocking voltage, dependability, and efficiency with less thermal constraint [7–9]. Thus, GaN,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, and SiC have a bandgap which is two to four times that of Silicon. A bigger energy bandgap makes it more challenging to break the bonding and generate free charge carriers for a current conduction, which results in a less conductive material and transistors with lower leakage currents and a more excellent stability at high temperatures. On the contrary,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> devices have a substantially greater breakdown voltage compared to Si devices when their on-resistances are comparable. Moreover, GaN devices have a larger saturation on-current than Si devices due to the higher saturated electron velocity of GaN. Additionally, the carrier drift velocity directly connects with the switching speed of semiconductor devices, and this device has a quicker recovery time and a lower reverse recovery current. On the other hand, SiC presents a thermal conductivity three times higher than Si and GaN and 16 times higher than  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>. The characteristics of Si are compared to those of WBG semiconductors such as SiC,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, and GaN in Figure 9 [10–12].



**Figure 9.** Comparison of wide bandgap materials with Si.

However, numerous figures of merit (FOM) have been proposed to compare the merit of several semiconductor materials for a provided application. A higher figure of merit number indicates a better performance. Hence, Johnson's figure of merit (JFOM) provides an indication of the material suitability for high-power applications at high frequencies, which can be estimated by using Equation (1) [13]:

$$\text{JFOM} = \left( \frac{E_c V_{\text{sat}}}{2\pi} \right)^2 \quad (1)$$

Here,  $V_{\text{sat}}$  denotes the saturation electron velocity, and  $E_c$  denotes the critical electric field. On the contrary, to analyze the optimum results of field effect transistors in low-

frequency power switching applications, Baliga's figure of merit (BFOM) was devised where conductive loss predominates, as shown in Equation (2) [14]:

$$\text{BFOM} = \epsilon_r \mu E_g^3 \quad (2)$$

Here,  $\epsilon_r$  denotes the semiconductor's dielectric constant, and  $\mu$  denotes the electron mobility. For a high frequency, the Baliga high-frequency FOM (BHFFOM) in Equation (3) evaluates the devices where the switching losses are the most significant [14]:

$$\text{BHFFOM} = \frac{\mu E_c^2 V_g^{\frac{1}{2}}}{2 V_{BR}^{\frac{3}{2}}} \quad (3)$$

Here, the gate drive voltage is  $V_g$ , while the breakdown voltage is  $V_{BR}$ . By using the device's on-state specific resistance,  $R_{on}$ , and the critical electric field,  $E_c$ , the latter is coupled to an experimental figure of merit on Equation (4). Eventually, to account for the high power, high temperature, and high-frequency performance simultaneously, the combined FOM (CFOM) was devised, as shown in Equation (5) [15]:

$$\text{FOM} = \frac{V_{BR}^2}{R_{on}} = \epsilon_r \mu \frac{E_c^3}{4} \quad (4)$$

$$\text{CFOM} = \chi \epsilon_r \mu V_{sat} E_c^2 \quad (5)$$

Table 1 shows the multiple figures of merit for the  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> potential high-frequency and high-power performance compared to other competing semiconductor materials. According to this table,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is a great contender for high-frequency power applications. In JFOM, the  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is more remarkable than approximately 1.5 times that of GaN, 10 times that of SiC, and about a thousand times that of Si. Consequently,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> outperforms Si, GaN, and SiC in terms of its high-frequency/high-power performance. Similarly, in BFOM,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is more remarkable than around four times that of GaN, ten times that of SiC, and a thousand times that of Si [16]. Moreover, wide-bandgap semiconductors, regardless of their FOM, provide better performance features for high-power, high-frequency applications. Thus, due to the high values of the Baliga FOM and the breakdown field,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is a promising candidate for the next generation of high-power devices, including HEMT, Schottky barrier diodes (SBDs), and field-effect transistors (FETs).

**Table 1.** Figures of merit of GaN and competing semiconductor materials in power electronics [12].

Material	Johnson's Figure of Merit, (JFOM)	Keyes Figure of Merit, (KFOM)	Baliga's Figure of Merit, (BFOM)	Baliga's High Frequency Figure of Merit, (BHFFOM)	Combined Figure of Merit, (CFOM)
Si	1.0	1.0	1.0	1.0	1.0
SiC	277.8	3.6	317.1	46.3	248.6
GaN	1089.0	1.8	846.0	100.8	353.8
$\beta$ -Ga <sub>2</sub> O <sub>3</sub>	2844.4	0.2	3214.1	142.2	37.0

### 2.1. Lattice Structure and Polarization of GaN-Based Semiconductors

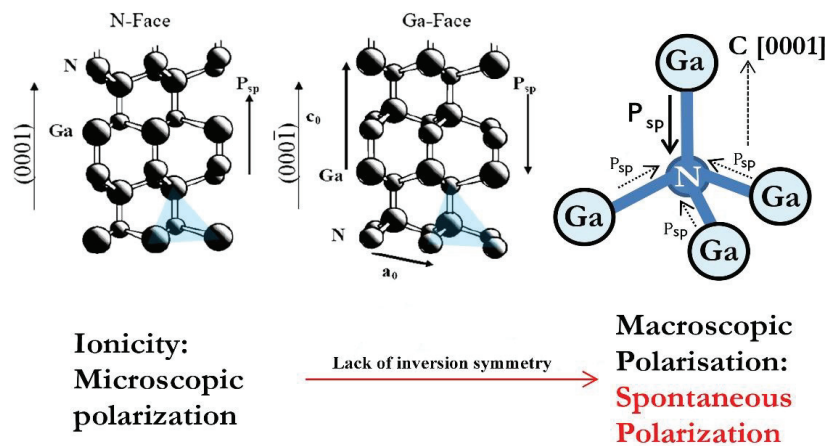
Wurtzite hexagonal close-packed (HCP) ( $\alpha$ -phase), rock-salt, and cubic zincblende ( $\beta$ -phase) are examples of III-N-based semiconductors, mainly GaN-based semiconductors [17,18]. Figure 10 depicts the wurtzite crystal structure, which is particularly important for electronics and optoelectronics applications today. The hexagonal unit cell of wurtzite comprises two intersecting hexagonal close packed (HCP) sub-lattices. As illustrated in Figure 10, it is defined by two lattice parameters, the height of the cell  $c_0$ , and the length of a side of the hexagonal base  $a_0$ , in an ideal ratio  $\frac{c_0}{a_0} = \sqrt{\frac{8}{3}} \approx 1.633$ . Each sub-lattice is made

up of one kind of atom. In relation to one another, the internal cell parameter  $u_0 = 3/8$  moves them along the c-axis. Table 2 presents the structural and polarization properties of III-Ns.

**Table 2.** Structural and polarization parameters of III-N wurtzite semiconductors [17].

Parameter	GaN	AlN	InN
$a_0(\text{Å}^\circ)$	3.197	3.108	3.580
$c_0/a_0$	1.6297	1.6033	1.6180
$\epsilon_1 = (u_0 - u_{\text{ideal}}) \times 10^{-3}$	1.9	6.4	3.7

These ideal values are absent in the typical nitride compounds GaN, InN, and AlN and their associated alloys. The  $c_0/a_0$  ratio deviates from the ideal lattice's 1.633 as the non-ideality of the lattice grows [19].



**Figure 10.** The alignment of  $P_{sp}$  and the tetrahedral bond structure of Ga-face and N-face heterostructures. Reproduced with permission [20]. Copyright 2019, Elsevier.

Because of the very high electronegativity of the N atom, which is 3.04 on Pauling's scale, and for Aluminum (1.61), Gallium (1.81), and Indium (1.78) atoms [19], consequently, the data for  $u_0$  and  $c_0/a_0$  deviate from the optimum values given earlier [21]. Group III-N semiconductors have a particularly high polarization due to the crystal structure's intrinsic electronic charge redistribution, which means a spontaneous polarization,  $P_{sp}$ , [19]. The directions  $\langle 0001 \rangle$  and  $\langle 000\bar{1} \rangle$  are not comparable due to a lack of inversion symmetry shown along its c-axis in the wurtzite structure. Hence, cation-face, i.e., Ga-face and anion-face, i.e., N-face, are the alternative polarities of GaN. The polarization field points change their position in the cation-face, i.e., Ga-face, surface towards the substrate. On the contrary, the polarization field points move in the opposite direction in the anion-face, i.e., N-face.

Because of the lack of this inversion symmetry, when the group III-N semiconductors' lattice is imposed by stress in the  $\langle 0001 \rangle$  direction, the ideal lattice values of the crystal structure's  $c_0$  and  $a_0$  will shift to adapt to the stress. As a result, the strength of the polarization would shift. In the strained group III-N crystals, this extra polarization is known as piezoelectric polarization,  $P_{pz}$  [22]. For instance, the in-plane constant of the lattice  $a_0$  would drop, and the vertical constant of the lattice  $c_0$  would rise if the crystal of the nitride is subjected towards a biaxial compressive stress. Due to the piezoelectric and spontaneous polarizations working in opposing directions, the ratio of  $c_0/a_0$  will climb to 1.633 of the perfect lattices, and the overall polarization strength will be reduced in the crystal. Moreover, when the tensile stress is imposed on the crystal, the spontaneous and

piezoelectric polarization work simultaneously. As a result, the total polarization will rise. The piezoelectric coefficients  $e_{33}$  and  $e_{13}$  are evaluated for the piezoelectric polarization,  $P_{pz}$  [23,24], as shown in Equation (6),

$$P_{pz} = e_{33}\varepsilon_3 + e_{13}(\varepsilon_1 + \varepsilon_2) \quad (6)$$

Here,  $a_0$  and  $c_0$  are the lattice parameter equilibrium values,  $\varepsilon_3 = (c - c_0)/c_0$  is the strain along the  $c$  axis, and  $\varepsilon_1 = \varepsilon_2 = (a - a_0)/a_0$  is the isotropic in-plane strain. The various strains in the lattice are connected in Equation (7). The elastic constants denoted by  $c_{13}$  and  $c_{33}$ . Combining Equations (1) and (2) provides the corresponding formula in Equation (8):

$$\varepsilon_3 = -2 \frac{c_{13}}{c_{33}} \varepsilon_1 \quad (7)$$

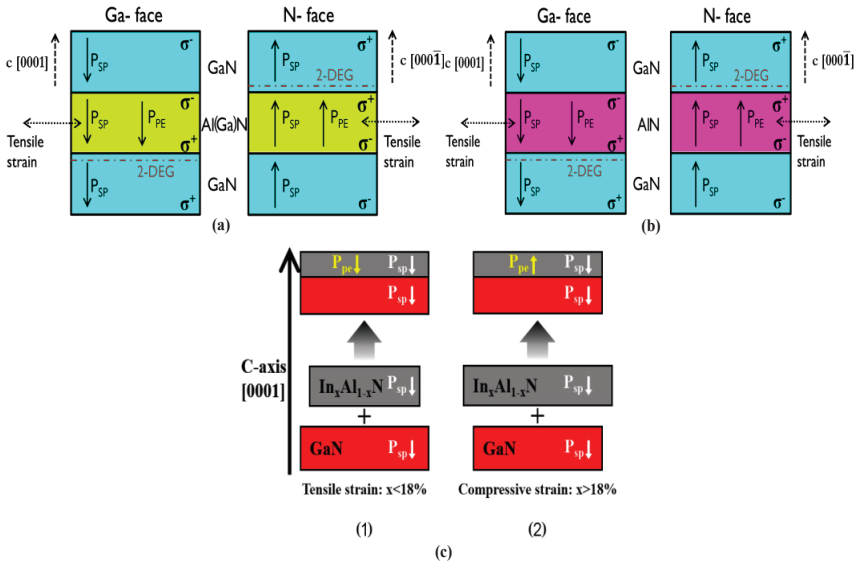
$$P_{pz} = 2 \frac{a - a_0}{a_0} \left[ e_{13} - e_{33} \frac{c_{13}}{c_{33}} \right] \quad (8)$$

The equation  $\left( e_{13} - e_{33} \frac{c_{13}}{c_{33}} \right)$  will be negative if  $e_{33}$ ,  $c_{13}$ , and  $c_{33}$  are positive, and the piezoelectric coefficient  $e_{13}$  is negative in wurtzite III-nitrides [25]. Thus, it is claimed that piezoelectric and spontaneous polarization are parallel under tensile stress layers, but they are anti-parallel under compressive stress layers. Polarization and gradients induce fixed sheet charges at the surfaces and interfaces of the AlGaIn/GaN heterostructures. As a result, there are high electric fields within the heterostructure. The electric field in nitrides may approach  $3 \times 10^6$  V/cm, which enhances the hole or electron formation at the AlGaIn/GaN contacts. This is called polarization-induced doping, which is the root of the two-dimensional electrons gas (2DEG) (discussed more in the below segment).

Figure 11a shows that growing a tiny epi AlGaIn layer on top of a thicker GaN layer generates an AlGaIn/GaN heterostructure. A 2DEG is generated at the interface between the AlGaIn barrier and the GaN channel because of the  $P_{sp}$  and  $P_{pz}$ , which may be a conduction channel consisting of exceptionally high mobility electrons even without any n-type doping, which is ideal for transistors. Both GaN and AlGaIn have a significant  $P_{sp}$ . When the material is strained, a  $P_{pz}$  component develops in GaN, AlN, or AlGaIn. The piezoelectric polarization arises in the thin layer of AlGaIn because it is beneath the tensile strain. In contrast, the layer of GaN is considerably thicker and nearly relaxed in an AlGaIn/GaN heterostructure.  $P_{sp}$  and  $P_{pz}$  are parallel when the AlGaIn layer is under a tensile strain (Figure 11a) [23]. So, to acquire the AlGaIn characteristics and determine the actual polarization-induced charge densities, we apply Equations (9) through to (14) [26].

Similarly, 2DEG is generated at the interface between the AlN barrier and the GaN channel for the reason of the  $P_{sp}$  and  $P_{pz}$ , as illustrated in Figure 11b. However, due to the large difference in the spontaneous and piezoelectric polarizations between the GaN and AlN layers, the 2DEG, which forms near the AlN/GaN interface, can reach over  $3 \times 10^{13} \text{ cm}^{-2}$  for an extremely thin AlN barrier layer thickness ( $d < 5 \text{ nm}$ ), along with a high mobility ( $>1000 \text{ cm}^2/\text{V}\cdot\text{s}$ ) and a very low sheet resistance ( $R_{sh} < 150 \text{ }\Omega/\square$ ) [27]. On the contrary, due to the high aluminum content and the associated degree of bond polarity, a spontaneous polarization in the  $\text{In}_{0.18}\text{Al}_{0.82}\text{N}/\text{GaN}$  heterostructures generates two-dimensional electrons gas (2DEG) densities which are competitive with AlGaIn/GaN structures without the need for a strain-induced piezoelectric component. For InAlN alloys, the strain state can go from tensile when the In % is lower than ~18%, to compressive when the In % is higher than ~18%, as shown in Figure 11c ((1), (2)), respectively; when the InAlN is the lattice matched to the GaN buffer, the In % is around 18%. Moreover, the implementation of the InAlN barriers with the In % around 18% allows for the strain to be controlled in the InAlN/GaN heterostructure, and a lattice-matched  $\text{In}_{0.18}\text{Al}_{0.82}\text{N}$  layer to the GaN sheet charge density is almost three times higher than for the conventionally grown  $\text{Al}_{0.25}\text{Ga}_{0.75}\text{N}$  barriers on the GaN channels [28].





**Figure 11.** Polarization charges in an (a) AlGaN/GaN, (b) AlN/GaN, and (c) InAlN/GaN heterostructure. Reproduced with permission [20]. Copyright 2019, Elsevier.

Spontaneous polarization can be observed in Equation (9). As an alternative, for a precise interpolation, a bowing parameter *b* might be utilized in Equation (10) [29]. The constants of the lattice for Al<sub>x</sub>Ga<sub>1-x</sub>N are in Equations (11) and (12) where *x* = Al mole fraction. The elastic constants are presented in Equations (13) and (14).

$$P_{sp}(x) = (-0.052x - 0.029) \frac{c}{m^2} \tag{9}$$

$$P_{sp}(x) = ((xP_{sp}(AlN) + (1 - x)P_{sp}(GaN) + bx(1 - x)) \tag{10}$$

$$a_0(x) = (-0.077x + 3.189) \times 10^{-10} \text{ m} \tag{11}$$

$$c_0(x) = (-0.203x + 5.189) \times 10^{-10} \text{ m} \tag{12}$$

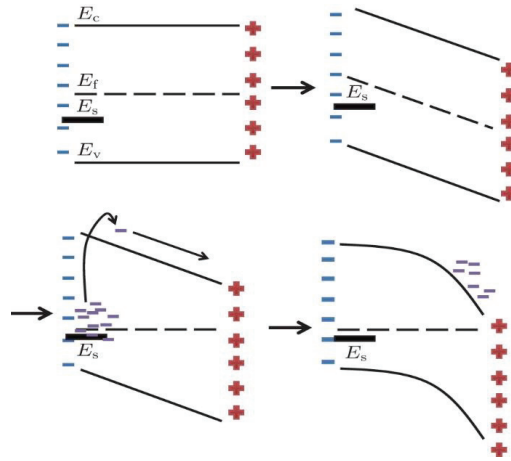
$$c_{13}(x) = (5x + 103) \text{ GPa} \tag{13}$$

$$c_{33}(x) = (-32x + 405) \text{ GPa} \tag{14}$$

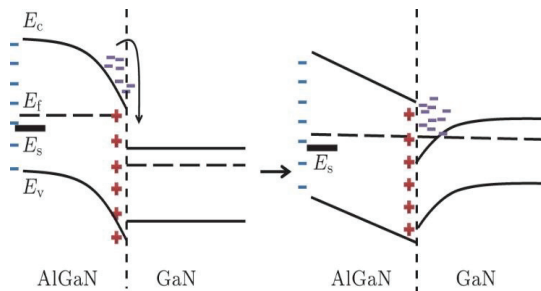
The above equations indicate that if the Al content in the AlGa<sub>x</sub>N layer rises, the overall polarization will soar. A polarization charge density (*ρ<sub>p</sub>*) corresponds to a polarization gradient (*P*) in space (*ρ<sub>p</sub>* = ∇*P*). Therefore, at the AlGa<sub>x</sub>N/GaN abrupt contact, a fixed polarization charge would be induced. In the case of AlGa<sub>x</sub>N/GaN, fixed positive induced polarization charges form at the interface. Even without n-type doping, the positive polarization-induced charges at the interface of AlGa<sub>x</sub>N/GaN attract the free electrons. Because of this, in the AlGa<sub>x</sub>N/GaN interface, 2DEG is generated. The carrier density of 2DEG may also be estimated analytically by using polarization [30].

The 2DEG creation is explained in a few Figures. Thus, in the undoped AlGa<sub>x</sub>N/GaN heterojunction, the 2DEG creation may be described on the AlGa<sub>x</sub>N surface by introducing donor states. An the isolated AlGa<sub>x</sub>N material energy band gap is depicted in Figure 12 with the presence of surface donor states. The isolated AlGa<sub>x</sub>N material is believed to be free of compressive/tensile forces. The Fermi level is attained if the density of the AlGa<sub>x</sub>N material is enough. So, the electrons are advanced to the conduction band and drawn to the other side by polarization-induced electric fields after the Fermi level exceeds the donor state-level *E<sub>s</sub>*. The Fermi level causes the dropping of the electrons into the GaN side

when the AlGaN and GaN materials come into contact. The 2DEG results from a buildup of electrons at the interface, as displayed in Figure 13. Thus, combined with the ionized surface donor, it produces an electric field that points between the interface and the surface in the AlGaN layer to minimize the polarization field [31].



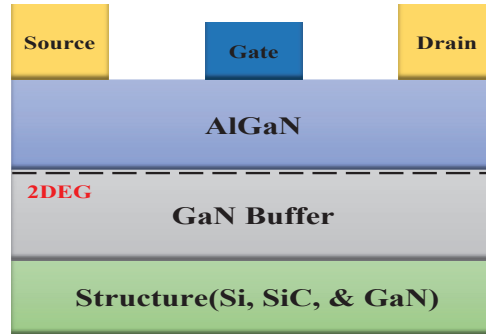
**Figure 12.** An undoped AlGaN material with  $E_5$  surface donor states has an energy band. Electrons are advanced into the conduction band and gravitate toward the electric field created by positive polarization. Reproduced with permission from Chin. Phys. B. [31].



**Figure 13.** In the 2DEG quantum well, the buildup of electrons is shown in the energy band of an undoped AlGaN/GaN heterojunction. Reproduced with permission from Chin. Phys. B. [31].

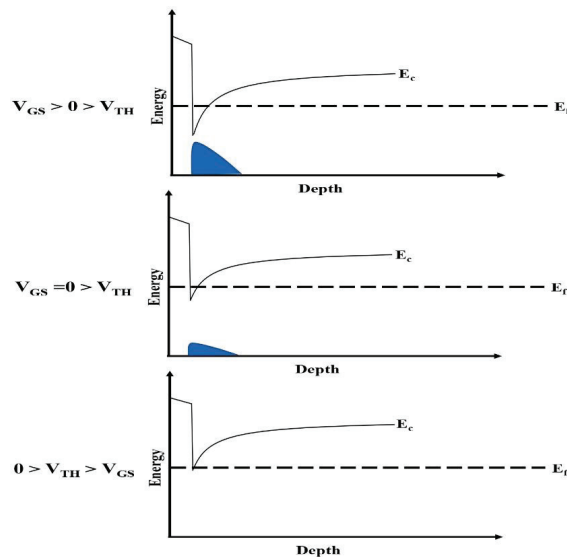
As noted previously, the creation of 2DEG occurs naturally at the interface when a tiny strained AlGaN layer is developed on top of a thicker relaxed GaN layer. Due to the confinement of high mobility electrons, this 2DEG exhibits very conductivity in the quantum well. Because of the reduced surface scattering, the electron mobility rises between the unstrained GaN and 2DEG areas at roughly  $1000 \text{ cm}^2/\text{V}\cdot\text{s}$  and  $1500\text{--}2000 \text{ cm}^2/\text{V}\cdot\text{s}$ , respectively. For HEMTs, a transistor channel with a higher mobility and electron concentration seems appropriate. Figure 14 depicts a basic AlGaN/GaN HEMT design. The substrates are mostly SiC, silicon, sapphire, or GaN, and a buffer layer is formed to relieve the strain induced by a foreign substrate's lattice mismatch. The 2DEG creates a native channel between the source and drain of the device. In most early AlGaN/GaN transistors, a Schottky gate electrode is formed by the deposition of Ni/Au or Pt metal on top of the AlGaN layer [32]. The GaN HEMT, with the 2DEG present at the interface of the AlGaN/GaN, was first shown in early 1993 [33]. The channel is regulated by supplying a gate voltage ( $V_{GS}$ ) and, therefore, a vertical electrical field to deplete or augment the

channel, making it less conductive in the off-state or more conductive in the on-state. Later, researchers from all over the globe have progressively reported high-performance GaN HEMTs for high-power and RF applications [34,35].



**Figure 14.** AlGaIn/GaN HEMT layout and 2DEG generated in AlGaIn/GaN contact are shown by the dashed line.

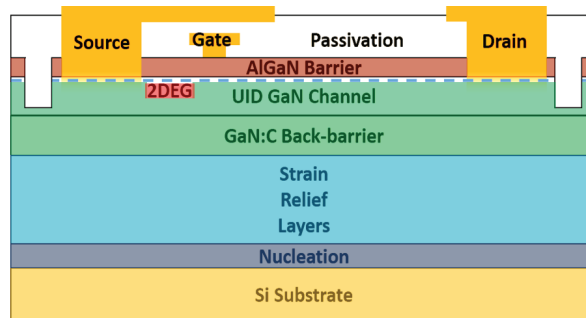
As said previously, when no bias voltage is applied from the gate to the source at the AlGaIn/GaN interface, i.e.,  $V_{GS} = 0$  V, the 2DEG channel exists. This kind of HEMT is known as a normally-on HEMT or a depletion-mode (D-mode) HEMT. It signifies that a current may freely flow between the source and the drain. It also indicates that the AlGaIn/GaN HEMT's threshold voltage ( $V_{TH}$ ) is less than 0 V, requiring a  $V_{GS}$  to deplete the 2DEG and switch off the HEMT, as shown in Figure 15. Meanwhile, this feature is also one of the primary problems for the state-of-the-art AlGaIn/GaN HEMTs utilized in higher current and power applications [36]. It has several practical limitations, including a high consumption, possible electrical safety risk, intrinsic fail-safe functioning, and complex circuit layout [32,36]. As a result, a normally-off operation, or an enhance-mode (E-mode) HEMT, is needed due to a high and positive threshold voltage ( $V_{TH}$ ).



**Figure 15.** The band diagrams for the three locations of the 2DEGs  $V_{GS} > 0 > V_{TH}$ ,  $V_{GS} = 0 > V_{TH}$  and  $0 > V_{TH} > V_{GS}$ .

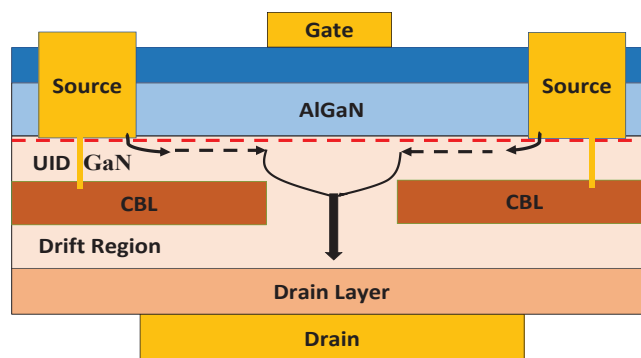
## 2.2. Lateral and Vertical GaN Power Transistors

Power transistors based on GaN are considered for two types of design: lateral and vertical structures. The lateral structure of the GaN HEMT is illustrated in Figure 16, where 2DEG formed at the AlGaN/GaN heterostructure interface. A high electron mobility ( $2000 \text{ cm}^2/\text{Vs}$ ) and electron velocity ( $1.3 \times 10^7 \text{ cm/s}$  saturation velocity and  $2.5 \times 10^7 \text{ cm/s}$  peak velocity) characterize the AlGaN/GaN structure. Furthermore, due to a significant spontaneous and piezoelectric polarization, the GaN HEMT structure exhibits a density of sheet carriers over  $1 \times 10^{13} \text{ cm}^{-2}$  in III-nitride materials. GaN HEMTs have a low on-resistance because of the device's carrier density and high electron mobility. This structure is discussed deeply in the normally-off GaN HEMT section.



**Figure 16.** Typical lateral AlGaN/GaN HEMT structure. Reproduce from IOP science under the terms of the Creative Commons Attribution 3.0 license [36].

Similarly, the vertical layout is beneficial for obtaining a high breakdown voltage and low on-resistance characteristics, as displayed in the current aperture vertical electron transistor (CAVET) in Figure 17 [36]. Here, the drain at the bottom, the gate, and the source are on the top of the structure. The gate controls the current via an aperture among the current blocking layers (CBLs) into the drain, where vast amounts of material flow, which is commonly produced by an isolation implantation or P-type doping of the GaN layer. The AlGaN/GaN layer's horizontal high mobility electron channel is combined with a thick GaN drift region to obtain a low  $R_{ON}$  and a high breakdown voltage. Compared to the lateral designs, vertical devices into the bulk material of the device maintain the blocking voltage in the vertical direction, resulting in a lower chip area for a particular operation current.

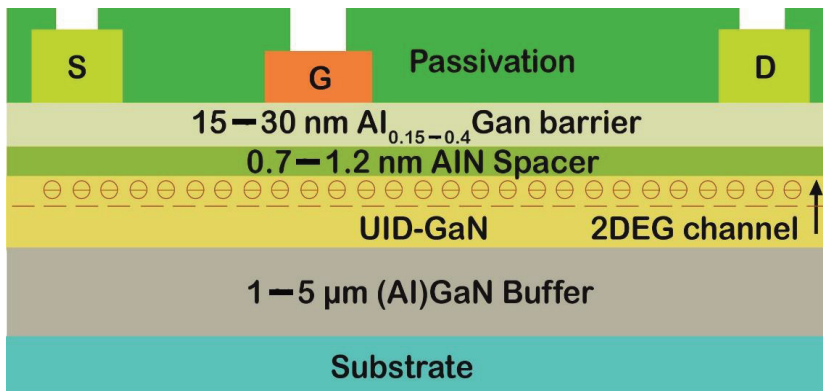


**Figure 17.** Vertical CAVET AlGaN/GaN HEMT structure. Reproduce from IOP science under the terms of the Creative Commons Attribution 3.0 license [36].

### 3. Normally on and off GaN HEMT Power Device Structure

#### 3.1. GaN HEMT Technology (Normally on)

When the AlGaIn/GaN HEMT structure is normally on, it is known as the depletion-mode (D-mode) structure. Figure 18 illustrates one of the examples of it. Where the buffer layer (1–5  $\mu\text{m}$ ) is deposited on the substrate for compensating the lattice mismatch stress, after that, to form a heterojunction, the GaN (UID) layer, AlN layer (0.7–1.2 nm), and  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  barrier (15–30 nm) layer is deposited. The thickness and Al molar fraction  $x$  of the  $\text{Al}_x\text{Ga}_{1-x}\text{N}$  (usually 0.15 to 0.4) varies to maintain the number of acceptable electric charges under the relaxation's critical thickness [37]. The heterojunction's energy bands are bent downward to produce a quantum well with a sharp, where electrons of a high intensity are confined at the interface of AlGaIn/GaN due to a bandgap offset and the polarization impact of AlGaIn/GaN [38]. Then, the 2DEG channel generates the high-density current from the Ohmic-contact source to the drain [39]. Consequently, a Schottky gate is needed for the pinching off the 2DEG channel, which is normally on. When sufficient negative voltages are applied to the device gate, the height of the Schottky barrier increases, allowing for the conduction band to pass through the AlGaIn barrier's gate region; thereby, the HEMT is turned off. Eventually, for the device surface protection, passivating layers (often  $\text{SiO}_2$  or  $\text{SiN}_x$ ) are required [40–42].



**Figure 18.** Device layout for a GaN HEMT structure that is normally on.

#### 3.2. GaN HEMT Technology (Normally off)

In the field of power conversion, a negative bias is required to turn off the devices, which is the major issue for the normally-on devices. On the contrary, a normally off operation is widely wanted for safety reasons. Consequently, academia and industry (e.g., Gan Systems, Infineon, Panasonic, STMicroelectronics, and On Semiconductors) are working to create and market dependable normally-off HEMTs [43]. Thus, the threshold voltage  $V_{\text{TH}}$  in AlGaIn/GaN HEMT is determined by numerous variables relating to the heterojunction and gate metal characteristics, shown in Equation (15) [44]:

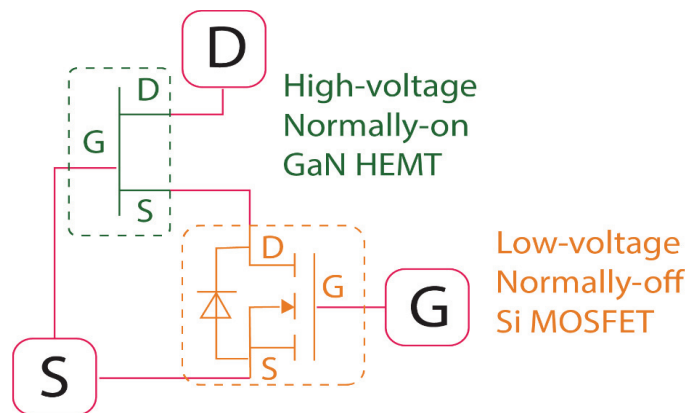
$$V_{\text{TH}}(x) = \varphi_B(x) - \Delta E_C(x) - \frac{\sigma(x)}{\epsilon_0 \epsilon_{\text{AlGaIn}}(x)} t - \frac{qN_D}{2\epsilon_0 \epsilon_{\text{AlGaIn}}(x)} (t)^2 \quad (15)$$

where between the gate metal and the AlGaIn barrier layer,  $\varphi_B(x)$  denotes the Schottky barrier height,  $\sigma(x)$  denotes the polarization charge at the interface of the AlGaIn/GaN,  $\Delta E_C(x)$  denotes the conduction band discontinuity at the interface of the AlGaIn/GaN,  $\epsilon_{\text{AlGaIn}}(x)$  denotes the AlGaIn layer permittivity,  $\epsilon_0$  denotes the permittivity vacuum,  $t$  denotes the AlGaIn thickness,  $N_D$  denotes the doping,  $q$  denotes the electric charge, and  $x$  denotes the Al content in the barrier layer. As  $x$  increases at a zero bias, more significant polarization discrepancies between the AlGaIn and GaN and thicker AlGaIn barriers result

in a more negative  $V_{TH}$ . Hence, it is clear from the equation that the AlGaIn barrier layer or modifying Schottky barrier height relies on the thickness and Al content to tune the  $V_{TH}$ . Therefore, various approaches have been suggested for obtaining the normally-off GaN HEMTs: the (a) cascode configuration, (b) fluorine implantation and thin/ultrathin-barrier, (c) p-GaN Gate, and (d) recessed gate.

### 3.2.1. HEMTs with Cascode Configuration (Normally off)

Figure 19 reflects a cascode setup of high-voltage normally-on GaN HEMTs and low-voltage normally-off Si MOSFETs [45,46]. When the  $V_{TH}$  of a Si MOSFET less than the positive gate-to-drain voltage is applied to the system, the GaN HEMT's gate-source voltage is 0 V; as a result, the opening of a GaN HEMT is normally on. By contrast, deactivating the Si MOSFET results in the GaN HEMT having a significant negative gate to source voltage, thus, the 2DEG channel is pinching off. Evidently, the cascode setup generates a positive  $V_{TH}$  for regulating the GaN HEMT switch that is normally on. Additionally, normally-off GaN HEMTs with the cascode design are commercially available at 600 V [43,45]. However, the parasitic effects of the packing and the high-temperature stability of the Si MOSFETs remain significant disadvantages [47,48]. If the GaN HEMT has a relatively high on-resistance compared to the Si MOSFET, the "cascode" configuration performs well at that time. In fact, since the on-resistance increases with the rated breakdown voltage, the "cascode" approach is advantageous when the normally on GaN HEMT is one of a high-voltage, and the Si MOSFET is low-voltage [49]. As an illustration, the Si MOSFET will provide just a 3% on-resistance to a 600 V GaN HEMT "cascode". On the contrary, for a lower targeted breakdown, the on-resistance of the GaN HEMT decreases; thus, the Si MOSFETs contribution becomes significant. Hence, the "cascode" approach is practically advantageous for applications above 200 V [49].

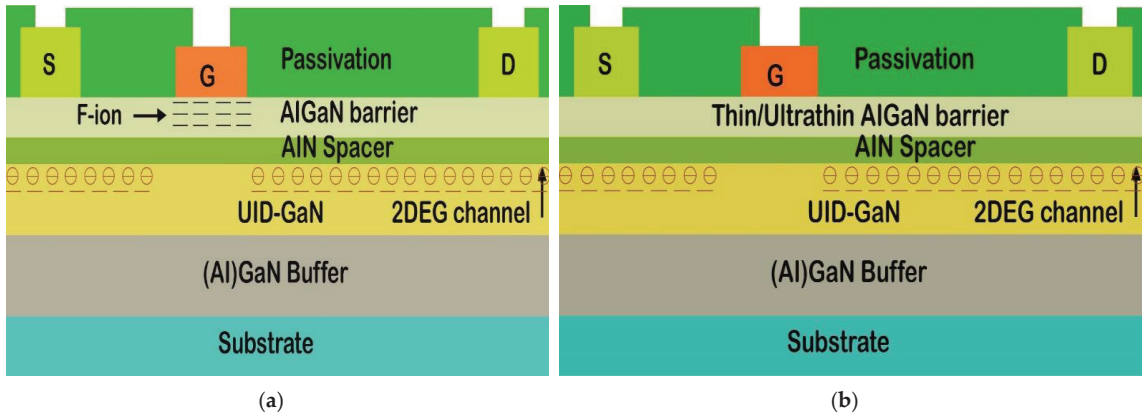


**Figure 19.** Normally-off HEMTs with cascode configuration structure.

### 3.2.2. HEMTs with Fluorine Implantation and Thin/Ultrathin Barrier (Normally off)

Figure 20a shows an alternative method of performing the normally-off operation to avoid the dry etching, which could cause damage to the device operation. Due to their considerable electron-negativity, fluorine given by the ion implantation and in the AlGaIn layers may easily boost the AlGaIn barrier electron potential and empty the 2DEG channel [50]. Likewise, by adjusting the height of the AlGaIn conduction band, the 2DEG can be depleted by a GaN HEMT design with a thin/ultrathin barrier [51,52], as displayed in Figure 20b. When the AlGaIn barrier thickness falls below a critical value, the  $V_{TH}$  shifts to a negative bias in the recessed-gate configuration. However, in various application issues, like for fluorine gates, the injection method must be repeatable, and for thin barrier HEMT designs, the output current is low, restricting these two devices [51,53].

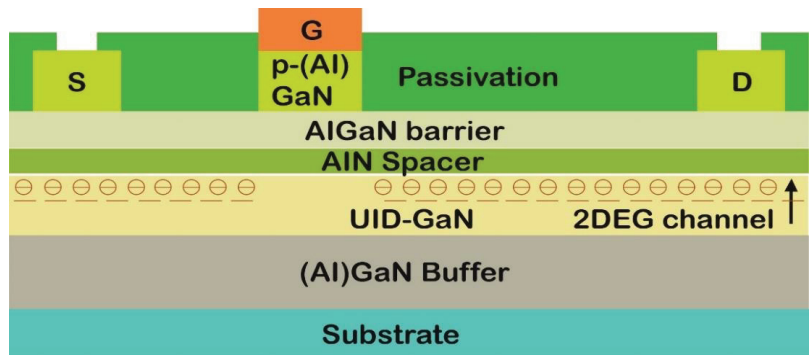




**Figure 20.** (a) Normally-off HEMTs with fluorine implantation structure.; (b) normally-off HEMTs with thin/ultrathin-barrier structure.

### 3.2.3. HEMTs with p-GaN Gate (Normally off)

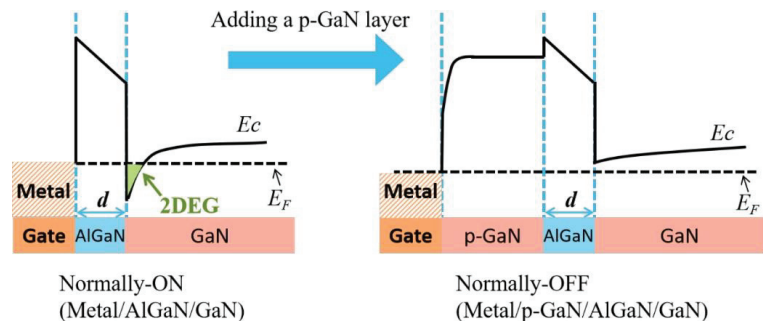
A p-GaN (or p-AlGaIn) layer is applied to the AlGaIn/GaN heterostructure at the gate region. As illustrated in Figure 21, it is probably the most promising technique to accomplish a normally-off operation [54–56]. In fact, it is presently the only commercially available normally-off GaN HEMT technology. GaN HEMTs of this sort have received much attention from the scientific community and the industry. The p-GaN gate HEMTs working principle is generally represented in Figure 22. The AlGaIn conduction band is elevated by the p-GaN cap layer on the AlGaIn, resulting in 2DEG depletion. Hence, it is possible to obtain the device's normally-off mode [57]. Earlier, Uemoto et al. [55] proposed a GaN HEMT with a p-AlGaIn gate that is normally off, with a  $V_{TH}$  of 1.0 V and a  $BV_{DSS}$  of 800 V.



**Figure 21.** Normally-off HEMTs with p- GaN (or p-AlGaIn) layout.

The characteristics of the AlGaIn/GaN heterostructure should be specified appropriately to enable an effective depletion of the 2DEG and a high  $V_{TH}$  ( $V_{TH} > 0$ ) [48–60]. The layer thickness of the AlGaIn barrier is usually between 10 and 15 nm, whereas the content of Al is between 15 and 25%. For the effective depletion of 2DEG, a high amount of doping in the p-GaN layer ( $>10^{18} \text{ cm}^{-3}$ ) is frequently needed [61]. In this regard, increasing the Mg electrical activation is one of the most critical factors in improving the threshold voltage  $V_{TH}$  of the p-GaN layer for a specific Mg concentration. Adequate growth parameters for the p-GaN layer and annealing conditions may achieve the latter goal [62,63]. On the

contrary, because of the high energy of ionization (in the range from 150 to 200 m eV) of Mg as a p-type dopant, i.e., an acceptor, obtaining a high activation of Mg in p-GaN is problematic [64,65]. In most cases, an acceptor concentration of  $2\text{--}5 \times 10^{19} \text{ cm}^{-3}$  is employed, roughly two orders of magnitude more than the concentration of holes. A greater Mg concentration in p-GaN might cause the layer's crystalline quality to deteriorate, reducing the electrically active acceptors [66,67]. As a result, in the p-GaN gate HEMTs, getting a high  $V_{\text{TH}}$  is difficult. Earlier, a Pd-based Ohmic gate was implemented on the cap layer of p-AlGaIn, which improved the device's hole injection and current capabilities. Therefore, the transistor was also known as a "gate injection transistor" (GIT) [55]. The GaN-GIT structure was modified to a hybrid drain-embedded GIT (HD-GIT) by Kaneko et al. [68]. The Panasonic group contains a p-doped GaN area adjacent to the ohmic drain. The injected holes discharge the trapped electrons near the drain edge in the off-state from the p-GaN layer, which helps prevent the current collapse. Compared to the standard GIT structure, this new modification boosts the breakdown voltage to 850 V with a slight increase in the device's leakage current and the on-resistance of  $2.6 \text{ m}\Omega\text{-cm}^2$ .



**Figure 22.** Metal/AlGaIn/GaN energy band diagram with and without a p-GaN gate under equilibrium. Reproduced with permission [57]. Copyright 2017, Elsevier.

In contrast, the metal/p-GaN/AlGaIn/GaN system TCAD simulations indicate that on the p-GaN, a Schottky metal gate must have a higher  $V_{\text{TH}}$  and less leakage than an Ohmic gate [55,63,64]. In the on-state, Meneghini et al. [60] demonstrated that a Schottky gate based on WSiN to the p-GaN rather than a typical Ni/Au Ohmic contact could improve the gate voltage swing of a transistor and lower the gate leakage current by roughly four orders of magnitude. Generally, the continuous power consumption of GaN HEMTs is due to the gate leakage and heat generation in the gate driver. The lack of a considerable gate side current injection due to the significant Schottky barrier is thus essential for HEMTs with a p-GaN gate for a decreased power consumption. Because of this, on the p-GaN, the Schottky gate is preferable over the Ohmic gate solution nowadays. Furthermore, several data from the literature are shown in Table 3, where some metals have been used in the Schottky gate contact to the p-GaN. Subsequently, because of its thermal and chemical durability and processing compatibility, adopting a TiN gate is now a good choice [69]. Eventually, several device and reliability difficulties still need to be investigated further, such as the low  $V_{\text{TH}}$ , high gate leakage currents, the poor gate BV, and the influence of fabrication techniques on the device's performance [57,70].

Table 3. Survey of literature data on different Schottky Contact.

Matel Gate	Doping $n_{dop}$ and p-GaN Thickness T	$V_{TH}$ (V)	$R_{ON}$ ( $\Omega$ -mm)	Ref
Ti (40 nm)/Au (100 nm)	$n_{dop} = 4 \times 10^{19} \text{ cm}^{-3}$ , T = 100 nm	1.82	11.9	[71]
Ti (25 nm)/Au (120 nm)	$n_{dop} = 1 \times 10^{18} \text{ cm}^{-3}$ , T = 70 nm	3	13.9	[72]
Ni/Au	$n_{dop} = 3.5 \times 10^{18} \text{ cm}^{-3}$ , T = 50 nm	1.5	8	[73]
Ti (50 nm)/Au (150 nm)	N/A, T = 70 nm	1.2	N/A	[74]
Ni (20 nm)/Au (200 nm)	$n_{dop} = 5 \times 10^{19} \text{ cm}^{-3}$ , T = 100 nm	1.5	N/A	[75]
Ni (25 nm)/Au (200 nm)	$n_{dop} = 1 \times 10^{18} \text{ cm}^{-3}$ , T = 60 nm	1.7–2.1	5.65 & 5.05	[76]
Ni/Au	$n_{dop} = 3 \times 10^{19} \text{ cm}^{-3}$ , T = 85 nm	1.5	29.5	[77]
Ni (25 nm)/Au (120 nm)	N/A, T = 100 nm	1.5	20	[78]
Ni/Au	$n_{dop} = 4 \times 10^{19} \text{ cm}^{-3}$ , T = 70 nm	1.02	15.4	[79]
Ni (15 nm)/Au (280 nm)	$n_{dop} = 4 \times 10^{19} \text{ cm}^{-3}$ , T = 70 nm	2.2	43.6	[80]
Ti/Au	$n_{dop} = 4 \times 10^{19} \text{ cm}^{-3}$ , T = 85 nm	2.1	21	[81]
TiN	$n_{dop} = 3 \times 10^{19} \text{ cm}^{-3}$ , T = 80 nm	1.6	17.8	[82]
W	$n_{dop} = 1 \times 10^{19} \text{ cm}^{-3}$ , T = 75 nm	2.1	49	[83]
TiN	N/A, T = 60 nm	2.1	15	[62]
Pd	$n_{dop} = 3 \times 10^{19} \text{ cm}^{-3}$ , T = 100 nm	1.7	8.5	[84]
Mo (100 nm)/Ni (20 nm)	$n_{dop} = 3 \times 10^{19} \text{ cm}^{-3}$ , T = 80 nm	1.08	10.7	[85]
W	$n_{dop} = 1 \times 10^{19} \text{ cm}^{-3}$ , T = 75 nm	1.6	26.5	[86]
Ti (25 nm)/Au (120 nm)	N/A, T = 75 nm	3.2 & 1.8	16	[87]
Ti (45 nm)/Au (200 nm)	$n_{dop} = 2 \times 10^{18} \text{ cm}^{-3}$ & $2 \times 10^{19} \text{ cm}^{-3}$ , T = 50 nm	1.30 & 1.45	9.66 & 9.51	[88]
Ti/Au/Ni	$n_{dop} = 4 \times 10^{17} \text{ cm}^{-3}$ , T = 50 nm	1.5	N/A	[89]

### 3.2.4. HEMTs with Recessed Gate (Normally off)

This method reduces the layer thickness of the AlGaN barrier under the gate via a plasma etching, which is the last option offered for achieving an HEMT (normally off) [90]. Because the leakage current of the gate is caused by a tunneling phenomenon that is very sensitive to the barrier layer thickness and uniformity, this approach necessitates a perfect control of the AlGaN etching process. Furthermore, etching-induced damage might increase the leakage current of the gate and non-uniformity effects in  $V_{TH}$  [91]. Additionally, there are two types of gates recessed available such as the slight MIS-HEMT of the recessed-gate design underneath the gate dielectric, a thin AlGaN barrier, and the complete MIS-FET of the recessed-gate design, known as a MOS-HFET hybrid, as shown in Figure 23a,b [92,93].

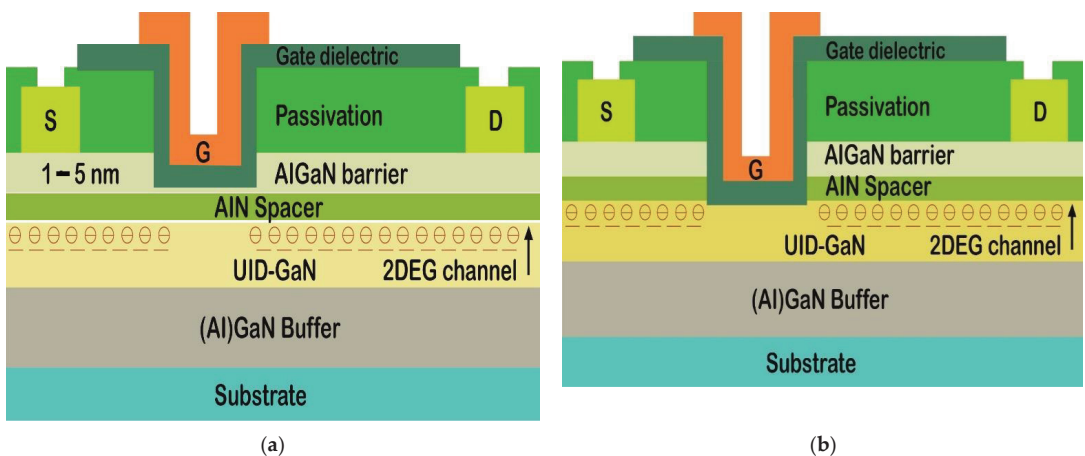


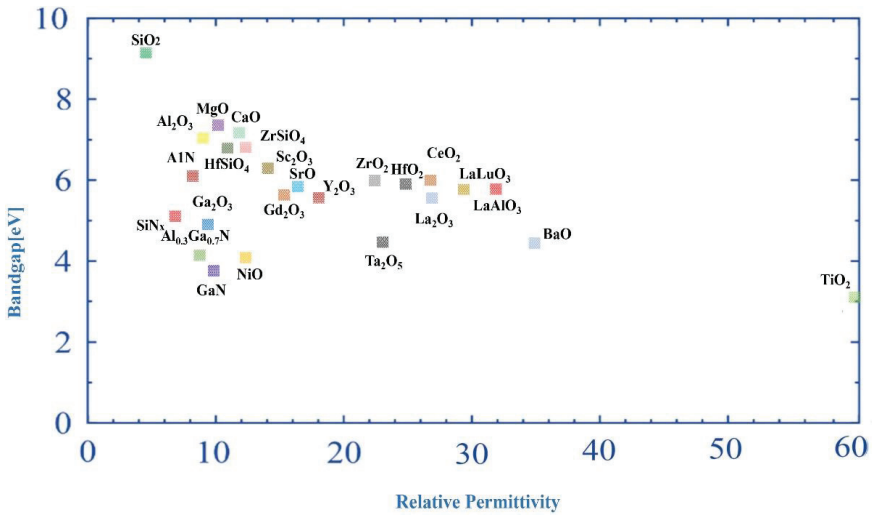
Figure 23. (a) Normally-off HEMTs with slight MIS-HEMT of recessed-gate design; (b) normally-off HEMTs with complete MIS-FET of recessed-gate design.

Standard MIS-FETs may obtain an E-mode performance by entirely eliminating the AlGa<sub>N</sub> barrier layer underneath the gate, resulting in the device turning off at a zero gate voltage. Whenever the positive voltage of the gate exceeds  $V_{TH}$ , an accumulation layer of an electron forms at the interface of the gates, which operates the devices' conductive channel and is switched on. It has benefited from a high threshold voltage ( $V_{TH}$ ) but suffers from a decrease in the channel mobility ( $\mu_{FE}$ ) due to rough surfaces in the recessed region and electrically active faults in the MIS structure. In addition, a poor channel mobility will raise the device on-resistance ( $R_{ON}$ ) and system power consumption. Therefore, a slight MIS-HEMT of the recessed-gate has been offered to improve the device's channel mobility ( $\mu_{FE}$ ) and decline its on-resistance ( $R_{ON}$ ), where the thin layer of the AlGa<sub>N</sub> barrier will hinder the 2DEG channel from the MIS interface. As a result, the channel mobility ( $\mu_{FE}$ ) increased and reduced the on-resistance ( $R_{ON}$ ) [94]. Thus, the channel mobility ( $\mu_{FE}$ ) was defined as Equation (16):

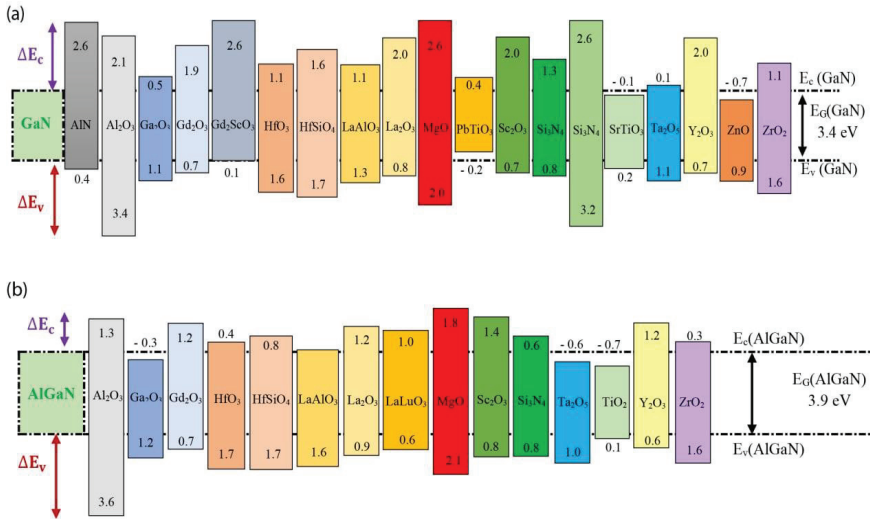
$$\mu_{FE} = \frac{L_g}{WC_{ox}V_{DS}} \left( \frac{\partial I_{DS}}{\partial V_{GS}} \right) \quad (16)$$

Here,  $L_g$  and  $W$  donate the channel length and width, while  $C_{ox}$  donates the gate insulator capacitance per unit area. Moreover, Fiorenza et al. [95] have evaluated in MISHEMTs of the recessed gate the field-effect mobility by using gate insulator SiO<sub>2</sub> with several variables (the roughness of the surface, the temperature, the field of electric, the quality of the dielectric, and so on). This study demonstrated in the insulator/GaN system the necessity of reducing the interface state density to enhance the field effect's mobility and decrease the precise on-resistance. Eventually, these two recessed gates improved the threshold voltage, device performance, channel mobility, the reliability of the device, and overcame the gate leakage issue [96–98]. Additionally, the gate dielectric for the gate recessed depends on several characteristics, such as the permittivity, the (Al) GaN band offset, the bandgap, and the insulator chemical stability [38,94,95]. Especially for power-switching devices, a wide bandgap material is also significant. The (Al) GaN band offsets are required to reduce the gate leakage currents appropriately, even while operating the forward gate bias. On the contrary, a high permittivity value is advantageous for obtaining high transconductances [43]. In the case of MIS-HEMTs, the capacitive contribution of the gate dielectric is minimized by a high permittivity dielectric, facilitating a stronger connection between the 2DEG channel and the gate and therefore maintaining high transconductances, which is especially important for RF devices. In addition, compared to Schottky gate HEMTs, the high permittivity materials may limit the changing of the values of the threshold voltage from positive to negative of normally-on MIS-HEMTs, which helps lower the static power usage and improve the performance and the energy efficiency of the device [99].

In GaN-based insulated-gate transistors, Figure 24 demonstrates the bandgap-permittivity connection for nitride compounds and the insulators for different gate dielectrics [38,95,96]. Figure 25a illustrates that Robertson et al. [100] calculated the insulators on the GaN band offsets; they were the first to forecast the band alignment of the GaN and the insulators using charge neutrality levels (ECNL) calculations. Figure 25b shows the dielectrics on the Al<sub>0.3</sub>Ga<sub>0.7</sub>N band offsets recently obtained by Reddy et al. [101] using the same approach. As a gate dielectric, SiO<sub>2</sub> on AlGa<sub>N</sub>/GaN MIS-HEMTs was first implemented by Khan et al. [102] and they noticed that it enhances the gate voltage swing capabilities and controls the leakage currents in the gates for its attractive characteristic-like large band offset to (Al)Ga<sub>N</sub>, the chemical stability, and the large bandgap.



**Figure 24.** For primary insulators and GaN compounds, the energy bandgap (eV) vs. permittivity is shown. Reprinted with permission [42]. Copyright 2017, the author(s). Published by Elsevier.



**Figure 25.** Various dielectric materials regarding (a) GaN [100] and (b)  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}$  [101] have different valence and conduction band offsets ( $\Delta E_V$  and  $\Delta E_C$ ).

In contrast, for MIS gate designs utilizing dielectrics such as  $\text{Ga}_2\text{O}_3$ ,  $\text{SiN}_x$ , because of its small conduction band offsets, resulted in large gate leakage currents [103–105]. Likewise, the minor AlN and (Al)GaN lattice mismatch has been shown in a few investigations, whereby it is appropriate for the gate insulator and passivation layer [106,107]. Moreover, numerous high-permittivity dielectrics have been used in the MIS gate architectures of GaN HEMTs [108], including  $\text{HfO}_2$ ,  $\text{ZrO}_2$ ,  $\text{Ta}_2\text{O}_5$ ,  $\text{La}_2\text{O}_3$ ,  $\text{CeO}_2$ , and  $\text{TiO}_2$  [109–111]. Thus, Table 4 represents the data gathered from the literature study of normally-off HEMTs with a recessed gate where several types of gate insulators ( $\text{SiN}$ ,  $\text{SiO}_2$ ,  $\text{Al}_2\text{O}_3$ , and processing (PECVD, LPCVD)) are shown.

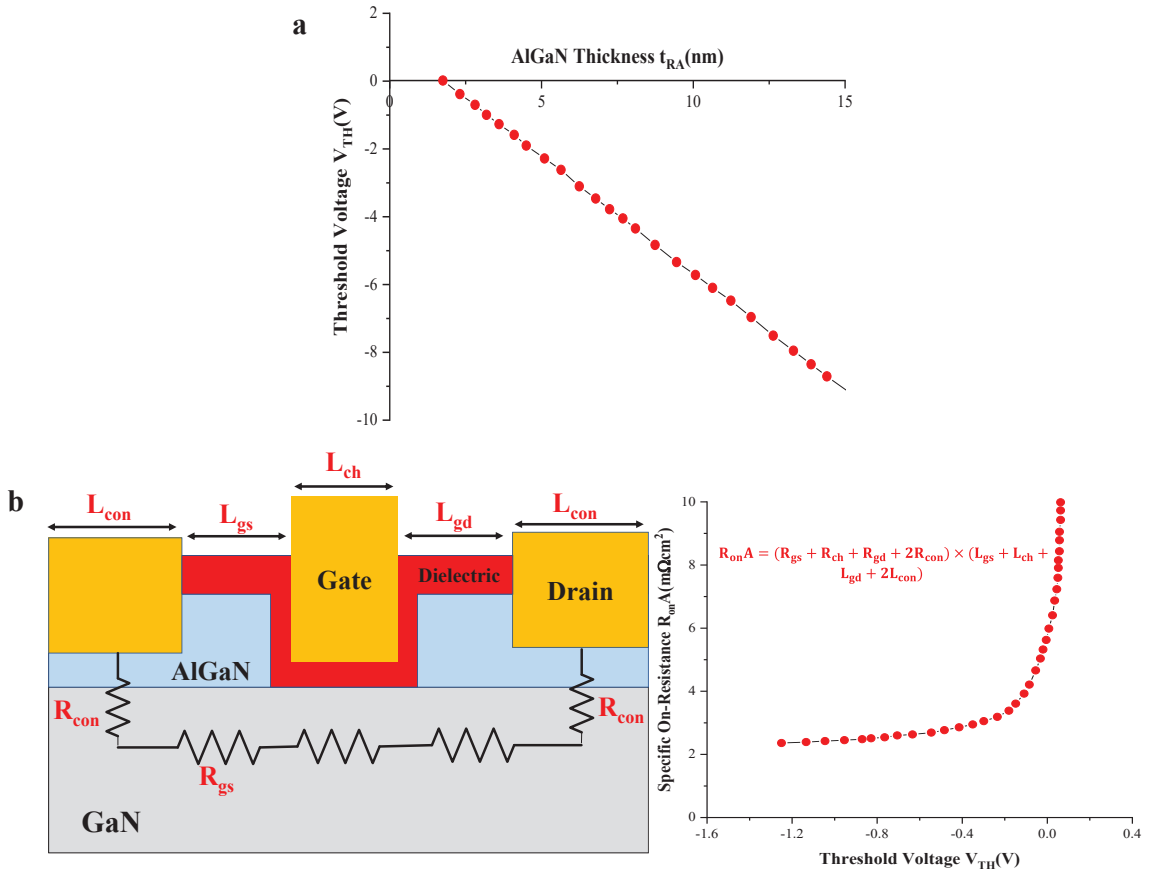
**Table 4.** Survey literature data on difference types of gate insulators and processes.

Gate Insulator	Insulator Processing	$\mu_{FE}$ ( $\text{cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$ )	$V_{TH}$ (V)	$R_{ON}$ ( $\Omega \cdot \text{mm}$ )	On/off Ratio	$C_m$ (mS/mm)	Ref
SiN <sub>(30 nm)</sub> / SiO <sub>2</sub> (3 nm)	SiO <sub>2</sub> ALD + post annealing at 890 °C in N <sub>2</sub> + SiN LPCVD at 665 °C	116	2.4	15.9 $\Omega \cdot \text{mm}$ at $V_{GS} = 12 \text{ V}$	$6 \times 10^8$	52	[112]
SiN <sub>(100 nm and 300 nm)</sub> / ZrO <sub>2</sub> (23 nm)	SiN PECVD + ZrO <sub>2</sub> ALD at 200 °C	850	2.19	9.2 $\Omega \cdot \text{mm}$ at $V_{GS} = 8 \text{ V}$	$\sim 10^9$	135	[113]
	PECVD + post annealing at 850 °C in N <sub>2</sub>	110	0.7	N/A	N/A	N/A	[95]
Al <sub>2</sub> O <sub>3</sub> (25 nm)	ALD + TMA and ozone	N/A	5	12.9 $\Omega \cdot \text{mm}$ at $V_{GS} = 19.7 \text{ V}$	N/A	44	[114]
HfO <sub>2</sub> (13 nm)	ALD+ ozone	1482	3.1	6.0 $\Omega \cdot \text{mm}$ at $V_{GS} = 8 \text{ V}$	$10^5$	N/A	[115]
Al <sub>2</sub> O <sub>3</sub> (15 nm)	ALD+ ozone	1991	2.6	5.5 $\Omega \cdot \text{mm}$ at $V_{GS} = 8 \text{ V}$	$10^5$	N/A	[115]
SiN (2 nm)/ SiN (15 nm)	LT-PECVD at 850 °C + HT-LPCVD at 780 °C	160	2.37	13.2 $\Omega \cdot \text{mm}$ at $V_{GS} = 15 \text{ V}$	N/A	17	[116]
SiN (15 nm)	HT-LPCVD at 780 °C	38	1.28	20 $\Omega \cdot \text{mm}$ at $V_{GS} = 15 \text{ V}$	N/A	2	[116]
TiO <sub>2</sub> (3.4 nm)	Thermal oxidation	1270	4.2	N/A	$2.3 \times 10^8$	N/A	[110]
Al <sub>2</sub> O <sub>3</sub> (25 nm)	ALD + post annealing at 830 °C in N <sub>2</sub>	2033	2.5	6.8 $\Omega \cdot \text{mm}$ at $V_{GS} = 12 \text{ V}$	$10^8$	92	[117]
	LPCVD on photo-electrochemical recess	49	0.8	26 $\Omega \cdot \text{mm}$ at $V_{GS} = 15 \text{ V}$	N/A	2	[118]
SiN (15 nm)	SiN LPCVD at 780 °C	141	1.3	12 $\Omega \cdot \text{mm}$ at $V_{GS} = 15 \text{ V}$	N/A	13	[118]
SiN (30 nm)/ AlN (5 nm)	AlN PEALD + SiN LPCVD	198.80	6.28	11.62 $\Omega \cdot \text{mm}$ at $V_{GS} = 15 \text{ V}$	$10^8$	85.75	[119]
HfO <sub>2</sub> (20 nm)	ALD + post annealing at 600 °C in N <sub>2</sub>	N/A	2.5	3.8 $\Omega \cdot \text{mm}$ at $V_{GS} = 6.5 \text{ V}$	$2.1 \times 10^9$	81.38	[120]
Al <sub>2</sub> O <sub>3</sub> (30 nm)	ALD + post annealing at 850 °C in N <sub>2</sub>	1602	2.6	10.2 $\Omega \cdot \text{mm}$ at $V_{GS} = 10 \text{ V}$	N/A	58	[121]
AlN (7 nm)/ SiN (7 nm)	MOCVD	180	1.2	N/A	$(5-6) \times 10^8$	60	[122]
Al <sub>2</sub> O <sub>3</sub> (4 nm)	ALD + post annealing at 900 °C in O <sub>2</sub>	1450	1.55	7.1 $\Omega \cdot \text{mm}$ at $V_{GS} = 12 \text{ V}$	N/A	54	[123]
SiNx (20 nm)/ SiON (10 nm)	SiON PECVD at 350 °C in SiH <sub>4</sub> , NH <sub>3</sub> , N <sub>2</sub> O, and N <sub>2</sub> atmospheres + SiNx LPCVD at 780 °C with an ammonia flow of 280 sccm, a SiH <sub>2</sub> Cl <sub>2</sub> flow of 70 sccm.	1793	0.81	31.2 $\Omega \cdot \text{mm}$ at $V_{GS} = 12 \text{ V}$	N/A	N/A	[124]
Al <sub>2</sub> O <sub>3</sub> (18 nm)	ALD + post annealing at 400 °C in N <sub>2</sub>	65	7.6	19.5 $\Omega \cdot \text{mm}$ at $V_{GS} = 14 \text{ V}$	N/A	N/A	[125]
Al <sub>2</sub> O <sub>3</sub> (30 nm)	ALD + post annealing at 850 °C in N <sub>2</sub>	1670	0.53	24.4 $\Omega \cdot \text{mm}$ at $V_{GS} = 10 \text{ V}$	$\sim 10^8$	42	[126]
Al <sub>2</sub> O <sub>3</sub> (5 nm)/ SiN (7 nm)	SiN LPCVD at 780 °C	122	1.7	12.9 $\Omega \cdot \text{mm}$ at $V_{GS} = 18 \text{ V}$	$\sim 10^8$	53	[127]
NiO <sub>x</sub> (100 nm)	Sputtering	N/A	0.45	9.42 $\Omega \cdot \text{mm}$ at $V_{GS} = 4 \text{ V}$	$10^8$	$\sim 75$	[128]
SiO <sub>2</sub> (20 nm)	ALD + post annealing at 780 °C	1700	1.56	7.4 $\Omega \cdot \text{mm}$ at $V_{GS} = 6 \text{ V}$	$10^{10}$	190	[129]
Al <sub>2</sub> O <sub>3</sub> (20 nm)	ALD + post annealing at 900 °C in N <sub>2</sub>	245	5	N/A at $V_{GS} = 12 \text{ V}$	$10^{10}$	19	[130]
Si <sub>3</sub> N <sub>4</sub> (10 nm)/TiO <sub>2</sub> (20 nm)	SiN PECVD + TiO <sub>2</sub> ALD	1200	1.81	43.81 $\Omega \cdot \text{mm}$ at $V_{GS} = 10 \text{ V}$	N/A	112	[131]

Subsequently, the AlGaIn thickness is another important factor for the threshold voltage ( $V_{TH}$ ). Medjdoub et al. [132] had shown the relation between the AlGaIn thickness with a threshold voltage. From Figure 26a, notice that if the AlGaIn thickness ( $t_{RA}$ ) reduces, the  $V_{TH}$  increases. Similarly, other authors, Saito et al. [133], presented the relationship between the  $V_{TH}$  and the specific on-resistance ( $R_{ONA}$ ) by calculating the equation, as displayed in Figure 26b. On the contrary, the on-resistance ( $R_{ON}$ ) will be increased if the 2DEG mobility is decreased. Thus, from Figure 26b, the equation for calculating the specific on-resistance ( $R_{ON}$ ) is denoted by Equation (17),

$$R_{ON}A = \left( R_{gs} + R_{ch} + R_{gd} + 2R_{con} \right) \times \left( L_{gs} + L_{ch} + L_{gd} + 2L_{con} \right) \quad (17)$$





**Figure 26.** (a) The AlGaN layer thickness and gate threshold voltage relation. (b) In the recessed-gate GaN HEMT, the calculation of specific on-resistance and the relation between the threshold voltage and the specific on-resistance. Reprinted under the open access policy from Bentham Open [132].

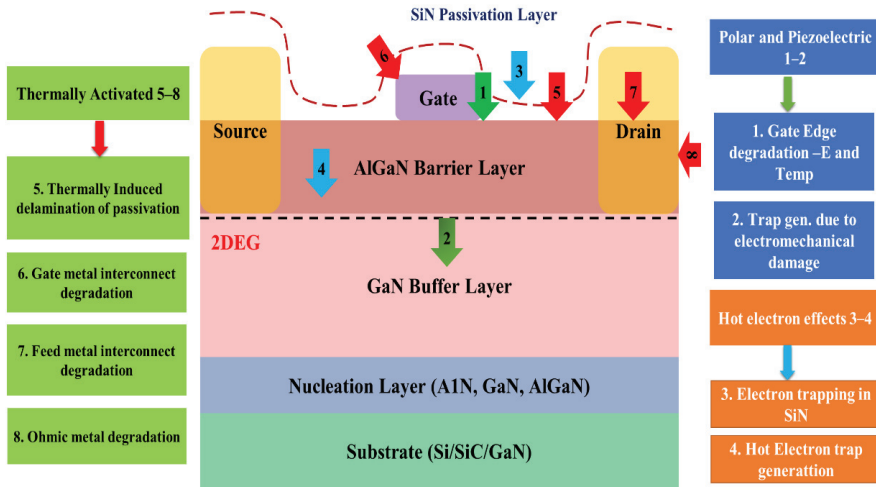
Additionally, the field plate has used a device structure to reduce the current collapse. For GaN-based devices, current collapse is a well-known phenomenon that results in a trade-off between the breakdown voltage and the on-resistance by inserting the source-gate field plate; the electric field at the gate-drain edge is redistributed [134–136], as shown in Figure 16. The current collapse is discussed in the below segment.

#### 4. Reliability of GaN HEMTs

##### 4.1. Degradation Creation

While GaN HEMTs have improved remarkably, several material-related challenges must be resolved before they are revealed as a reliable and sustainable technology. Al-GaN/GaN HEMTs' actual device performance has not yet reached the theoretically predicted levels. Even on unaged GaN HEMTs, parasitic effects could be noticed that degrade the performance metrics but do not significantly impact the reliability. Nevertheless, over time or under aging stresses, the degradation processes that accelerate with time impair not only the electrical response but also the device's resilience and dependability, resulting in shorter lifetimes and failure. The GaN industry's principal aim is to improve the dependability of its products while also reducing the parasitic effects. Further degradation

difficulties with GaN devices include thermal mismatches, heteroepitaxy, and polarization effects with the substrate, all of which are inherent to the material. Compared to other conventional technologies, AlGaN/GaN HEMTs can work at an extremely high bias, electric fields, and temperatures. Figure 27 demonstrates the various types of degradation affecting AlGaN/GaN HEMTs [137,138].



**Figure 27.** Several degrading problems affect AlGaN/GaN HEMTs with their origin. Reprinted with permission [138]. Copyright 2010, Cambridge University Press, and the European Microwave Association.

It is important to note that five to eight issues are associated with thermally induced degradation processes that have already been reported in other semiconductor systems (SiC, GaAs, Si, etc.). As a result, these failure mechanisms are simpler to explain and exclusive to the metallization scheme which has been adopted. Both three and four mechanisms are connected to the introduction of the hot electrons; it is a usual problem that field-effect transistors of a high voltage face. Other semiconductor devices have been proven to suffer from a deterioration, caused by hot electrons (Si, GaAs, InP, etc.). On the other hand, because of this semiconductor material's piezoelectric and polar properties, one to two issues are specific for GaN devices; consequently, those processes have not been fully defined or investigated. As a result, the GaN HEMT reliability analysis is a unique issue that needs to be devoted, as well as an in-depth physics-based study. Furthermore, high Schottky-gate leakage currents are also one of the main issues for degrading the device performance and reliability. Thus, the reduction in  $BV_{GD}$  raises the noise figure (NF) and decreases the power-added efficiency (PAE) due to the high gate leakage current [139]. In addition, there are numerous mechanisms of gate leakages, including the emission of a thermionic field [140], the emission of thermionic [141], the dislocation-assisted tunnelling [142], the trap assisted tunnelling [143], the Fowler–Nordheim tunnelling [144], the defect hopping [145], the space charged limited current [146], and the Frenkel–Poole emission [147].

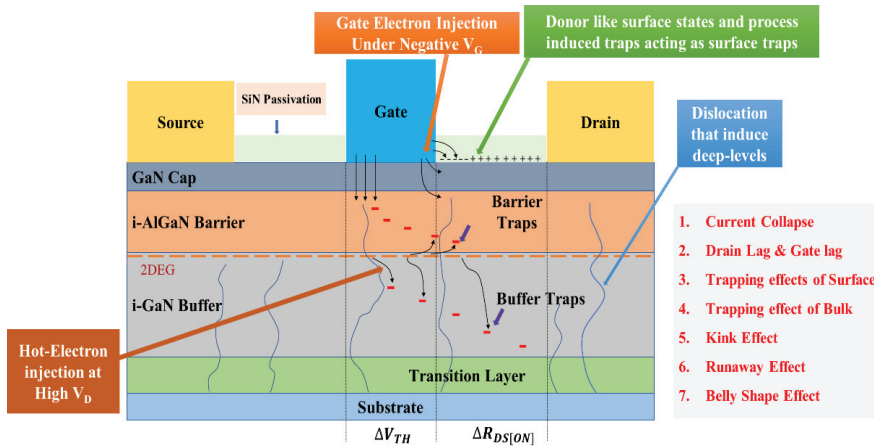
#### 4.2. Reliability Issues

These days, researchers focus on enhancing the AlGaN/GaN HEMTs reliability device because of the trapping effect during the AlGaN/GaN HEMT operation. One of the major obstacles causing performance degradation is the trapping effects in AlGaN/GaN HEMTs during operation, causing current dispersion between DC to RF or otherwise, DC to pulsed  $I_D - V_D$  characteristics. Trapping effects like the frequency dispersion of transconductance,

the sensitivity of the light, the drain lag and gate lag transients, and the limited microwave power output have all been detected [148].

As shown in Figure 28, there are various trapping mechanisms usually seen in AlGaIn/GaN HEMTs, such as:

- Under a high negative VGS, barrier traps and a gate electron are injected onto the surface;
- Under a high on-state VDS, the barrier/buffer traps are injected using hot electrons;
- During material growth, the electrons captured by the deep layers are induced.



**Figure 28.** The AlGaIn/GaN heterostructure is shown schematically, with several trapping methods and their effects on device performance. Reprinted with permission [149]. Under the terms of the Creative Commons Attribution 4.0 license.

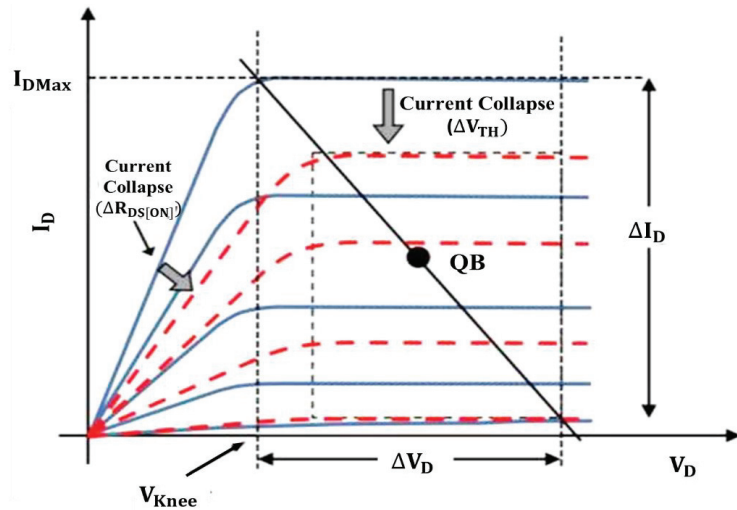
#### 4.2.1. Current Collapse

In order to maintain the charge neutrality, trapping electrons reduces in the 2DEG channel the density of the sheet carriers, resulting in a decreased current density in the drain. This decrease in the drain current is referred to as the “current collapse”. M. A. Khan et al. [150] released the first article on AlGaIn/GaN HFETs current collapse in 1994. The “drain-lag” and “gate-lag” conditions of the quiescent bias (Q-bias) are the main parameters used to characterize the current collapse phenomena [148]. In Figure 29, the characteristics curve of  $I_D-V_D$  demonstrates the current collapse’s effect on the output power of HEMT. The solid and dotted lines indicate the device’s  $I_D-V_D$  characteristics curve before and after the current collapse phenomena. The current collapse causes the knee voltage ( $V_{knee}$ ) to grow as the maximum current decreases ( $I_{Dmax}$ ). It reduces the maximum output power ( $P_{max}$ ) that may be achieved, which is provided by the given equation:

$$P_{max} = \frac{(\Delta V_D \times \Delta I_D)}{8} \quad (18)$$

The dissimilarity between the  $V_{knee}$  and the breakdown voltage ( $BV_{GD}$ ) equals the highest possible voltage swing ( $\Delta V_D$ ).  $I_{Dmax}$  specifies the maximum current swing.  $P_{max}$  is depicted in Figure 29 by the shaded region, and the current collapse phenomena have narrowed this operating window. Thus, the main reason for the current collapse is caused by the reduction in positive charges of polarization induced from the heterojunction transistor surface, followed by the loss of an equivalent number of electrons in the 2DEG [151].  $\Delta R_{DS[ON]}$  characterizes the current collapse, as illustrated in Figure 29, because the electrons are trapped in the gate-drain access area by the surface, buffer, or barrier traps. Similarly,

under the gate are the areas of electron trapping (see Figure 28), resulting in a threshold voltage shift ( $\Delta V_{TH}$ ), which characterizes a current collapse; therefore, the pulsing  $I_D$ - $V_D$  characteristics are caused by a drop in the drain current in the device's saturation zone, as seen in Figure 29.

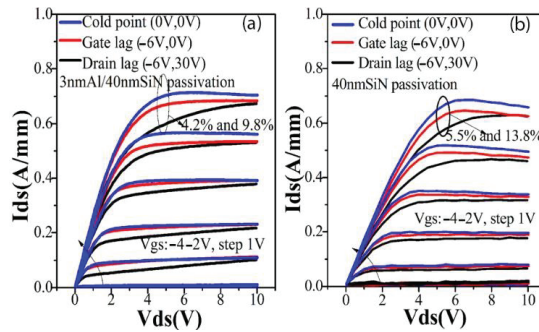


**Figure 29.** The  $I_D$ - $V_D$  characteristics curve of HEMT before (solid lines) and after (graded lines) current collapse is shown in this diagram. Reprinted with permission [152]. Copyright 2003, the American Vacuum Society.

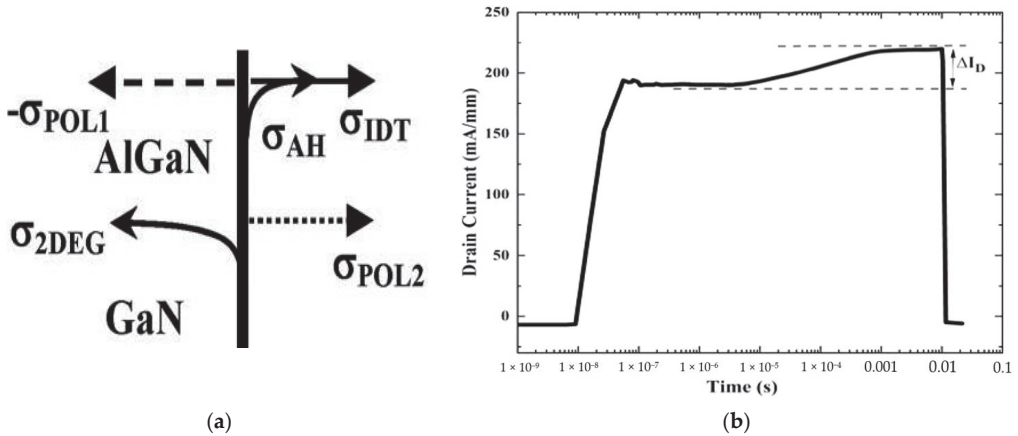
#### 4.2.2. Drain and Gate Lag

The gate lag refers to the drain current's transient response to the gate voltage, and a drain lag is the transient response of the drain current to the drain voltage, which remains constant when the drain or gate voltage matches. According to Figure 30, Zhang et al. [153] investigated the magnitudes of collapse between the saturation and the knee voltages for the various quiescent biases. Hence, the collapse considerably reduces the performance near the knee voltage. From curve (a), when  $V_{DS} = 4.5$  V, the collapse percentage was 4.2 and 9.8, respectively, with the Al/SiN passivation layer. On the contrary, the collapse rate increased by a 5.5 and 13.8 percentage, with the SiN passivation layer at the  $V_{DS} = 5$  V, approximately, on the curve (b).

However, the effects of acceptor- and donor-like traps on the HEMT device were analyzed by Tirado et al. [154] The accumulating hole near the surface counteracts the acceptor-like traps, and the device is insensitive to the acceptor-like traps. Therefore, the surface donor-like traps are the primary cause of the gate lag [155]. Figure 31a presents that in addition to the dipole charge owing to polarization-induced charges, the charge due to 2DEG, the charge due to the donor-like trap ionization, and the charge due to the holes accumulating close to the AlGaN surface, the filling and emptying of the donor-like traps in the surface can impact the density of the 2DEG. When a new device is strained, the electrons that directly tunnel through the Schottky gate contact can occupy the donor-like traps and turn them neutral [156]. The 2DEG density is dropped with the reducing donor-like traps due to the charge neutrality criteria, which causes an initial fall in the current in Figure 31b [154], where the drain current instantly rises as the on-state remains stable for a while. After that, until saturation, its soars again. At the final stage, the drain current change is referred to as the delay of the current, known as a gate lag.

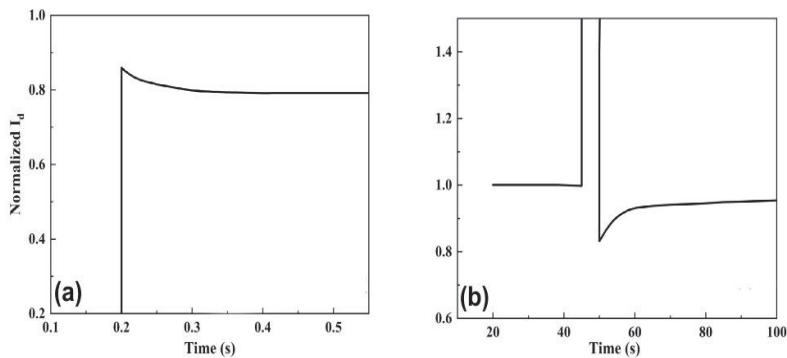


**Figure 30.** The gate lag and drain lag of (a) Al/SiN passivated and (b) SiN passivated AlGaIn/GaN HEMT devices were measured at different passivation layers. Reproduced with permission [153]. Copyright 2019, the author (s), published by AIP Publishing.



**Figure 31.** (a) Diagram of an HEMT device’s space charge element. The two-dimensional electron gas is referred to as  $\sigma_{2DEG}$ , the dipole charge induced by polarization is denoted by  $\pm \sigma_{POL1,2}$ , Ionized donor-like traps are referred to as  $\sigma_{IDT}$ , and  $\sigma_{AH}$  symbolizes the accumulation of holes near the AlGaIn surface. (b) AlGaIn/GaN HEMT gate lag phenomenon’s transient waveform of the drain current. Reproduced with permission from IOP Publishing [154].

When measured at the turn-on pulsing mode, the observed drain current tends to reduce with time, as shown in Figure 32a. When evaluated at the turn-off pulsing mode, Figure 32b indicates a decline in the drain current when the voltage at the drain returns to 0 V. These two varieties of the drain current curves are frequently referred to as the drain lag [157]. Due to the trapping of the electron in the channel, this current reduction occurred. Some electrons might tunnel through the AlGaIn barrier while the device is in the on-state and trapped by deep-level traps. Eventually, to overcome these issues, the passivation layer and field plate had to be used on the device, as presented in Figure 16.



**Figure 32.** For AlGaIn/GaN HEMTs, the transient waveform of the drain current from the drain lag phenomena. (a) turn-on pulsing mode (b) turn-off pulsing mode. Reproduced with permission [157]. Copyright 2009, the author (s), published by AIP Publishing.

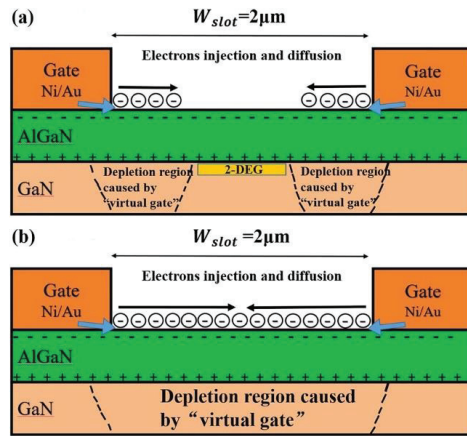
The gate lag measurements compare the prompt and steady-state  $I_D$  at a constant low field drain voltage (avoid self-heating contributions) while the gate bias is modulated from a quiescent point, usually below the pinch-off voltage  $\sim V_G = -6$  V, to an open channel condition such as  $V_G = 0$  V. At the pinch-off, a high amount of channel electrons are trapped in bulk or surface states, which do not immediately feed back into the channel instantaneously when the gate turns on. With the large-signal recovery time of constants up to the order of seconds, the responsible traps must have a significantly large activation energy and/or be fed by a “slow” conducting mechanism (like hopping) to explain the long time constants. The surface states are believed to dominate in the gate lag since the passivation significantly improves the current response.

For the drain lag measurements, the gate voltage is kept constant at around 0 V, while the drain voltage is shifted from a low equilibrium value of  $\sim 10$ – $100$  mV to a higher value of 15–30 V. The buffer traps are reported to be dominant here since the devices with higher buffer layer conductivities display lower drain lag ratios. High-drain biases inject electrons into the buffer, where they stay trapped. The passivation has a minimal effect, and the hot electrons can contribute significantly. The recovery time is often in minutes, and the reduction in the knee voltages and  $I_{D,max}$  is amplified. The threshold shifts associated with the current collapse are also accounted for with the drain lag effect.

#### 4.2.3. Trapping Effects of Surface

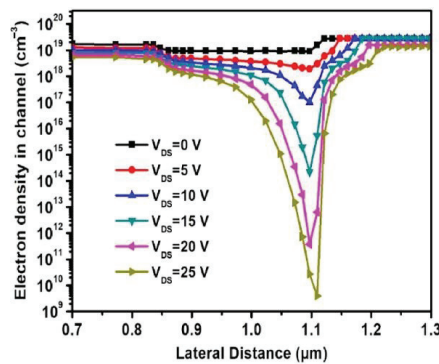
In GaN HEMTs, the effects of surface trapping are commonly used to describe electron trapping on the AlGaIn barrier surface. R. Vetry et al. [158] utilized the “virtual gate” idea to describe the current dispersion because of surface trapping on the ungated surface between the drain and gate contacts under negative  $V_{GS}$  and a positive drain bias. Thus, Figure 33a illustrates that, at first, due to the presence of a momentous initial drain current, the 2DEG channel must remain in the slot region; from the bilateral metal gates to the AlGaIn surface in the slot area, the electrons are injected and captured by the surface states when the off-state gate voltage is applied. Afterwards, from both the bilateral gate edges to the middle of the slot region, the negative trapped surface charges steadily deplete the 2DEG conduction channel, which, acting as a “virtual gate” on both sides, converges at the middle of the slot region, and the entire 2DEG channel in the slot region becomes wholly depleted. Eventually, it has gradually become a complete “virtual gate”, as presented in Figure 33b [159].





**Figure 33.** The device layout illustrates (a) electron injection in the slot region and the virtual gate in both areas. (b) the devices become fully virtual gates. Reproduced with permission [159]. Copyright 2019, the author (s), Published by AIP Publishing.

The impact of the virtual gate on the sheet carrier density is observed in Figure 34 [160], where the increased drain voltage at the gate edge of the drain side causes a linear reduction in the sheet carrier density. For this reason, electrons accumulate at the drain side's gate edge. Consequently, this accumulation of electrons not only influences the channel but also extends towards the lateral axis of the device, for instance, extending the depletion from 1.1  $\mu\text{m}$  to 1.2  $\mu\text{m}$  for the drain voltage from 0 V to 25 V.

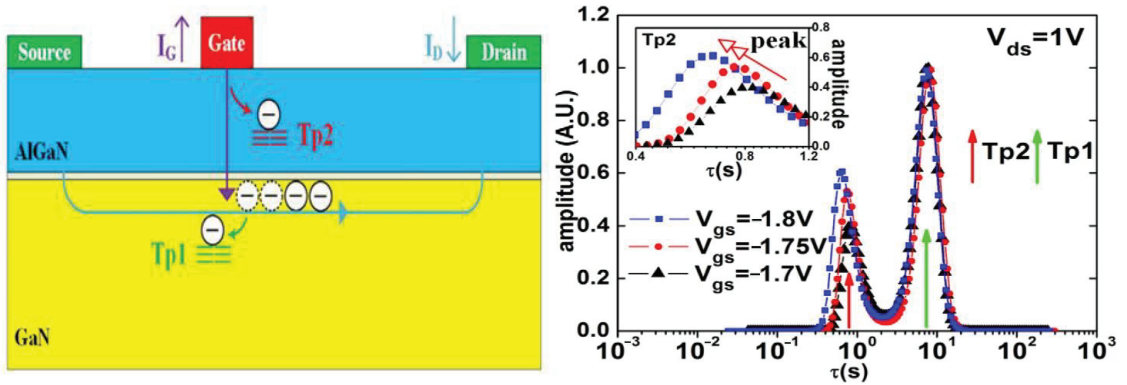


**Figure 34.** AlGaN/GaN HEMT sheet carrier density along the channel for different drain voltage. Reproduced with permission [160]. Copyright 2021, Elsevier.

#### 4.2.4. Trapping Effect of Bulk

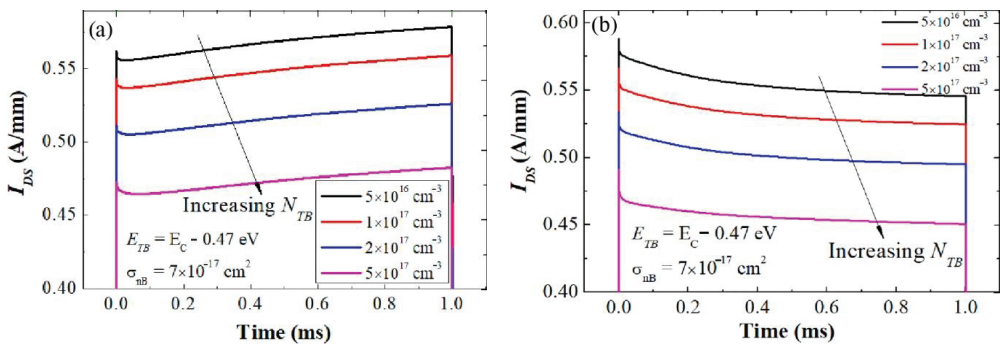
Bulk traps are traps of electrons which are found in the GaN buffer, AlGaN barrier, or other parts of the device heterostructure, as shown in Figure 27. J. Joh et al. [161] also reported that the injection of an electron into the bulk traps from the gate induced the bulk trapping effect to occur. Thus, X. Zheng et al. [162] illustrated that varying the  $V_{GS}$  has bulk trapping effects on the AlGaN barrier traps (TP2) and the GaN channel layer traps (TP1), presented in Figure 35. However, from the gate current ( $I_G$ ), TP2 can capture more electrons if the  $V_{GS}$  increases the negative bias voltage. TP2s electron trapping reduces the channel carrier concentration, which lowers the drain current. Additionally, the trapping process of TP2 is speeded up by a higher negative bias voltage of  $V_{GS}$ , which decreases the

action time of TP2. Meanwhile, TP1 is insensitive to the change in  $V_{GS}$ , causing little effect on TP1. Eventually, it is observed that the  $V_{GS}$  effect on TP1 is less than on TP2.



**Figure 35.** Trapping process of TP1 and TP2 with various values of  $V_{GS}$ . Reproduced with permission [162]. Copyright 2016, Elsevier.

P.V. Raja et al. [163] analyzed the buffer trapping effects on the AlGaIn/GaN HEMT device. For the gate lag transient, the  $V_{GS}$  pulsed from  $-3\text{ V}$  to  $0\text{ V}$  (from the off- to on-state) with a fixed  $V_{DS} = 10\text{ V}$ . The gate lag transient is simulated by changing the density of the buffer trap,  $N_{TB}$  (from  $5 \times 10^{16}$  to  $5 \times 10^{17}\text{ cm}^{-3}$ ), with a fixed electron trap at  $E_{TB} = E_C - 0.47\text{ eV}$  and an electron capture cross-section  $\sigma_{nB} = 7 \times 10^{-17}\text{ cm}^2$ . As a result, by increasing the  $N_{TB}$ , the signal magnitude of the gate transient is reduced, but variations of the transient are unchanged, as presented in Figure 36a. On the contrary, the  $V_{GS}$  remains at  $0\text{ V}$ , and the  $V_{DS}$  is switched from  $2\text{ V}$  to  $10\text{ V}$  in the drain lag transient. The parameters of  $N_{TB}$  and  $\sigma_{nB}$  remain the same on the buffer trapping. Consequently, reducing the magnitude of  $I_{DS}$  does not affect the current dispersion behavior, as displayed in Figure 36b.

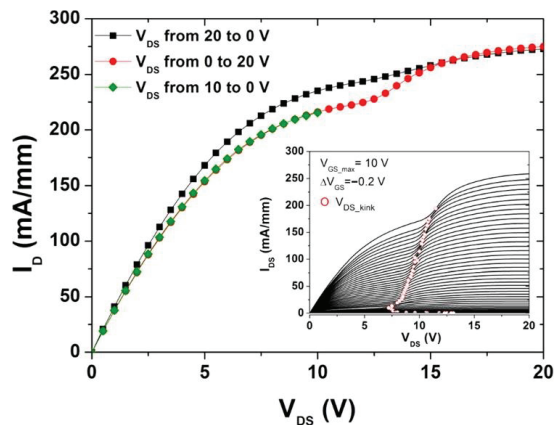


**Figure 36.** By varying buffer trap density, transient response of (a) gate lag and (b) drain lag are observed. Reproduced with permission [163]. Copyright 2021, Elsevier.

#### 4.2.5. Kink Effect

The kink effect refers to the output I–V characteristics of an undesirable change phenomenon caused by changes in the conductivity of the drain [164]. This is determined by the working point of the device, as well as the temperature, voltage, and current. As is evident in Figure 37, lengthy integration durations while comparing the output characteristics were achieved with a downward and upward  $V_{DS}$  pumping. When the  $V_{DS}$

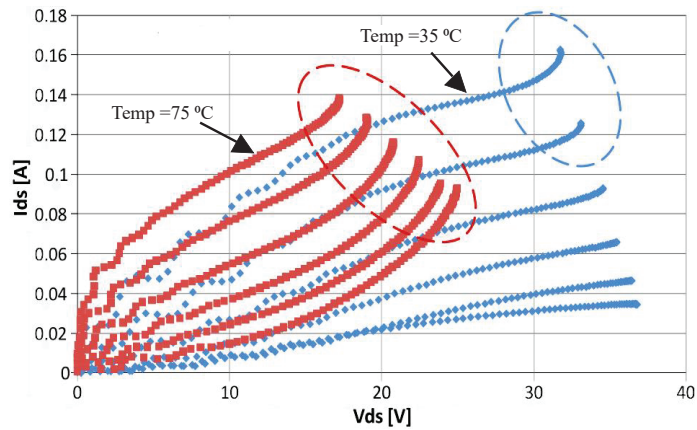
is pushed down from a high value, the drain current drops at the  $V_{DS\_kink}$  position, but it reappears when the  $V_{DS}$  is pumped up. As a result, the lower  $g_d$  is due to trapping the states and is connected among the source and drain electric field. This is also supported by the fact that the magnitude of the kink is unaffected by the running  $V_{GS}$  value, demonstrating that a large drain current is not required for a trap filling. The kink phenomenon has threshold characteristics related to the  $V_{DS\_kink}$ . There is no kink in the  $I_{DS}$  if the  $V_{DS\_max}$  does not exceed the  $V_{DS\_kink}$ . As the gate voltage ( $V_{GS}$ ) is increased from 0 V to  $V_{GS\_max}$ , the nonmonotonic behavior of the  $V_{DS\_kink}$  is noticed. In the region of a relatively high  $V_{GS}$ , the  $V_{DS\_kink}$  rose with  $V_{GS}$ . Nevertheless, the  $V_{DS\_kink}$  rose when  $V_{GS}$  reduced in the near pinch-off zone. The inset figure demonstrates the nonmonotonic behavior of the kink voltage ( $V_{DS\_kink}$ ) when the  $V_{GS}$  is stepping from 10 V to 0 V with  $\Delta V_{GS} = -0.2$  V. Each sweep of  $V_{DS}$ , is followed by a 5 min rest [165].



**Figure 37.** The kink effect in the  $I_D$  is clearly observed with a strong dependence on the  $V_{DS}$  sweep direction. Reproduced with permission [165]. Copyright 2016, the author(s), published by the American Vacuum Society.

#### 4.2.6. Runaway Effect

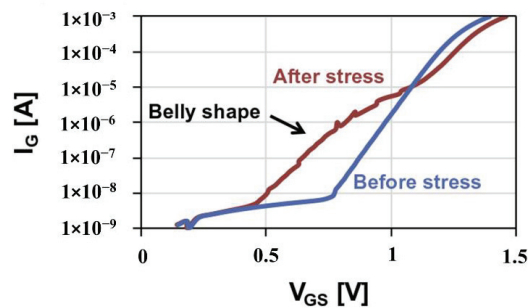
When the drain voltage is raised in the saturation regime, the runaway effect occurs, defined by a simultaneous increase in the drain and gate currents [166,167]. Usually, the gate-to-drain diode component dominates the gate leakage, which rises as the  $V_{DS}$  approaches the threshold. The gate leakage is projected to decrease when the  $V_{GS}$  is minimized. As shown in Figure 38, the absolute gate current in the runaway mode is larger for the lower  $V_{GS}$  levels. After the runaway-inducing aging testing, the reliability characterizations might be severely detrimental since a continuous rise in the  $I_G$  and  $I_D$  could result in catastrophe failures, turning the runaway into an end-of-life mechanism. For the runaways, the significant drain and gate voltage will be noticed. Under open channel situations, the runaway shifts to a lower  $V_{DS}$  and greater negative  $V_G$  values. Lower activation voltages result from higher temperatures and longer aging durations. According to conduction mechanism research, the runaway seems to be linked to the Fowler–Nordheim tunnelling process.



**Figure 38.** Output characteristics of the device reveal a runaway mechanism on the ellipse area with different temperatures. Reproduce with permission [167]. Copyright 2012, Elsevier.

#### 4.2.7. Belly Shape Effect

According to Brunel et al. [168], after the HTOL or HTRB reliability testing, the electrical parasitic phenomena known as the belly shape effect (BS) in which on the Schottky forward characteristic, an excess of the gate leakage current resembling a “belly shape” character is noticed [168,169]. Figure 39 shows a standard belly shape. After just a few hours of aging, a belly shape forms, with varying magnitudes during the aging process, indicating degradations due to variations in the epitaxial layers, metal, or surface states. Nonetheless, the mechanics of its development are still unknown, and additional research is needed to address the dependability manifestations. Without compromising the overall dependability, it may result in high leakage currents for fascinating research on the situation and internal physics.



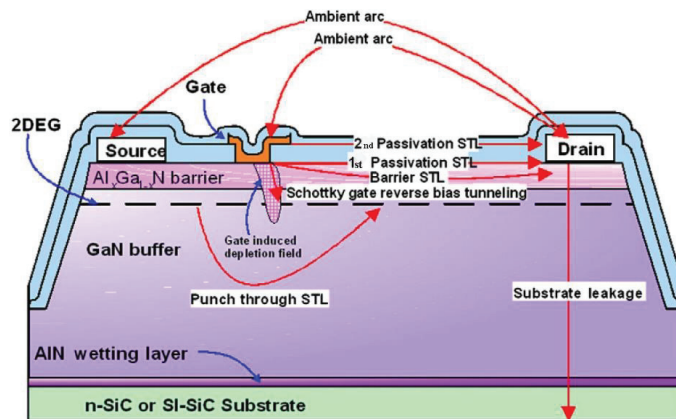
**Figure 39.** Before (blue) and after (red) 4000 h of HTRB stress, the forward characteristics of an HEMT with BS are shown. Reproduced with permission [168]. Copyright 2013, Elsevier.

#### 4.3. Breakdown Voltage in GaN HEMTs Device

Gallium nitride transistors are expected to play an essential role in the next-generation power converters, thanks to the high expected breakdown voltage, which is a direct consequence of the high breakdown field of GaN ( $>300$  V/ $\mu\text{m}$ ). Thus, in switching the operation, the transistors alternate between the on-state, where the gate opens the channel and allows the carriers to flow through the device, and the off-state, where the gate closes the channel and blocks the carriers' current. At the off-state, the gate potential,  $V_{GS}$ , is lower than the device's threshold voltage,  $V_{TH}$ , and is considered a subthreshold condition. For

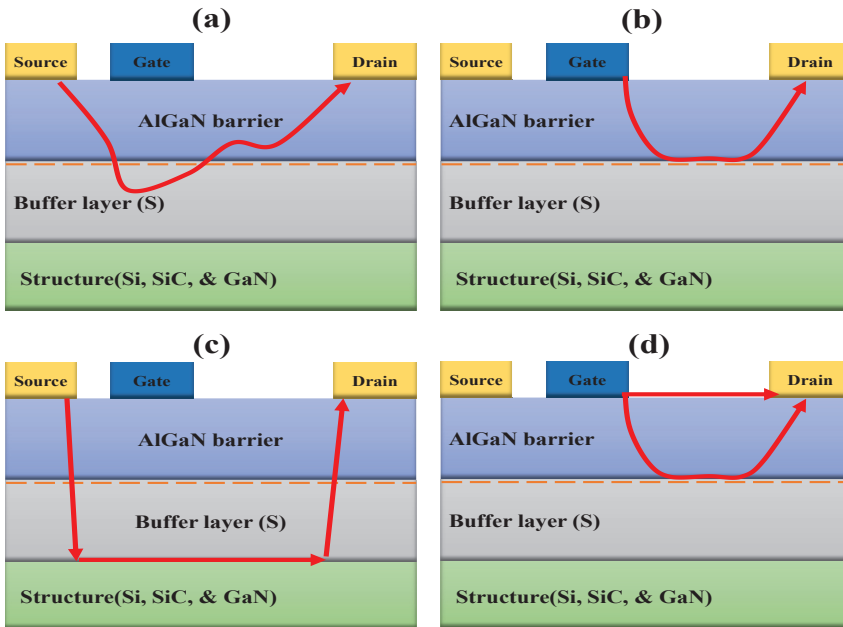
an efficient switching, the off-state operation point conditions should be at a high positive drain voltage and negligible drain current; therefore, a strong gate-blocking capability is required. At very high positive drain voltage conditions, the blocking capability of the device degrades and gives rise to the subthreshold leakage (STL) current. The subthreshold leakage current will increase and become significant, thereby reducing the efficiency of the switching. A significant leakage current is three orders of magnitude lower than the device's maximal output current. At high voltages, currents higher than this value may initiate destructive processes in the device; therefore, it is considered the starting point of the device breakdown. In most cases, the breakdown voltage is either the sub-threshold drain leakage, or the gate leakage increases above 1 mA/mm.

The main physical reasons for sub-threshold current leakages (STL) increased at a higher drain bias voltage are sketched in Figure 40. The STL has to be taken into account for a high voltage GaN device engineering and it is explained as follows:



**Figure 40.** Illustration of most important sub-threshold current leakages (STL) and breakdown paths might appear during high voltage in GaN-based HEMTs. Reproduced with permission [170]. Copyright 2011, Elsevier.

First, the electrons punch through in the buffer underneath the gated channel region [171]: this effect depends on the magnitude of the vertical electric field in the gate region and the ability of the buffer structure to confine electrons to the channel, as shown in Figure 41a. Second, the Schottky gate reverses the bias tunnelling: this originates from the drain side edge of the gate and is triggered by the high electric fields present in this particular device region, as displayed in Figure 41b. Third, Figure 41c presents the vertical device breakdown or the substrate leakage across the epitaxial layers to the conductive substrates such as n-SiC or Si: this is mainly an issue of the buffering technology and can be prevented by suitable epitaxial concepts [171]. High-voltage GaN devices place very stringent demands on high-voltage buffer structures since, in most cases, these devices are fabricated on conductive substrates (Si, n-SiC) which are usually connected to either the drain or the source terminal of the power devices. Fourth, surface-related breakdown: this is mainly associated with the quality of device passivation, whether the interface is between the passivation layers or the semiconductor surface itself, as indicated in Figure 41d. Finally, an ambient arcing between the closely spaced device electrodes may also occur if the devices are operated in the air. Thus, this has to be taken into account by the device layout design, the technology, and design of the passivation, and also the device packaging.



**Figure 41.** Schematic represents the main source of limiting the high voltage capability of AlGaN/GaN HEMT on substrates (Si, SiC, or GaN). (a) Punch through effect, (b) Breakdown along channel region, (c) Breakdown through buffer layer, (d) Leakage currents originating from the gate structure.

### 5. Challenges for GaN HEMTs Device

Next-generation power-efficient converters might be created using GaN-based power devices if the fundamental problems pertaining to the material's quality, device's fabrication, and its performance can be resolved. However, challenges arise, such as it is impossible to crystallize GaN from melted material because the bulk GaN crystal development process is more challenging compared to Si and SiC. Bulk GaN substrates require high temperatures,  $>2200\text{ }^{\circ}\text{C}$ , and a nitrogen pressure  $>6\text{ GPa}$ , plus they have tough growth methods, such as a hydride vapor-phase epitaxy (HVPE), sodium flux, and an acidic/basic ammonothermal method is required. On top of that, these GaN substrates have a defect density of between  $10^4$  and  $10^6/\text{cm}^2$ , which necessitates a careful examination before they can be used for commercial purposes [172]. Ion implantation is used to dope the conventional Si and SiC power devices selectively. However, for GaN, it is still a highly complex process requiring specialized instruments capable of high-temperature ( $>1200\text{ }^{\circ}\text{C}$ ) and high-pressure conditions ( $>1\text{ GPa}$ ) [173]. Bulk GaNs commercialization is hampered not only by the high cost and small size of these substrates, but also by the enormous initial investment required to set up GaN-specific fabs, which could drive up the average selling price (ASP) of discrete devices and further impede the adoption of these devices. Therefore, achieving significant advancements in both the cost and substrate size of these bulk GaN substrates is crucial.

Moreover, some other challenges, such as the GaN HEMT PAs, operate at high-frequency and high-power conditions, where the drain and the gate metals meltdown because of the Eddy current triggered by the magnetic field from the nearby coil. On the contrary, the high operating current may also facilitate the issue. The meltdown occurs at the Au layer, and several hints of Au can be traced in either subsequent layer [174]. The heavy ion irradiation makes the challenge for the GaN HEMT because this ion irradiation induces a device damage by creating lattice defects and accelerating the degradations of



the GaN HEMT under tests (CGHV1J006D, manufactured by Wolfspeed, Durham, NC, USA). On the other hand, a gate injection triggers an impact ionization in the channel, thus inducing failures under the off-state. Its breakdown drain bias becomes lower than the pristine one, owing to the defect generations between the channel layer and the buffer layer during the ion irradiation [175].

Furthermore, after wet etches are done to remove the ohmic contacts of electrically stressed devices; the formation of nano-cracks underneath the ohmic metal contacts of GaN HEMTs becomes challenging for the researchers [176]. This crack might grow from the metal inclusions under the influence of a vertically oriented electric field, which introduces biaxial stress in the channel layer. The hoop stresses introduced by the biaxial compressive stresses and the residual tensile stress introduced in the epitaxial process impel the cracks to extend from the alloyed S–D contacts into the channel.

## 6. Conclusions

GaN HEMTs appear to be a competitive semiconductor technology for the foreseeable future. The existing and projected demand for GaN-based products in power industries is outlined. The benefits and physics of III-N materials are explained to comprehend GaN-based device transistors better. The contest between Si, GaN, SiC, and  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is anticipated to heat up in the following years since these devices are forecast to represent a crucial function in the next generation of power converters. Research at both the academic and industry levels will lead to a significant advancement in device technology. On the other hand, reliability is still a big issue. Thus, the main GaN HEMT reliability concerns caused by the trap effects like a drain, a gate lag, a current collapse, and a breakdown voltage are explained briefly. Finally, we discussed the lateral type AlGaIn/GaN HEMT devices, but in the future, we will include the vertical type AlGaIn/GaN HEMT devices. Overall, the future growth of the GaN research field will be aided by the continued improvement of all these features, thanks to the more sophisticated machinery and higher-quality materials.

**Author Contributions:** Conceptualization, M.F.P.M., M.S. and H.K.; methodology, N.I.; software, N.I.; validation, H.K. and M.S.; formal analysis, M.F.P.M. and M.F.A.J.K.; investigation, N.I. and M.F.P.M.; resources, N.I. and M.F.P.M.; data curation, N.I., H.K. and M.F.P.M.; writing—original draft preparation, N.I.; writing—review and editing, N.I., S.F., M.S. and M.F.P.M.; visualization, N.I., S.F., M.S., M.F.A.J.K. and M.F.P.M.; supervision, S.F., M.S., M.F.A.J.K. and M.F.P.M.; project administration, M.F.P.M.; funding acquisition, S.F. and M.F.P.M. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research was funded by Universiti Sains Malaysia’s Research University Incentive (RUI) grant “1001/PELECT/8014134”.

**Data Availability Statement:** Not applicable.

**Acknowledgments:** The author would like to express his gratitude to USMs School of Electrical and Electronic Engineering, CEDEC, and INOR for providing the research facilities.

**Conflicts of Interest:** The authors declare no conflict of interest.

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Review

# Surface Dispersion Suppression in High-Frequency GaN Devices

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**Abstract:** GaN-based high electron mobility transistors (HEMTs) are shown to have excellent properties, showing themselves to perform well among the throng of solid-state power amplifiers. They are particularly promising candidates for next-generation mobile communication applications due to their high power density, frequency, and efficiency. However, the radio-frequency (RF) dispersion aroused by a high surface-state density inherent in nitrides causes the degradation of GaN devices' performance and reliability. Although various dispersion suppression strategies have been proposed successively—including surface treatment, passivation, field plate, cap layer, and Si surface doping—outcomes were not satisfactory for devices with higher frequencies until the emergence of a novel N-polar deep recess (NPDR) structure broke this deadlock. This paper summarizes the generation of dispersion, several widespread dispersion containment approaches, and their bottlenecks under high frequencies. Subsequently, we highlight the NPDR structure as a potential substitute, evaluate its technical benefits, and review the continuous exertions in recent years.

**Keywords:** GaN-based HEMTs; RF dispersion; suppression; NPDR structure; high-frequency

## 1. Introduction

Millimeter-wave technology is undoubtedly an ongoing research focus for fifth-generation mobile communication technology (5G) and beyond. GaN-based high electron mobility transistors (HEMTs) are taking the lead in the radio-frequency (RF) industry, especially for those applications that require abundant power density, thanks to the unparallel combined material properties of a wide bandgap ( $E_g \sim 3.4$  eV), large critical breakdown electric field, high electron saturation velocity, high electron mobility and sheet density achieved by 2-Dimensional electron gas (2DEG), and excellent thermal properties when prepared on silicon carbide (SiC) substrates [1–4]. However, the existence of direct current (DC)-RF dispersion (also known as the “current collapse”) leads to a significant decrease in output power density and causes reliability-related issues in GaN-based HEMTs, especially at higher frequencies, which limits the development and application of such devices. Research has shown that the widespread presence of trapping states (covering the semiconductor surface, barrier layer, interface, channel, and buffer layer) in III/V group compound semiconductors should be mainly responsible for the dispersion of GaN HEMTs [5]. In high-frequency devices, the closer proximity of 2DEG to the surface highlights the role of surface traps (surface states) on dispersion [6,7]. These surface states trapping electrons to form a “virtual gate” (similar to a gate function) further deplete the 2DEG channel, which strongly impacts the device output characteristics and reliability. Engineers have tried to solve this problem by using multiple processes, including surface treatment [8], passivation [9], field plate [10], cap layer [11], and Si surface doping [12] in recent years. With the increasing demand for higher operating frequencies, the reduced gate length and the aspect ratio in need of being maintained drive the 2DEG much closer to the surface compared with the lower frequency HEMT epitaxial structure, thus limiting the effectiveness of those techniques in improving the dispersion. In this vein, researchers working on high-frequency GaN devices have sought novel technologies to better solve this aporia.

**Citation:** Zhu, P.; Ni, X.; Fan, Q.; Gu, X. Surface Dispersion Suppression in High-Frequency GaN Devices.

*Crystals* **2022**, *12*, 1461. <https://doi.org/10.3390/cryst12101461>

Academic Editor: Dmitri Donetski

Received: 27 September 2022

Accepted: 14 October 2022

Published: 16 October 2022

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In this paper, we explain the origin of surface states and the mechanism causing dispersion in GaN devices. The current dominant methods for suppression dispersion and their bottlenecks in the high-frequency domain are summarized. Finally, we focus on the N-polar deep recess (NPDR) structure, addressing its uniqueness in controlling dispersion and reviewing the research advances in NPDR metal-oxide-semiconductor (MIS)-HEMTs.

## 2. Surface States and Virtual Gate

In GaN-based HEMTs, surface states are critical sources of 2DEG in the channel [13], allowing the device to achieve a very high electron concentration without the need for intentional doping (unlike GaAs-based 2DEG), which dramatically reduces ionized impurity scattering and enhances carrier mobility. On the other hand, GaN-based HEMTs are also plagued by the dispersion effect generated by surface states. This section mainly discusses the creation of surface states and the principle of dispersion caused by them.

### 2.1. Sources of Surface States

Surface states, a type of electron-bound state, can be categorized into two sorts based on their formation: intrinsic and extrinsic.

Intrinsic surface states arise due to the termination of the ideal crystal structure at the surface. It is common knowledge that GaN, like any crystal, cannot be extended infinitely in space. Therefore, the periodic potential field will be interrupted at the surface and cause additional energy levels in the forbidden band known as surface energy levels, whose corresponding electronic states are named surface states. Chemical bonding theory explains that the chemical bonds of GaN crystal break at the surface, and the unbonded electron pairs form dangling bonds, the corresponding electronic states being surface states [14]. Besides, those created by threading dislocations accessible at the surface, native oxide, N-vacancies, ions adsorbed from the surrounding environment (such as oxygen, carbon, and hydrogen, each with its unique energy level), and surface damage in the processing are referred to as extrinsic surface states [14–16]. These two different forms of generation pathways are shown in Figure 1.

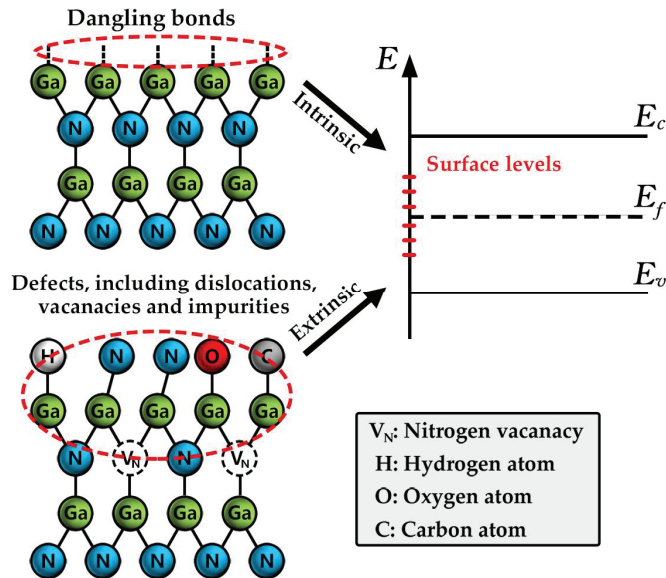


Figure 1. Mechanisms for the generation of intrinsic and extrinsic surface states.

2.2. Virtual Gate Model

Depending on their behaviors, surface states can be classified as either acceptors or donors. Table 1 shows the charge situations of these two categories of surface states in the empty and filled (after trapping the electrons) conditions. Under the strong influence of the polarized electric field, the donor surface state filled with electrons below the Fermi level will be partly ionized, allowing the electrons to escape into the channel to produce a high concentration of 2DEG and leave large positive charges on the surface [17]. As such, the surface of the GaN device should not show a negative surface potential. Vetury et al. [18] observed that a significant number of negative charges reside on the device’s surface, conflicting with the previous theory when they employed the floating gate approach to investigate the surface state impact of AlGaIn/GaN HEMTs in 2001. In response, they explained that these positive charge centers (empty surface states) located between the gate and drain act like traps to capture gate leakage electrons or those channel hot electrons escaping via the barrier to the surface [15,19,20]. During the process from off-state to on-state, electron emission from surface states with a slower period differs from RF signals, so the trapped electrons are not released when the device is turned on, which is equivalent to another gate existing between the gate and the drain electrodes, i.e., virtual gate [21,22]. As shown in Figure 2, the trapped electrons move and jump on the surface to form a negative charge region, causing the gate depletion region to expand laterally, depleting the 2DEG in the channel and resulting in the current collapse. This RF dispersion is generally determined by pulsed  $I_{DS}-V_{DS}$  measurement, depending on different stressed conditions, and can be defined as:

$$\text{Dispersion (\%)} = \frac{I_{DS,DC} - I_{DS,Pulsed}}{I_{DS,DC}} \times 100\% \tag{1}$$

Table 1. Electrical properties of donor and acceptor surface states.

Type	Empty	Filled
Donor surface states	Positive	Neutral
Acceptor surface states	Neutral	Negative

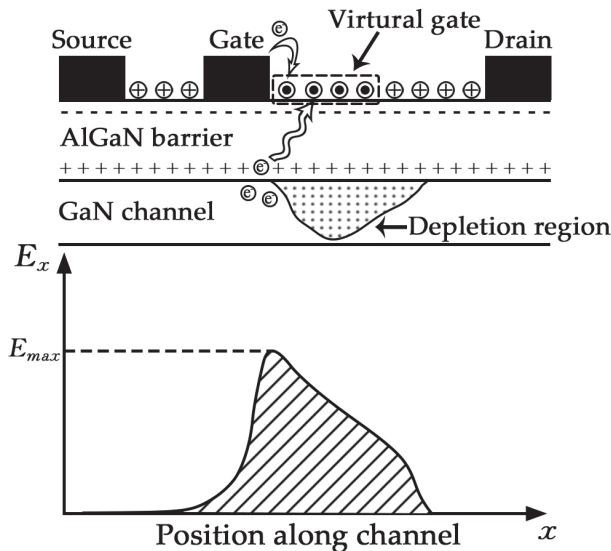
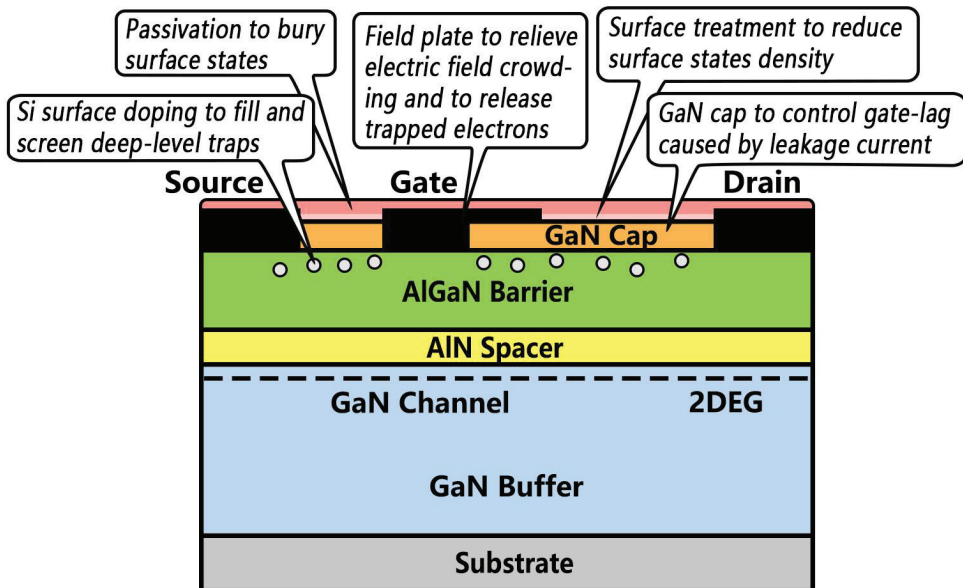


Figure 2. The device model shows the virtual gate’s location, schematic representation, and the electric field distribution in the channel.

### 3. Methods for Suppression Surface Dispersion and Their Bottlenecks

Based on the principle of extra depletion of the 2DEG channel by the virtual gate model, it can be concluded that one of the most critical tasks in dispersion control is to minimize trapping electron action attributable to surface states. Common solutions in AlGaN/GaN HEMTs are summarized in Figure 3. Five categories of methods have been developed and demonstrated to suppress the RF dispersion with mixed success: (1) surface treatment that intends to diminish surface state density to reduce the odds of surface states trapping electrons; (2) passivation, which intends to bury surface traps by depositing dielectrics on the device surface to prevent gate leakage electrons from being trapped in them; (3) the uses of field plate structure intend to alleviate the gate edge electric field crowding and enhance the emission rate of trapped electrons; (4) adding a GaN cap intends to control the gate-lag caused by the leakage current; (5) si surface doping intends to compensate for the trapping energy level to screen the 2DEG from the traps. This section summarizes the research advances of the above technologies and the bottlenecks they encounter at high frequencies.



**Figure 3.** Common methods for suppressing RF dispersion in AlGaN/GaN HEMTs.

#### 3.1. Common Methods for Suppression Surface Dispersion

##### 3.1.1. Surface Treatment

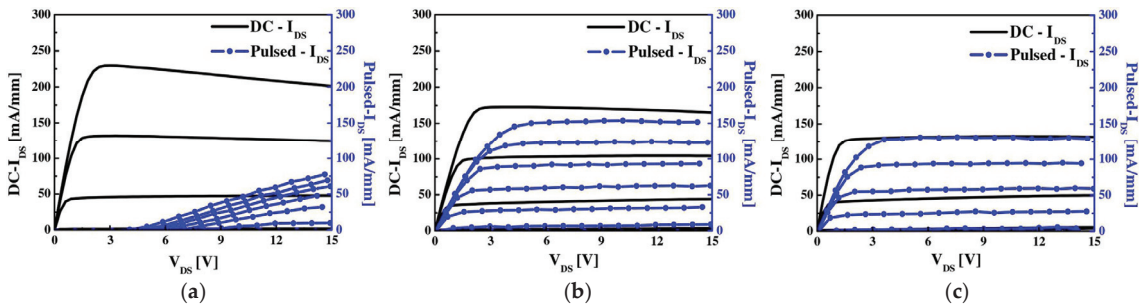
Natural oxides and organic matter adsorbed on the (Al)GaN surface create many interface states between the dielectric used for passivation and the barrier, which reduces the effectiveness of passivation. Consequently, surface treatment prior to dielectric deposition is of extraordinary importance to obtain a high-quality interface.

Organic matter and oxides are mainly composed of carbon and oxygen. UV/ozone surface treatment can proficiently remove carbon [23], while oxygen can be treated by some wet chemical cleaning methods. King et al. [24] found that HF and HCl were able to minimize oxygen coverage on AlN and GaN surfaces, and residual halogen ions ( $\text{Cl}^-$  and  $\text{F}^-$ ) tie up the dangling bonds preventing the surface from being oxidized again. The same result was found in the experiments of Diale et al. [25], who respectively compared the methods of cleaning GaN surfaces with HCl, KOH, and  $(\text{NH}_4)_2\text{S}$ . They concluded that KOH was effective for carbon removal but contributed to a rough surface. The sample cleaned in  $(\text{NH}_4)_2\text{S}$ , a chemical avoiding surface re-oxidation, acquired the optimum cleaning result with the lowest values



of both C and O, root mean square (RMS) roughness, and Ga/N ratio. Other wet chemical cleaning efforts mainly focus on  $\text{HNO}_3$ ,  $\text{H}_2\text{SO}_4$ ,  $\text{NH}_4\text{OH}$ , and  $\text{NaOH}$ .

Surface treatment using plasma like  $\text{NH}_3$ ,  $\text{N}_2$ , and  $\text{N}_2\text{O}$  is also valuable for suppressing dispersion to enhance performance [26–29]. By filling nitrogen vacancies and removing impurity oxygen atoms, nitrogen-related plasma treatment considerably enhances the quality of the  $\text{SiN}_x/\text{GaN}$  interface [28]. Romero et al. [27] treated the  $\text{AlGaIn}/\text{GaN}$  HEMT (which had been wet cleaned by  $\text{NH}_4\text{OH}$ ) with in situ  $\text{N}_2$  plasma ( $\text{N}_2\text{PP}$ ) at  $200^\circ\text{C}$  for 1 min prior to  $\text{SiN}_x$  passivation of the device. The treated GaN HEMT obtained an  $I_{\text{DS}}$ , which was 10% higher than the untreated one, and achieved a more advanced knee voltage. A 65% drop in the density of interface states was discovered after applying  $\text{N}_2\text{PP}$ , which was responsible for reducing gate leakage current by two to three times (from  $7.7$  to  $2.3 \times 10^{-2}$   $\text{A}/\text{cm}^2$  at  $V_{\text{GD}} = -20$  V), utilizing capacitance-voltage (C-V) and conductance-frequency (G-F) measurements. Furthermore,  $\text{NH}_3$  plasma-treated performs better than  $\text{N}_2$  in GaN HEMTs [26], with RF dispersion respectively decreasing from 63% (without pretreatment) to 1% and 9% (shown in Figure 4). This is probably due to the fact that  $\text{NH}_3$  plasma eliminates oxide and carbon residues while reducing the density of surface state defects.



**Figure 4.** DC and pulsed  $I_{\text{DS}}-V_{\text{DS}}$  characteristics for the GaN device. (a) Without pretreatment; (b) with  $\text{NH}_4\text{OH}/\text{N}_2$  pretreatment; (c) with  $\text{NH}_4\text{OH}/\text{NH}_3$  pretreatment. DC and pulsed  $I_{\text{DS}}-V_{\text{DS}}$  were measured at  $V_{\text{DS}} = 0$  to  $15$  V and  $V_{\text{GS}} = -3$  to  $1$  V. The pulse width and period were  $500$  ns and  $1$  ms. Adapted with permission from Ref. [26]. Copyright 2010, The Japan Society of Applied Physics.

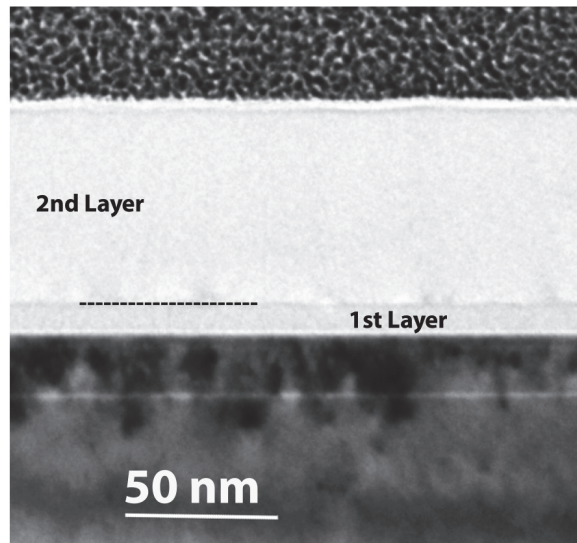
In addition, plasma can also be combined with heat treatments such as high-temperature annealing in vacuum [30] or  $\text{N}_2$  [31] and  $\text{NH}_3$  [32] atmospheres to enhance the desorption of contaminants further and assist in the elimination of remaining surface defects, thereby improving the surface quality of the device. It has to be emphasized, however, that the surface treatment also increases the risk of unreliability and is, therefore, mostly involved in laboratory research efforts.

### 3.1.2. Passivation

Since 2000, when Green et al. [15] deposited a layer of  $\text{Si}_3\text{N}_4$  for passivation on the surface of  $\text{AlGaIn}/\text{GaN}$  HEMT to obtain the highest power density ( $4$  W/mm at  $4$  GHz) during that period, passivation has become one of the most commonly used and effective techniques to solve RF dispersion after more than 20 years of development.

Previous studies have reported that  $\text{SiN}_x$ ,  $\text{AlN}$ ,  $\text{SiO}_2$ ,  $\text{SiNO}$ ,  $\text{Al}_2\text{O}_3$ , and  $\text{HfO}_2$  (high- $\kappa$  dielectric) can all be applied to GaN-based HEMTs [28,31,33–35]. However, some researchers believe that nitrides (compared to oxides) probably are more suitable for GaN devices because oxygen impurities can easily diffuse into the GaN crystal and generate a high density of deep (or slow) interface states, producing additional current collapse [36,37]. This conclusion is consistent with the report of Geng et al. [31], which evaluated  $\text{AlGaIn}/\text{GaN}$  MIS-HEMTs utilizing PECVD deposition of  $20$  nm  $\text{SiN}_x$ ,  $\text{SiO}_2$ , and  $\text{SiNO}$  as passivation layers, respectively. It is found that the interface-trapped charge density (or the deep energy level defects density with long emission time of electrons) for  $\Delta E > 0.657$  eV in  $\text{SiO}_2$  is  $4.13 \times 10^{12}$   $\text{cm}^{-2}$  (three times

larger than that of  $\text{SiN}_x$ ,  $\sim 1.38 \times 10^{12} \text{ cm}^{-2}$  in  $\text{SiN}_x$ ). Compared to only 11.06% dispersion in  $\text{SiN}_x$ , the current collapse in  $\text{SiO}_2$  reaches 84.14% at  $V_{gs} = -18 \text{ V}$ , proving the success of  $\text{SiN}_x$  passivation and the fact that  $\text{SiO}_2$  would not be appropriate for GaN devices. Based on taking  $\text{SiN}_x$  as a dielectric, Huang et al. [38] proposed an improved structure using bilayer LPCVD  $\text{SiN}_x$ ; a Si-rich  $\text{SiN}_x$  layer (Si/N = 59/41) with a thickness of  $\sim 10 \text{ nm}$  was first deposited, followed by a  $\sim 67 \text{ nm}$  Si-poor  $\text{SiN}_x$  layer (Si/N = 50/50, high-resistive). Figure 5 exhibits a TEM cross-sectional image of this bilayer  $\text{SiN}_x$  passivation, and the black dotted line refers to the boundary between the first and second layers. The Si-rich  $\text{SiN}_x$  layer upper to surface is argued to remove the deep-level traps at the AlGaIn/SiN<sub>x</sub> interface, which makes microwave GaN HEMTs show a much smaller degradation of about 9.7% ( $\sim 30\%$  dispersion in 70 nm Si-poor  $\text{SiN}_x$  sample) while maintaining a low gate leakage current owing to the second high-resistive layer.



**Figure 5.** TEM cross-sectional image shows a distinguishable bilayer structure of the passivation layer. Reprinted with permission from Ref. [38]. Copyright 2018 by IEEE.

### 3.1.3. Field Plate

The field plate is applied in GaN-based HEMTs to reduce the electric field crowding at the gate corner of the drain side, preventing electron injection from the gate into surface states, and forming a virtual gate. Moreover, the horizontal electric field near the end of the field plate will strengthen the process of electrons escaping from the traps and speed up the electrons hopping along the AlGaIn surface, further lowering the trapped electron density and, therefore, substantially suppressing current collapse [22]. The effectiveness of the field plate in suppressing current collapse is more robust with increasing field plate length. The trapped charges on the device surface decreased from  $1.58 \times 10^{12} \text{ cm}^{-2}$  (no field plate) to  $0.8 \times 10^{12} \text{ cm}^{-2}$  after using a  $1.5 \mu\text{m}$  field plate structure [39], the pulsed  $I_{DS}-V_{DS}$  characteristics and trapped charge density are displayed in Figure 6. The field plate this method has now been widely adopted and greatly influenced the high-voltage devices. Despite this, it is worth noting that it is thrown into an awkward situation in high-frequency applications. Because this design not only reduces the speed of the channel electrons owing to the weakened electric field but also introduces additional external capacitance that limits the efficiency and gain of the device. Accordingly, in order to ensure anticipant RF performance, the field plate has found very limited usage in high-frequency industries.

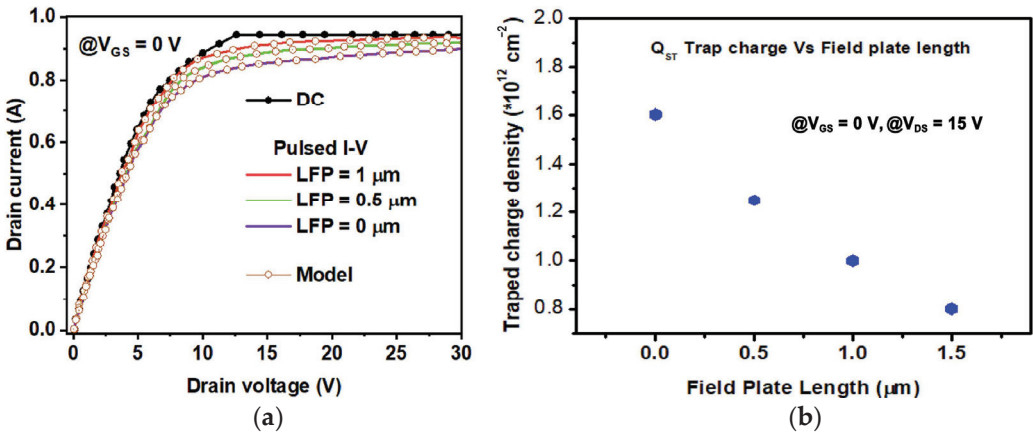


Figure 6. AlGaIn/GaN HEMT characteristics with different field plate lengths. (a) Pulsed  $I_{D_S}$ - $V_{D_S}$  characteristics with Quiescent Voltage ( $V_{G_S,Q} = -8$  V and  $V_{D_S,Q} = 50$  V); (b) trapped charge ( $Q_{ST}$ ). Adapted with permission from Ref. [39]. Copyright 2021 by Elsevier.

### 3.1.4. GaN Cap

GaN cap, a thin layer of GaN (about a few nanometers) on top of the barrier that forms a sandwich structure (e.g., GaN/AlGaIn/GaN), is another well-established technique in industry for managing the current collapse. This cap can be doped GaN (typically n-type doping by SiH<sub>4</sub> or p-type doping by Cp<sub>2</sub>Mg) or i-GaN. No matter what type of GaN cap is used, it degrades gate leakage levels [40], both vertically and horizontally. Vertically, raising the effective Schottky barrier by the GaN cap provides a stronger limitation on the emission and tunneling of hot electrons [11,41]. Horizontally, as presented by Sarkar et al. [11], the GaN cap passivates the access region to suppress lateral electrons hopping via surface traps, significantly reducing the total leakage current (shown in Figure 7a). In other words, the GaN cap can effectively screen 2DEG from dispersion-related traps. As shown in Figure 7b,c, 2 nm of GaN cap layer effectively controls the current collapse in GaN-based HEMTs, while enhancing the device’s frequency performance (62% improving in  $f_T$ ) at the expense of a small amount of gain.

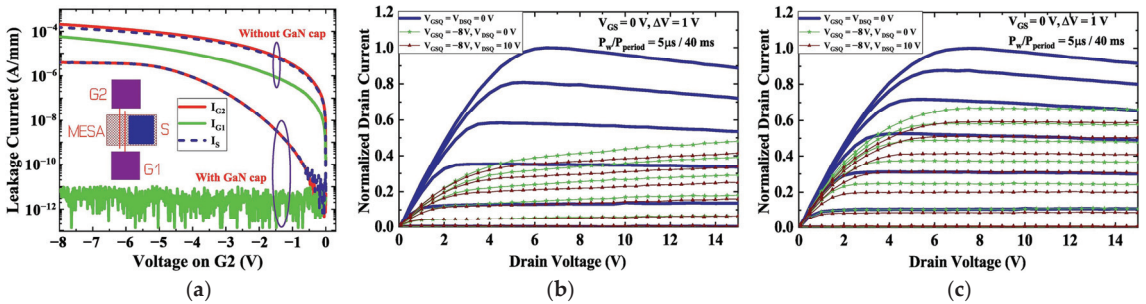


Figure 7. (a) Characteristics of the double gate.  $I_S$  is the vertical leakage current through 2DEG, and  $I_{G1}$  is the horizontal leakage current by electron hopping between surface states.  $I_{G2}$  is the total leakage current ( $I_{G2} = I_S + I_{G1}$ ). Pulsed output characteristics of HEMTs, (b) without GaN cap, and (c) with GaN cap. Adapted with permission from Ref. [11]. Copyright 2022 by Elsevier.

### 3.1.5. Si Surface Doping

Surface doping of GaN HEMTs with Si also contributes to the suppression of dispersion [42]. Si (as an electron donor) surface doping can prevent the slow process of

re-emitting trapped channel electrons from surface states by filling and screening the deep-level traps [12]. However, the method also causes an escalation in leakage levels (electrons can tunnel through the thinned potential barriers more easily), so attention to a concentration should be paid when doping the surface of the device to avoid the impact of poor leakage current and breakdown resistance on device reliability.

### 3.2. Bottlenecks Encountered at High Frequencies

At lower frequencies (below Ka-band), the previously mentioned techniques can be combined to control RF dispersion in GaN HEMTs. As the gate length is further decreased to increase the operating frequency, the distance from the polarized surface to the 2DEG channel also has to be reduced to maintain the desired aspect ratio and contain the short channel effect, whereas the corresponding cost is the 2DEG channel suffers from the surface RF dispersion more seriously, rendering the effect of all surface engineering techniques less effective. When the operating frequency is pushed over 30 GHz (which means just entering the millimeter-wave range), the capacitance penalty imposed by the field plate causes this structure to be disabled because of the severely degraded high-frequency performance. Therefore, researchers urgently need to find new techniques to alleviate the problem of surface state trapping electrons to ensure the device's reliability at high-frequency operation.

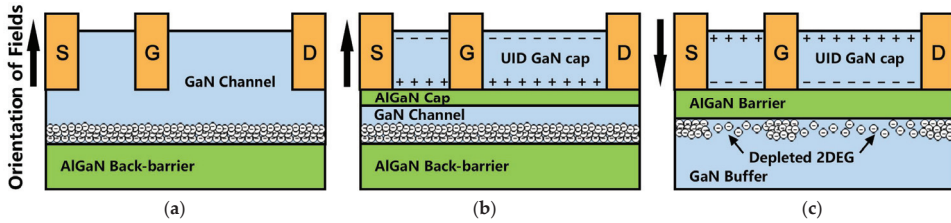
## 4. NPDR MIS-HEMTs for High-Frequency Device

Due to the comparatively good material quality and electrical features, Ga-polar GaN has dominated power devices for a long time. In recent years, the material growth technique has constantly been progressing on N-polar GaN; thus, related device research gradually gained significant interest [43,44]. On account of the opposing polarity, N-polar GaN HEMTs offer a series of natural advantages for higher frequency epitaxy and device design over the Ga-polar [45], such as (a) devices with a narrower top layer bandgap achieve lower contact resistance; (b) a natural back-barrier improves 2DEG confinement and minimize short channel effect while giving rise to higher transconductance. Additionally, the presence of the back-barrier allows the device to keep leakage current (from channel to substrate) at a low range even when there is no doping (e.g., Fe, C) in the buffer, avoiding the dispersion introduced by slow deep energy level discharge [46]; (c) flexible device aspect ratios accommodate shorter gate lengths resulting from increased frequency. These features are tailored to the needs of high-frequency devices so that the N-polar GaN transistor stood distinctly above all others in 2012, with a  $f_T = 270$  GHz and  $f_{max} = 370$  GHz [47]. However, the most outstanding value of N-polar GaN materials is the ability to make the deep recess structure dramatically mitigate RF dispersion to guarantee reliability at higher frequencies [48]. Here, the basic structure of NPDR is displayed, the reason why deep recess can only be applied on the N-polar GaN (rather than Ga-polar) is discussed, and the research advances on NPDR are summarized.

### 4.1. What and Why Is NPDR?

The most basic structure of NPDR is to directly thicken the GaN channel above the back-barrier, as shown in Figure 8a, and the 2DEG at the bottom of the channel is isolated from the surface to control dispersion. The gate is buried deep in the GaN channel to considerably boost vertical scaling and strengthen the gate's modulation of 2DEG. To avoid gate leakage currents and regulate the dispersion created by the sidewall, a thin layer of dielectric (normally MOCVD  $\text{SiN}_x$ ) is commonly placed for initial passivation before depositing gate metal. In the improved design of the NPDR structure (shown in Figure 8b), the insertion of an AlGaN cap layer (as etch stop layer) is considered necessary because the difference in components allows for more precise selective etching, while the cap provides better Schottky contact for the device. Apart from these two causes, the polarization electric field generated by N-polar AlGaN also mitigates the injection of gate leakage electrons during reverse bias [49]. Since the thick GaN cap keeps the surface away from the channel (differs from passivation, thick

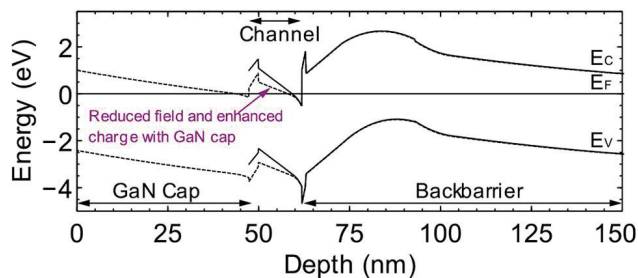
dielectric does not change the surface position due to the absence of polarization), even if a virtual gate is formed on the surface of the access region, there is almost no depletion of charge in the channel. The scattering associated with the surface is also effectively controlled, thus substantially increasing the 2DEG mobility. As mentioned earlier, the traditional passivation of HEMTs using *ex situ* SiN<sub>x</sub> dielectrics still has massive trapping states, whether in bulk or at the interface. However, no significant interfacial states are presented in the NPDR structure because the GaN cap has no difference in lattice constants from the channel. There should also be no more bulk traps within the UID GaN cap than in the channel, which ensures an ultra-low trap density near the 2DEG. To sum up, the deep recess structure is impressive for eliminating the RF dispersion in GaN HEMTs.



**Figure 8.** Schematic diagrams of on-state device operation for deep recess GaN HEMT with different structures. (a) N-polar; (b) N-polar with AlGaN cap; (c) Ga-polar.

In fact, deep recess structures were first proposed for Ga-polar devices [50–52], but the results did not meet the expectations. As the polarization of the GaN cap caused the conduction band to be pulled up, the 2DEG would be depleted below the access region (shown in Figure 8c). Shen et al. speculated that suitable Si doping could compensate for the negative polarization charge and prevent the accumulation of holes. They proposed direct Si delta-doping at the GaN/AlGaN interface [52], but unfortunately, the introduction of Si would cause higher gate leakage and, thus, a reduction in breakdown voltage. Another method that inserts a Si-doped graded AlGaN between the UID GaN cap and the AlGaN barrier is introduced for similar motivations [50]. Although the lower Al component of AlGaN can partially alleviate the 2DEG depletion by polarization, it is difficult to overcome the process because of the high requirements for precise etching. The additional graded AlGaN is also detrimental to the device aspect ratio. Hence, it can be confirmed that using a deep recess structure on the Ga-polar must be compromised for device performance.

In contrast to the Ga polarity, the electric field created in the access region of the N-polar GaN HEMTs partially counteracts the electric field provided by the gate. It pushes the conduction band to the Fermi energy level (Figure 9), thus augmenting the 2DEG concentration [53]. This provides an intrinsic advantage wherein the Ga-polar devices cannot be duplicated, and demonstrates that only the N-polar GaN HEMTs are appropriate for the deep recess.



**Figure 9.** Energy band diagram comparing the N-polar GaN HEMT with and without a GaN cap. Reprinted with permission from Ref. [53]. Copyright 2018 by IEEE.

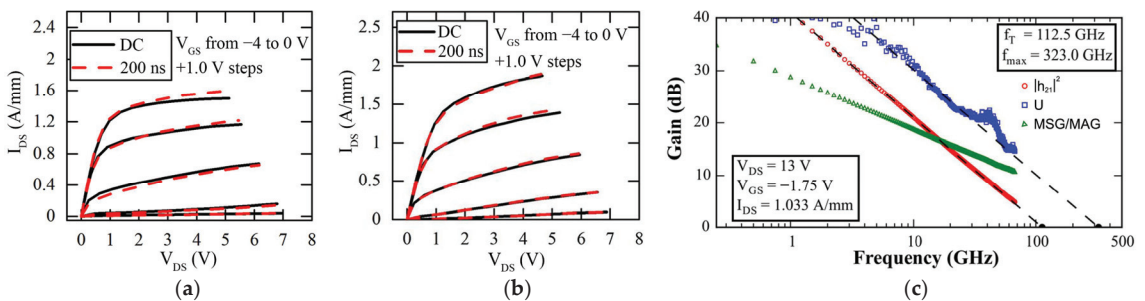


#### 4.2. Research Advances

In 2011, Kolluri et al. [54] first designed and fabricated an N-polar GaN HEMT with a thick unintentionally doped (UID) GaN cap, i.e., NPDR MIS-HEMT, and found that a 120 nm UID GaN cap was sufficient to remove any RF dispersion in the device. Since the last decade, extensive efforts have been devoted to NPDR structures to eliminate RF dispersion in solid-state power devices.

Wienecke et al. [55] from UCSB broadened the operating frequency to W-band (80–100 GHz) by fabricating NPDR MIS-HEMT on a sapphire substrate in 2016, with a 75 nm gate length and T-shaped gate. After implementing a T-gate design, weakened parasitic capacitance enhances device RF performance (both  $f_T$  and  $f_{max}$ ) to some extent [56].

The controlling dispersion ability is assessed using DC and 200 ns pulsed I–V tests. Figure 10a supports that the device’s on-resistance ( $R_{on}$ ) and  $I_{max}$  are 0.58  $\Omega$  and 1.5 A/mm, respectively, under the DC condition. Only a minimal current collapse occurs even in the pulsed measurement, demonstrating the deep recess structure’s efficient dispersion administration in high-frequency devices. Thanks to this, the device achieves a 2.9 W/mm  $P_{out}$  with an associated PAE of 15.5% at a load of 94 GHz. The following year, this team significantly improved the NPDR structure design, i.e., gate-sidewall overlapping [49]; the 3D model is presented in Figure 11. A 30 nm overlap on the sidewall was introduced when depositing the gate metal (the gate was aligned to the bottom of the notch structure in the previous design). This design is believed to assist the drain-side gate in relieving the edge electric field while allowing the device to handle more significant voltage fluctuations (over 12 V) and raise this device’s power density to double the previous density. As can be seen from the pulse diagram (Figure 10b), the wrapping of the metal gate around the sidewall does bring about amazing dispersion management (details of which will be discussed later), resulting in the absence of any current collapse and knee-out phenomenon. Furthermore, in the small-signal RF measurement (shown in Figure 10c), the  $f_T$  and  $f_{max}$  of this HEMT are extrapolated to be 113 and 323 GHz, respectively, when the  $V_{DS}$  and  $V_{GS}$  bias are set to 13 V and  $-1.75$  V. N-polar GaN HEMTs passivated by MOCVD and PECVD  $\text{SiN}_x$  during the same period, on the contrary, tend to exhibit an undesirable dispersion behavior [57,58].



**Figure 10.** (a) DC and pulsed  $I_{DS}$ – $V_{DS}$  measurements of the NPDR MIS-HEMT, fabricated by Wienecke et al. in 2016. Adapted with permission from Ref. [55]. Copyright 2016 by IEEE. (b) DC and pulsed  $I_{DS}$ – $V_{DS}$  measurements and (c) small-signal RF performance of the NPDR MIS-HEMT with gate-sidewall overlapping, fabricated by Steven et al. in 2017. Adapted with permission from Ref. [49]. Copyright 2017 by IEEE.

The relationship between gate metal coverage of recessed regions and dispersion was further discussed by Wienecke [59]. In the case of a fully exposed sidewall, the dispersion aroused by the gap (refers to the space between the bottom of the gate metal and the groove, schematic diagram as shown in Figure 12) was first determined. Figure 13 exhibits the dispersion vs. the drain-side and source-side gap and the effect of different gate coverage on the output power and gate leakage current, respectively. When the gate metal covers the entire gate depression area (no gap and the sidewall is completely covered), the dispersion



induced by those surface states on the sidewall is wholly removed. If the gap is minute (for example, 5 nm), the produced dispersion is negligible and can be acceptable. Once the gap approaches 50 nm or more, the RF dispersion will increase dramatically; hence, wide gaps over 50 nm are forbidden in NPDR structures. The gap discussed above relates to the drain side, whereas the source-side sidewall is completely covered, and a 50 nm field plate is used so that the experimental dispersion is mainly from the drain side. The same test procedure is applied to the source side, and a similar dispersion behavior is obtained. Results of gate coverage contribution to device performance suggest that the full metal coverage sample achieved the highest RF  $P_{out}$  of any transistor under the drain bias. However, it will cause a slight degradation in  $f_T/f_{max}$  due to the larger  $C_{gs}$  and  $C_{gd}$  [60]. The  $I_g$  drops rapidly with the increase of sidewall coverage, but the device with a 15 nm gap is even lower than that of the one with half of the sidewall covered; thus, the mechanism of gate metal deposition coverage on the gate leakage current should be further investigated. Weighing the device's frequency characteristics, breakdown and output power performance, Full Metal Coverage is considered the best trade-off solution. Most reports on NPDR structures currently use a self-alignment process to cover the entire gate depression region.

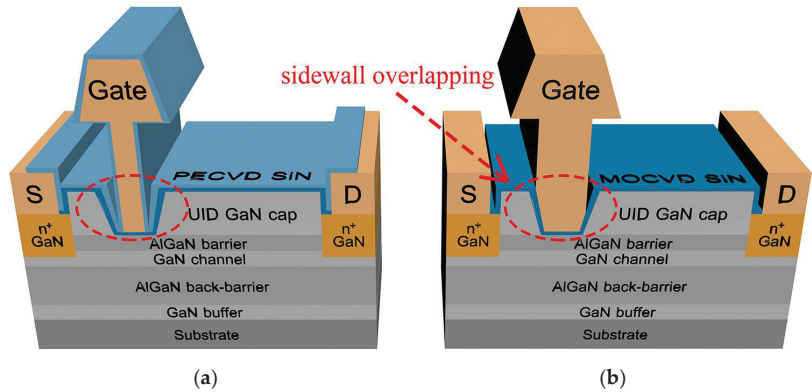


Figure 11. 3D model of NPDR MIS-HEMTs. (a) Without gate-sidewall overlapping; (b) with gate-sidewall overlapping.

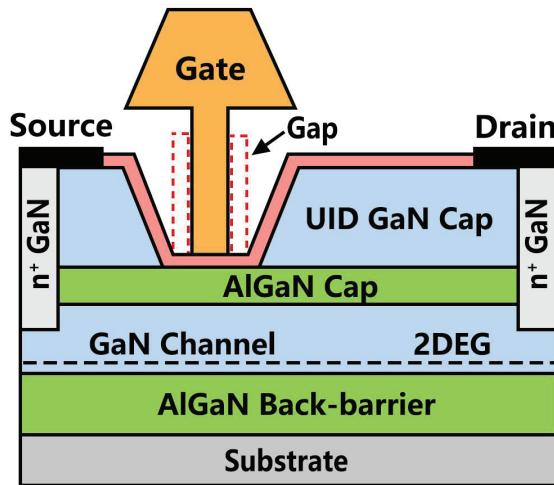
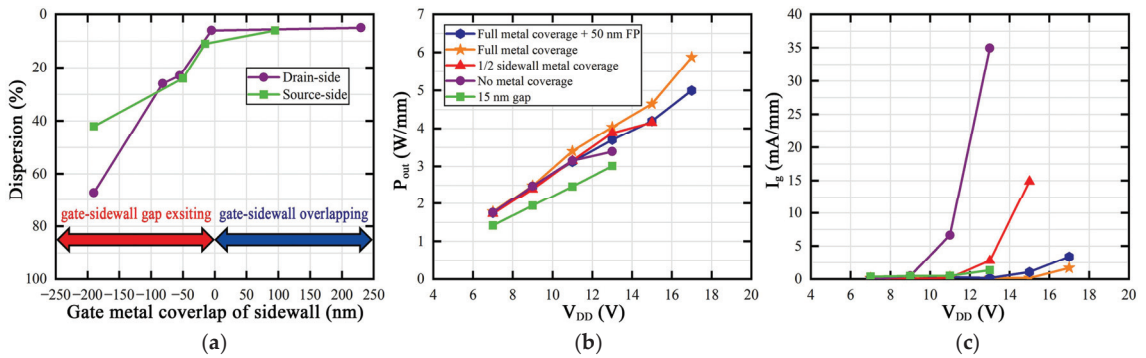


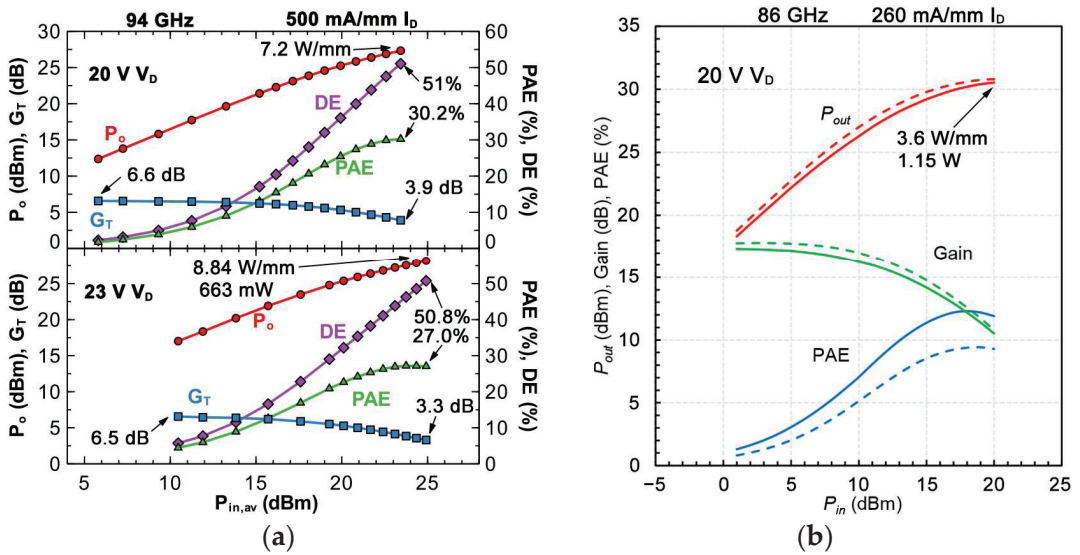
Figure 12. Schematic diagram of the gap between the gate metal and the GaN cap sidewalls.



**Figure 13.** (a) Plots of the dispersion vs. source-side and drain-side gap. (b,c) The performance of output power and gate leakage current at different gate coverage. Reworked from Ref. [59].

The UID GaN cap thickness is also one of the crucial parameters in the NPDR structure. It is clear that the thicker the cap is, the further the channel is from the device surface, which minimizes the surface charge impact on the 2DEG and achieves superior dispersion control. 47.5 nm GaN cap thickness was found to be the most suited in earlier research until lately, this classic thickness has been replaced by 20 nm, primarily to reduce the fringing capacitance while still maintaining the high access region channel conductivity [61]. This action helps improve the device's gain and  $f_T/f_{max}$  combination but perhaps leads to incomplete dispersion control. While additional PECVD passivation can be used to compensate for the reduced ability to regulate dispersion and obtain the desired results.

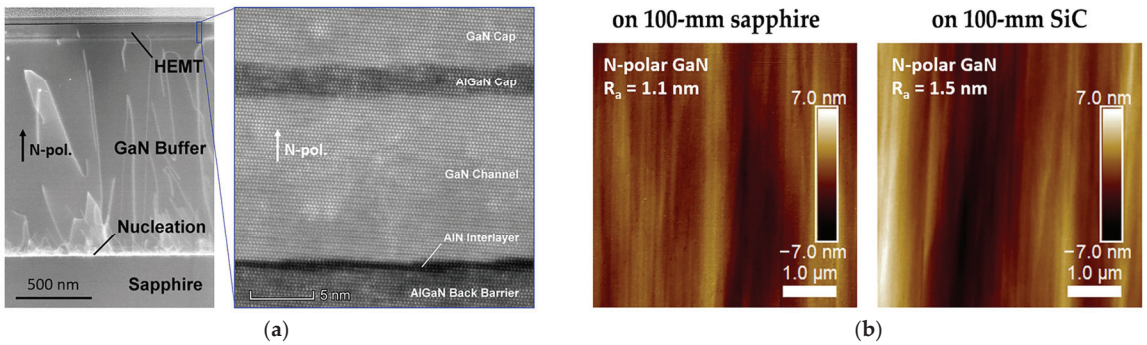
UID GaN cap with PECVD  $\text{SiN}_x$  passivation to commonly suppress dispersion has been demonstrated and fabricated many times in N-polar GaN devices [55,61–63]. Utilization of the double-layer structure makes it possible to achieve excellent performance without the original thick cap, preventing parasitic channels caused by the strong polarization effect (PECVD  $\text{SiN}_x$  does not produce polarization). At the same time, gate misalignment inside the trench is inevitable during the gate deposition, and PECVD  $\text{SiN}_x$  is also effective in eliminating the remaining dispersion left by gate misalignment [55]. Regardless of the rationale, the additional  $\text{SiN}_x$  passivation does have beneficial effects on the breakdown and power performance of the device. Romanczyk found that depositing 40 nm PECVD  $\text{SiN}_x$  on the surface of a typical 47.5 nm UID GaN cap yielded higher output power at 10 GHz and allowed the HEMT to operate at higher  $V_{DS,Q}$  (the  $\text{SiN}_x$  passivation increased  $V_{T,access}$  so that the channel can withstand higher voltages without being depleted) [62]. Under pulsed  $I_{DS}-V_{DS}$  measurement (650 ns pulse with and 0.065% duty cycle), the  $I_D$  of the device drops only 8.5%, even with the stress as high as 23 V. Figure 14 compares the performance of this NPDR GaN HEMT with the superior Ga-polar monolithic microwave integrated circuit (MMIC) at W-band. When the load-pull measure is boosted to 94 GHz, a peak output power of 8.84 W/mm with 27% associated PAE ( $V_D = 23$  V) made it the best-performing device among the N-polar GaN device family. A slight reduction in voltage (to 20 V) would show a peak PAE of 30.7%, also unprecedented in N-polar GaN devices to date. This result far exceeds the leading level in the W-band reported for Ga-polar devices (an MMIC reported by Niida et al. [64] achieving 3.6 W/mm  $P_{out}$  with a maximum PAE of 12.3%, and an AlN/GaN HEMT reported by Harrouche et al. [65] achieving 4 W/mm  $P_{out}$  with a PAE of 14.3% in 2019), proving the absolute dominance of NPDR structures in the millimeter-wave RF field.



**Figure 14.** Power characteristics of devices in the W-band. (a) NPDR GaN HEMT reported by Romanczyk. Adapted with permission from Ref. [62]. Copyright 2020 by IEEE. (b) Advanced Ga-polar MMIC, the solid and dashed lines are the results in the actual measurement and simulation scenarios, respectively. Adapted with permission from Ref. [64]. Copyright 2016 by IEEE.

A thin double-cap layer structure, 2.6 nm of AlGaIn deposited on top of 10 nm UID GaN as the cap layer, facilitates gain enhancement and suppresses parasitic channels [66]. At a 1  $\mu$ s gate pulse width and an 800 ns drain pulse width, the test findings demonstrate that only around 10% dispersion ( $V_{GS,Q} = -6$  V,  $V_{DS,Q} = 0$  V) is observed. The gain enhancement due to the thin double-cap design facilitates the modulation effect of the gate on the 2DEG. It reduces the signal distortion of the device, enabling it to be more suitable for receivers that operate at low drain bias voltages.

More recently, Transphorm Inc. [67] has grown NPDR epitaxial stack on a 4-inch off-axis sapphire and a 4-inch off-axis C-face SiC substrates, respectively, and obtained excellent material quality characteristics for both, which demonstrates the feasibility of commercializing GaN NPDR MIS-HEMTs in the future. The STEM and typical AFM topography of the epitaxial stack are indicated in Figure 15. It can be seen in the STEM that the GaN buffer gradually filters out the linear dislocations starting from the nucleation layer to ensure the material quality in the upper HEMT region. In addition, there is a good hierarchical structure between the GaN and Al(Ga)N, with a low center-to-edge non-uniformity of about 0.3%. The low roughness average ( $R_a$ ) of only 1.1 nm (on 100 mm sapphire) and 1.5 nm (on 100 mm SiC) reveals that the N-polar epitaxial layer has a smooth surface, implying success in the large-size N-polar GaN wafers' growth. Researchers at Transphorm Inc. also found a low average  $R_{sh}$  of 234.3  $\Omega$ /sq for the 2DEG channel (with a 2% non-uniformity) owing to the 2DEG with an electron density of about  $1.44 \times 10^{13}$   $\text{cm}^{-2}$  and high electron mobility (is approximately 1850  $\text{cm}^2/\text{V}\cdot\text{s}$ ). It is worth mentioning that these values are the average mobility measured in both the parallel and perpendicular directions to the miscut steps. Thus, higher mobility and lower  $R_{sh}$  may be obtained if the current moves precisely in the parallel direction (along the terrace direction) of the actual deep recess devices.



**Figure 15.** (a) STEM cross-section of the N-polar GaN epitaxy and NPDR MIS-HEMT layers; (b) AFM topography image of N-polar GaN epitaxy on 100 mm sapphire and 100 mm miscut C-face SiC substrates. Adapted with permission from Ref. [67]. Copyright 2021 by IEEE.

The parameters and the performance of NPDR MIS-HEMTs operating in a range of frequencies are summarized in Table 2 for reference. The superior results imply that the NPDR structure is an efficient solution for suppressing surface dispersion of high-frequency devices, which may be commercially available and employed in the future RF industry, especially in the growing demand of the 5G market. However, it is necessary first to consider the poor heat dissipation caused by the current recovery. GaN-on-diamond may be a prospective option to address the thermal aggregation of NPDR GaN HEMTs in the future [68–70].

**Table 2.** Characterization of NPDR MIS-HEMTs applied to various wave bands, including epitaxial structures, output performances, and dispersion suppression.

Ref.	Band	Freq. (GHz)	Peak P <sub>o</sub>			Peak PAE			Disp. (%)	Cap Thk. (nm)	SiN <sub>x</sub> Thk. (nm)	Substrate
			V <sub>D</sub> (V)	P <sub>o</sub> (W/mm)	PAE (%)	V <sub>D</sub> (V)	P <sub>o</sub> (W/mm)	PAE (%)				
[55]	W	94	10	2.9	15.5	8	1.7	20	110	18	Sapphire	
[60]			14	4.2		8	1.6	16.5	22	NO	Sapphire	
[61]			16	5.5	20.6	12	3.7	25.9	20	20	Sapphire	
[71]			11	3.7		9	3.0	27.8	<5	47.5	NO	SiC
[72]			18	6.2	33.8	16	5.6	34.8		47.5	24	SiC
[49]			16	6.7	14.4	15	4.8	16.9	NO	47.5	NO	SiC
[73]			20	7.1	25.1	14	4.6	27.5		47.5	NO	SiC
[53]			20	7.9	26.9	16	5.3	28.8	<10	47.5	NO	SiC
[62]			23	8.8	27	20	7.2	30.2	8.5	47.5	40	SiC
[74]				87			8	2.5	34.2	NO	47.5	NO
[66]	Ka	30	20	8.1	52.5	14	5.6	55.9	10	12.6	20	SiC
[53]			26	10.3	47.4				<10	47.5	NO	SiC
[63]										47.5	40	SiC
[53]	X	10	20	7.8	54.9	14	5.1	58.1	<10	47.5	NO	SiC
[54]	C	4	24	5.5	74				NO	120	NO	Sapphire

### 5. Conclusions

GaN-based HEMTs have shown great performance in the microwave RF field. Nevertheless, the inherent high-density surface states of GaN and the inevitable defects during fabricating are potential sources of surface traps. In the switching transition of the device, the behaviors of trapping and delayed releasing electrons by the surface states are the leading causes of RF surface dispersion and pose a significant challenge to HEMTs to maintain high output power and stability. Accordingly, how to suppress RF dispersion in GaN devices is an interesting research problem.

Surface treatment, passivation, field plate, GaN cap layer, and Si surface doping are demonstrated to effectively suppress RF dispersion and are widely used in the industry.

While these methods provide varying degrees of dispersion suppression, as higher frequencies are explored, the exacerbated surface trapping effect or excessive parasitic capacitance makes these techniques progressively less effective.

N-polar GaN has many special advantages in high-frequency applications due to the opposite polarity, especially allowing the growth of a thick GaN channel (or thick UID GaN cap on the access region), providing an alternative way to minimize the dispersion caused by surface trapping at high frequencies. The utilization of a thick GaN layer keeps the surface far from the 2DEG channel to control the surface states and minimize the impact of surface charging on device operation. The isolation between the channel and the surface enables the NPDR structure to be considered the most promising approach for solving RF dispersion in GaN-based high-frequency power devices. In the past decade, the structural design of NPDR has been continuously improved, such as self-alignment for full coverage of the depression region with gate metal, simultaneous use of deep recess structure and SiN<sub>x</sub> passivation, and a double-layer structure for the receiver side. From the results, NPDR is expected to significantly contribute to the elimination of RF dispersion in high-frequency GaN HEMTs, restore their stability and inherent high power density, and is likely to be used in commercial 5G millimeter-wave RF devices in the future. However, the high price of SiC substrates, the high-quality requirements for N-polar GaN epitaxy, and heat dissipation are the primary impediments to large-scale industrial fabrication. Therefore, if more substantial progress can be achieved in addressing these obstacles, the application prospects of high-frequency GaN HEMTs will extend further.

**Author Contributions:** Conceptualization, P.Z. and X.G.; investigation, X.N. and Q.F.; resources, X.N. and Q.F.; data curation, P.Z. and X.G.; visualization, P.Z.; writing—original draft preparation, P.Z.; writing—review and editing, X.G.; funding acquisition, X.G. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research was funded by the National Nature Science Foundation of China, grant number 62074033.

**Data Availability Statement:** Not applicable.

**Acknowledgments:** The authors would like to thank Maxwell QH from Dulwich College Suzhou for his contribution to the English language and style in this work.

**Conflicts of Interest:** The authors declare no conflict of interest.

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Review

# Process of Au-Free Source/Drain Ohmic Contact to AlGa<sub>N</sub>/Ga<sub>N</sub> HEMT

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**Abstract:** AlGa<sub>N</sub>/Ga<sub>N</sub> high electron mobility transistors (HEMTs) are regarded as promising candidates for a 5G communication system, which demands higher frequency and power. Source/drain ohmic contact is one of the key fabrication processes crucial to the device performance. Firstly, Au-contained metal stacks combined with RTA high-temperature ohmic contact schemes were presented and analyzed, including process conditions and contact formation mechanisms. Considering the issues with the Au-contained technique, the overview of a sequence of Au-free schemes is given and comprehensively discussed. In addition, in order to solve various problems caused by high-temperature conditions, novel annealing techniques including microwave annealing (MWA) and laser annealing (LA) were proposed to form Au-free low-temperature ohmic contact to AlGa<sub>N</sub>/Ga<sub>N</sub> HEMT. The effects of the annealing method on surface morphology, gate leakage, dynamic on-resistance ( $R_{ON}$ ), and other device characteristics are investigated and presented in this paper. By using a low-temperature annealing atmosphere or selective annealing method, gate-first Si-CMOS compatible AlGa<sub>N</sub>/Ga<sub>N</sub> HEMT technology can be realized for high frequency and power application.

**Keywords:** AlGa<sub>N</sub>/Ga<sub>N</sub>; HEMT; ohmic contact; Au-free low-temperature

**Citation:** Zhang, L.-Q.; Wu, X.-L.; Miao, W.-Q.; Wu, Z.-Y.; Xing, Q.; Wang, P.-F. Process of Au-Free Source/Drain Ohmic Contact to AlGa<sub>N</sub>/Ga<sub>N</sub> HEMT. *Crystals* **2022**, *12*, 826. <https://doi.org/10.3390/cryst12060826>

Academic Editors: Peng Chen, Zhizhong Chen and Dmitri Donetski

Received: 24 April 2022

Accepted: 6 June 2022

Published: 10 June 2022

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## 1. Introduction

Traditional Si-based radio frequency (RF) and power devices, due to the physical limitation of Si material, cannot meet the requirements of higher-speed and higher-power in a 5G generation communication system. GaN-based HEMTs are regarded as promising candidates for high-frequency and high-power electronic devices due to their superior material properties [1–4]. The GaN-based materials are always heterogeneous and grown on other substrates, such as Si, SiC, and sapphire [5–8]. Among the heterojunction device structures, the AlGa<sub>N</sub>/Ga<sub>N</sub> HEMT exhibits the best electronic characteristics [9–11]. Furthermore, the AlGa<sub>N</sub>/Ga<sub>N</sub>-on-Si is the structure most commonly selected for power application for the following reasons [12–15]: the fabrication process is compatible with Si CMOS process flow, which helps to reduce the manufacturing cost. Realization of a large-size AlGa<sub>N</sub>/Ga<sub>N</sub>-on-Si wafer can also further reduce the cost. The regular epitaxial AlGa<sub>N</sub>/Ga<sub>N</sub> layers are grown on a high-resistivity Si substrate by metal organic chemical vapor deposition (MOCVD), which is shown in Figure 1. From Si bottom to top, a GaN buffer layer with a thickness of about 3 μm is deposited for reducing stress caused by lattice mismatch. After that, the device layer is formed by depositing an unintentional doped (UID) Ga<sub>N</sub> device layer (~100 nm), AlN interlayer (~1 nm), and Al<sub>x</sub>Ga<sub>1-x</sub>N barrier layer (~25 nm, x varies from 0.15–0.4). The two-dimensional electron gas (2DEG) is formed at

the AlGaN/GaN interface due to the polarization effect [16,17]. Finally, the GaN cap layer (~3 nm) is deposited for protecting the device surface.

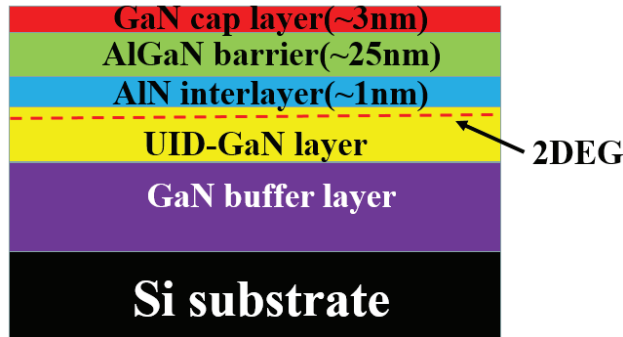


Figure 1. Schematic AlGaN/GaN-on Si device structure.

For RF application, the gate of the fabricated device is always formed in a T-shape for smaller gate resistance [18–20]. The process flow, which can be seen in Figure 2, consists of mesa isolation, source/drain ohmic contact formation, SiN passivation, T-shape gate formation, gate electrode deposition, via formation, and testing electrode deposition.

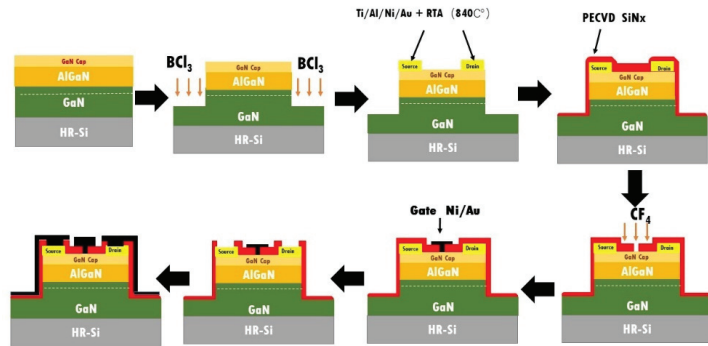


Figure 2. Schematic process flow of T-shaped AlGaN/GaN HEMT.

For power application, the gate is fabricated in a regular shape, as shown in Figure 3. The fabrication process consists of mesa isolation, source/drain ohmic contact formation, gate electrode deposition, SiN passivation, via formation, and testing electrode deposition.

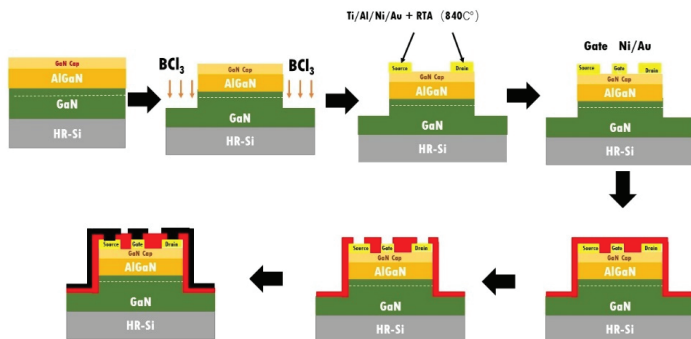


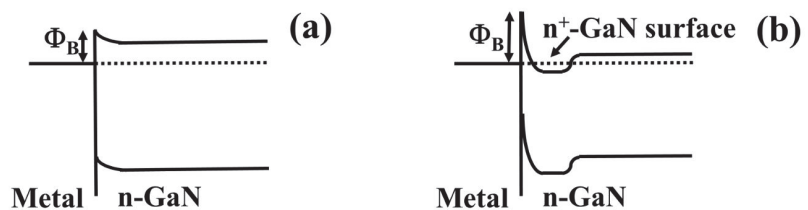
Figure 3. Schematic process flow of regular AlGaN/GaN HEMT.

The quality of source/drain ohmic contact has a great impact on the performance of AlGaIn/GaN HEMT, such as on-resistance ( $R_{on}$ ), output current ( $I_{DS}$ ), extrinsic transconductance ( $G_m$ ), and current gain cut-off frequency ( $f_T$ ) [11,21–25]. Always, the source/drain regions form ohmic contact to reduce  $R_{ON}$  and improve output current and  $f_T$  characteristics. Thus, the source/drain ohmic contact technique should be investigated. Over the years, researchers have systematically investigated ohmic contact to  $n^+$ -GaIn and AlGaIn/GaN for achieving low contact resistance ( $R_C$ ).

The most popular metallization schemes of ohmic contact in AlGaIn/GaN HEMT is Ti/Al/X/Au, where X can be Ni, Mo, Pt, Ta, Ir, etc. [26–30]. Ti/Al/X/Au Au-contained schemes will be discussed in Section 2. However, the Au-contained metal scheme is not suitable for Si-based CMOS fabrication lines because Au has a high diffusion coefficient in silicon, which can lead to heavy metal contamination [31,32]. The use of Au will increase the fabrication cost, and long-term Au diffusion will lead to ohmic contact degradation [31,33]. Thus, an Au-free ohmic contact metal scheme should be proposed and investigated for achieving the purpose. In Section 3.1, the most advanced Au-free ohmic contact techniques for AlGaIn/GaN HEMTs are displayed and discussed. Thermal budget is another issue that should be considered in AlGaIn/GaN HEMT source/drain ohmic contact formation. Traditional rapid thermal annealing (RTA) usually needs a high-temperature atmosphere to form ohmic contact between a metal stack and an AlGaIn/GaN heterojunction, which will lead to the oxidation of the AlGaIn surface and create N defects [34], degrading the dynamic performance of AlGaIn/GaN-based HEMTs. Also, TiN protrusions of random sizes take shape during the high-temperature annealing process [35]. Rough surface morphology and unideal ohmic metal edge sharpness can be observed to easily form short contact between the source/drain metal stack and gate metal electrode [36]. This phenomenon will be more severe for the Q band and Ka band small-sized AlGaIn/GaN HEMT. In addition, the high-temperature process is incompatible with the gate-first fabrication technique [37]. Thus, instead of pursuing the optimized annealing temperature of the RTA technique, a novel annealing technique may be employed as an alternative to form low-temperature Au-free AlGaIn/GaN HEMT ohmic contact with the existing Au-free metal schemes, including microwave annealing (MWA) and laser annealing (LA), etc. Details about MWA and LA techniques to form ohmic contact to AlGaIn/GaN HEMTs will be discussed in Section 3.2, which is promising for the realization of gate-first technology and a Si-CMOS compatible GaIn HEMT technique.

## 2. Ti/Al/X/Au Au-Contained Ohmic Contact Technique

Considering the wide bandgap of (Al)GaIn, two methods are adopted to form good quality ohmic contact: (1) reduce the barrier height( $\Phi_B$ ) by selecting the appropriate metal and (2) increase the possibility of tunneling by forming an  $n^+$ -(Al)GaIn surface. The energy band diagram of metal/(Al)GaIn by two methods are shown in Figure 4.



**Figure 4.** Energy band diagram of metal/(Al)GaIn by reducing the barrier height( $\Phi_B$ ) (a) and increasing the possibility of tunneling by forming  $n^+$ -(Al)GaIn surface (b).

For the first method, researchers selected Al, Ti, Au, Ni, Mo, Pd, Pt, Cr, etc. as contact metals and investigated their contact characteristics with (Al)GaIn [38–46]. The work function ( $W_m$ ), specific contact resistivity ( $\rho_c$ ), and  $\Phi_B$  characteristics of different metal materials can be seen in Table 1.

**Table 1.**  $W_m$ ,  $\rho_c$ ,  $\Phi_B$  characteristics of different metals to (Al)GaN.

Metal	$W_m$ (eV)	$\rho_c$ ( $\times 10^{-6} \Omega/\text{cm}^2$ )	$\Phi_B$ (eV)	Refs.
Al	4.28	8	0.8	[38,45]
Ti	4.33	3	0.58	[38–41,43]
Au	5.1	2.35	0.9	[38,43,44]
Ni	5.15	6.99	1.4	[38,41,44]
Mo	4.6	5.3	0.81	[42]
Pd	5.12	9.78	1.9	[38,46]
Pt	5.65	11	1.6	[38,41]
Cr	4.5	11.8	0.39	[41]

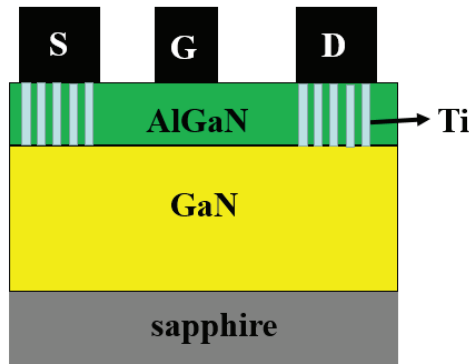
The results indicate that it is challenging to form good quality ohmic contact between single layer metal and (Al)GaN due to the higher  $W_m$  of the selected metal material. Also, the Ti, Al, etc. single layers are prone to oxidation during the high-temperature annealing process. Thus, a multilayer metal stack combined with a high-temperature annealing scheme became the common choice for GaN-based devices' source/drain ohmic contact formation [47]. The multilayer metal stack, as shown in Figure 5, always consists of four metal layers: the barrier layer, coating layer, diffusion barrier layer, and cap layer. The most popular metal scheme is Ti/Al/X/Au, where X can be Ni, Mo, Pt, Ta, Ir, etc. During the annealing process, the barrier layer Ti reacts with the AlGaIn layer to form TiN [48]. TiN carries out lower work function [49], which lowers the Schottky barrier height and therefore helps in ohmic contact formation. Also, the created N vacancies formed in the reaction process make the AlGaIn layer underneath the contact metal  $n^+$ -doped, which makes electron tunneling easy for ohmic contact formation [50]. Coating layer Al reacts with Ti under the high-temperature atmosphere to form  $\text{Al}_3\text{Ti}$ , which helps in ohmic contact formation [51]. The diffusion layer Ni, Mo, Pt, and Ta etc., which owns high melt point prevents Au indiffusion and Al outdiffusion [52]. Furthermore, the surface morphology of the contact metal can be affected by the metal layer. Au, which acts as a cap layer, prevents the Ti, Al layer oxidation within the high-temperature annealing atmosphere. Also, the Au layer improves the contact conductivity [53].

**Figure 5.** Schematic structure of metal stacks used for forming ohmic contact to AlGaIn/GaN HEMT.

Ohmic contact resistance  $R_C$ ,  $\rho_c$ , surface morphology, and thermal stability are the important indexes of ohmic contact quality. The  $R_C$  value can be affected by the selected metal stack, the metal thickness, ohmic recessing of the AlGaIn layer, surface pre-treatment prior to ohmic metallization, annealing time and temperature,  $n$ -type doped in the semiconductor, etc. [52,54–63]. These affecting factors were investigated and optimized by universities and research institutions. Jacobs B et al. [54] have systematically studied the influence of the metal stack, Ti, Al, Ni thickness, Ti/Al ratio, and annealing condition on  $R_C$ . In their results, the achieved optimized  $R_C$  is  $0.2 \Omega\text{-mm}$  with Ti thickness of 30 nm, Ti/Al

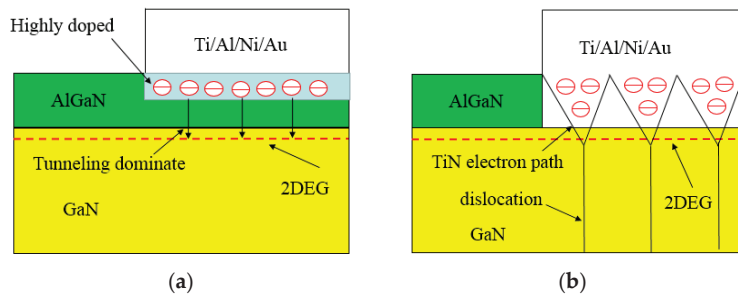


ratio of 6, Ni thickness of 40 nm, and annealing temperature of 900 °C for 30 s. Yan et al. [59] demonstrated that the  $R_C$  can be further reduced by a multi-step annealing process. With the improvement of AlGaIn/GaN material growth, ohmic contact formation for metal and AlGaIn/GaN becomes challenging. Buttari D et al. [60] developed a low-damage  $Cl_2$  reactive ion etching (RIE) recess etch on an AlGaIn layer (7nm), decreasing  $R_C$  from 0.45  $\Omega \cdot mm$  to 0.27  $\Omega \cdot mm$ . By Si ion implantation in the source/drain region, Nomoto K et al. [61] proved that the on-resistance can be decreased dramatically. By etching holes that were  $0.8 \mu m \times 0.8 \mu m$  in size and etching a depth of 10 nm, Wang et al. [62] developed a pattern of square holes technique in the source/drain AlGaIn layer and achieved an  $R_C$  as low as 0.1  $\Omega \cdot mm$ , as shown in Figure 6. The fabricated AlGaIn/GaN HEMTs exhibits comparable output current, peak transconductance and threshold voltage characteristics with conventional AlGaIn/GaN HEMTs. Before ohmic contact metal deposition, Fujishima T et al. [63] developed a  $SiCl_4$  and  $BCl_3$  plasma treatment on the source/drain surface and achieved low  $R_C$  values of 0.41  $\Omega \cdot mm$  and 0.17  $\Omega \cdot mm$ , respectively. By optimizing the affecting factors of Ti/Al/X/Au schemes, the achieved  $R_C$  can be as low as 0.3  $\Omega \cdot mm$ , and even much lower. The obtained low  $R_C$  can meet the requirements for the RF and power applications of AlGaIn/GaN HEMT by using Ti/Al/Ni/Au metal schemes.



**Figure 6.** Schematic structure of AlGaIn/GaN HEMT with holes etching in the ohmic region.

Universities and industries have conducted studies on the ohmic contact formation mechanism. Two methods are regarded as the mechanism to form ohmic contact to AlGaIn/GaN HEMT: (1) a field emission (FE) tunneling mechanism [64–66] via the formation of a thinner high doping or a lower barrier; and (2) a spike mechanism [67,68] by TiN direct electron path formation along the dislocation. In the FE tunneling mechanism, Ti reacts with the GaN or AlGaIn layer to form TiN. N should be extracted from GaN or AlGaIn, generating a highly n-doped interface region, which is responsible for the occurrence of FE tunneling. The work function of TiN (3.74 eV) is lower than Ti (4.33 eV), which is believed to lower the Schottky barrier for low-resistance ohmic contact formation. In the spike mechanism, the TiN projections forming along the dislocation places penetrate through the AlGaIn layer under a high temperature, which sets up a direct electron path connecting the 2DEG and the ohmic metal. This method is believed to be more efficient in electron transferring than the FE tunneling mode. With the improvement of AlGaIn/GaN material growth, the spike phenomenon, which penetrates through the whole AlGaIn layer, becomes less likely to happen. The cross-sectional diagrams of both physical models are shown in Figure 7, which reveals the ohmic contact formation mechanism.



**Figure 7.** Physical models of Ti/Al/Ni(x)/Au ohmic contact to AlGaN/GaN HEMT: FE tunneling mechanism (a) and spike mechanism (b).

### 3. Au-Free Ohmic Contact Technique

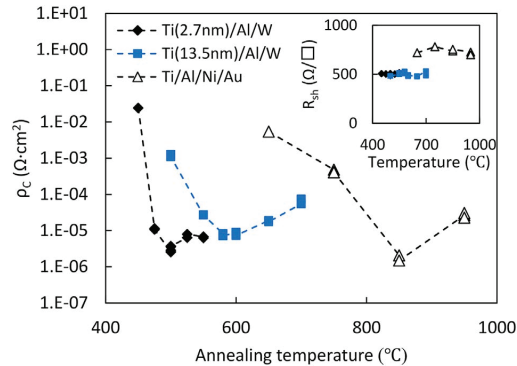
#### 3.1. Existing Advanced Au-Free Ohmic Contact Technology

The cap layer of Au is proposed to prevent the oxidation of ohmic metal under a high-temperature atmosphere. Au is also proposed to form Ga vacancies in AlGaN or GaN layers to decrease the contact resistance [31]. It is challenging to form high-quality ohmic contact with low contact resistance by using Au-free metal schemes. However, as mentioned in the introduction section, Au-contained metal schemes suffer from Si-based CMOS technology non-compatibility, rough surface morphology, and degradation of dynamic device performance. Also, the use of Au will increase the fabrication cost. Thus, Au-free ohmic contact metal schemes should be proposed and investigated for achieving the purpose. Over the years, groups from all over the world have studied and proposed a number of metal schemes, such as Ti/Al/W [33], Ta/Al/Ta [69], Ti/Al/Ti/TiN [70,71], Ta/Si/Ti/Al/Ni/Ta [72], Ti/Al/Ni/Pt [73], Ti/Al/TiN [74], Ti/TiN [75], Ti/Al/NiV [76], Ti/Al/Ti/W [77,78],  $Ti_xAl_y$  [79], and Ti/Al/Ni/Ti [80]. In these schemes, the cap layer of Au is replaced by W, TiN, and Ta, etc. For the Ti/Al-based method, Lee H S et al. [81] used a fully recessed AlGaN structure in the source/drain region, followed by a Ti/Al/W deposition and 870 °C annealing process, reducing the  $R_C$  to 0.49  $\Omega \cdot \text{mm}$ . This method enables the direct contact between Ti/Al/W and 2DEG. The Ti/Al/W metal stacks also exhibit much smoother morphology and a much lower voltage drop property for the same output current level, which is a very important characteristic for high-voltage power electronics. The source/drain AlGaN layer can be partially recessed to achieve ohmic contact with an  $R_C$  of 0.21  $\Omega \cdot \text{mm}$  using Ti/Al/Ti/TiN at the low temperature of 550 °C [71]. By optimizing the Ti thickness (2.5 nm) and annealing temperature (550 °C), the low  $R_C$  ohmic contact can be realized. High-resolution transmission electron microscopy (HR-TEM) and electron dispersive X-ray spectroscopy (EDS) were adopted to investigate alloy distribution and the ohmic contact formation mechanism. From the TEM and EDS results as shown in Ref. [71], they deduced that Ti plays a catalytic role for the Al-N reaction and N extraction. The formation of a continuous AlN thin layer at the contact interface accounts for the low resistance of Au-free ohmic contacts on AlGaN/GaN at a low annealing temperature.

Yoshida T et al. [33] reduced the  $R_C$  to 0.358  $\Omega \cdot \text{mm}$  at the low temperature of 500 °C by optimizing the thickness (a thin Ti layer of 2.7 nm) of Ti using Ti/Al/W, as shown in Figure 8. The fabricated devices have a maximum drain current density ( $I_{DS}$ ),  $R_{ON}$ , and peak transconductance ( $G_m$ ) of 0.422 A/mm, 9.7  $\Omega \cdot \text{mm}$  and 73.2 mS/mm, respectively. These characteristics are comparable to Au-contained AlGaN/GaN HEMTs.

Furthermore, the cap layer can be replaced by Pt, Ni, and NiV. Liu et al. [73] used a Ti/Al/Ni/Pt Au-free metal stack and achieved an  $R_C$  of 0.6  $\Omega \cdot \text{mm}$  at 975 °C annealing temperature. The maximum drain current and  $G_m$  achieved 700 mA/mm and 140 mS/mm, respectively. Tham W H et al. [76] used a Ti/Al/NiV source/drain metal stack scheme and achieved an  $R_C$  of 0.8  $\Omega \cdot \text{mm}$  featuring the low temperature of 500 °C. The AlGaN/GaN MIS-HEMTs were fabricated and measured. The achieved specific on-state resistivity

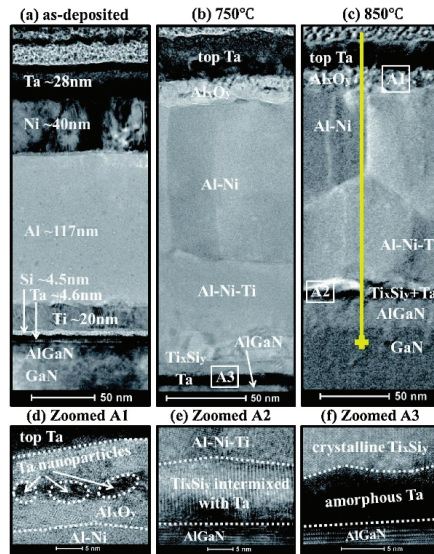
and maximum saturation drain current were  $2.3 \text{ m}\Omega \text{ cm}^2$  and  $0.21 \text{ A/mm}$ . Gao et al. [80] demonstrated a two-step Ti/Al/Ni/Ti Au-free ohmic contact technique (Ti/Al deposited by EBE and Ni/Ti grown by magnetron sputtering) and achieved an  $\rho_c$  of  $5.59 \times 10^{-5} \Omega/\text{cm}^2$ . The achieved maximum saturation drain current and  $R_{\text{ON}}$  reached around  $0.4 \text{ A/mm}$  and  $15.6 \Omega\text{-mm}$ .



**Figure 8.** Specific contact resistivity  $\rho_c$  vs. annealing temperature. All samples were annealed for 1 min, except for samples with Ti (2.7 nm)/Al/W, which were annealed for 10 min. The inset shows the corresponding channel sheet resistances  $R_{\text{sh}}$ . Reprinted with permission from Ref. [33]. Copyright 2018, Wiley.

Ta-based schemes were also proposed to form ohmic contact to AlGaIn/GaN heterojunctions. Li et al. [82] deposited a Ta/Si/Ti/Al/Ni/Ta metal stack and achieved a low  $R_C$  of  $0.22 \Omega\text{-mm}$  by optimizing the annealing temperature. The ohmic contact formation was also investigated by using X-ray diffraction (XRD), TEM, and EDS analysis, as shown in Figure 9. It was deduced that the formation of  $\text{Ti}_x\text{Si}_y$  alloy with a low work function and intermixing with Ta results in a low ohmic contact resistance  $R_C$ . Johnson D W et al. [69] used a  $\text{Cl}_2$  plasma etch to recess the whole AlGaIn barrier layer in the source/drain region and deposit a Ta/Al/Ta layer with optimized thickness. The achieved  $R_C$  can be as low as  $0.2 \Omega\text{-mm}$  with the annealing temperature lower than  $600^\circ\text{C}$ . Maximum drain current is found to be  $236 \text{ mA/mm}$  at  $V_{\text{DS}} = 10 \text{ V}$ . Maximum transconductance and  $R_{\text{ON}}$  were  $55 \text{ mS/mm}$  and  $41.3 \Omega\text{-mm}$ , respectively. Considering the recess ohmic contact technique increased the fabrication complexity, in 2021, Fan et al. [79] developed a non-recessed Ti-Al alloys Au-free scheme instead of Ti/Al-based multilayers. By optimizing the ratio of Ti in  $\text{Ti}_x\text{Al}_y$  and annealing temperature, the low  $R_C$  of  $0.063 \Omega\text{-mm}$  can be obtained with  $\text{Ti}_5\text{Al}_1$  under the optimal annealing condition. The EDS and TEM results as shown in Ref. [79] show that the Al outdiffusion can be suppressed and Ti can deeply diffuse into the AlGaIn barrier layer by using  $\text{Ti}_x\text{Al}_y$  alloy. The extracted N atoms increase with an increasing Ti ratio of  $\text{Ti}_x\text{Al}_y$ . Therefore, a higher Ti ratio  $\text{Ti}_x\text{Al}_y$  is beneficial in forming a highly doped n-type AlGaIn region, resulting in a much lower ohmic contact  $R_C$ . Furthermore, their group proposed an Au-contained  $\text{Ta}_{0.83}\text{Al}_{0.17}/\text{Au}$  metal scheme to realize a low ohmic contact of  $0.14 \Omega\text{-mm}$  at  $900^\circ\text{C}$  [83]. Unlike the spike mechanism in the Ti/Al/Ni/Au method, the Ta-Al-Au mixed more uniformly with each other so that Au-dominated alloy fully penetrated the AlGaIn barrier layer for electron path formation. Thus, the  $R_C$  could be decreased drastically.

Au-free ohmic contact formation can also be realized by intentional ion implantation in the AlGaIn/GaN within the source/drain region [84]. In addition, selective regrowth of the source/drain region after the partial AlGaIn etching can also realize Au-free ohmic contact formation [85,86]. However, these methods require strict process conditions, increase the fabrication cost, and make the fabrication process more complex. Therefore, only few universities and institutions investigate these techniques.



**Figure 9.** Cross sectional high-resolution TEM images of (a) as-deposited, (b) 750 °C-annealed, (c) 850 °C-annealed non-gold ohmic contacts. (d,e): zoomed-in TEM images of Ta/Ni interface (A1) and metal/AlGaIn interface (A2) of 850 °C-annealed non-gold contact in (c), respectively, and (f): zoomed-in TEM image of metal/AlGaIn interface (A3) of 750 °C -annealed non-gold (Ta/Si/Ti/Al/Ni/Ta) ohmic contact in (b). Reprinted with permission from Ref. [82]. Copyright 2013, IOP science.

The AlGaIn/GaN HEMTs devices' electrical characteristics, with the existing advanced Au-free ohmic contact technique, can be summarized in Table 2. The results show that AlGaIn/GaN HEMTs with Au-free ohmic contacts exhibit similar electrical characteristics comparable to Au-contained AlGaIn/GaN HEMTs. The surface morphology of Au-free ohmic metals is more flat than the Au-contained ones due to the smaller root mean square (RMS) surface roughness.

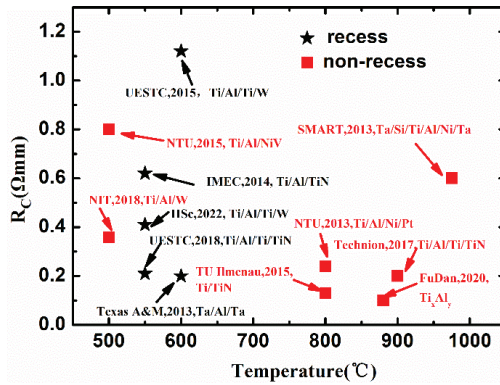
**Table 2.** Survey of literature data on GaN HEMTs using different Au-free ohmic contact schemes.

Au-Free Schemes	$R_C$ ( $\Omega$ ·mm)	$I_{dmax}$ (mA/mm)	$R_{ON}$ ( $\Omega$ ·mm)	Specific On-State Resistivity ( $m\Omega/cm^2$ )	$G_m$ (mS/mm)	Root-Mean-Square (RMS) Surface Roughness (nm)	Ref.
Ti/Al/W	0.358	422	9.7	/	73.2	/	[33]
Ta/Al/Ta	0.2	263	41.3	/	55	/	[69]
Ti/Al/Ti/TiN	0.21	/	/	/	/	/	[71]
Ta/Si/Ti/Al/Ni/Ta	0.24	830	/	/	250	/	[72]
Ti/Al/Ni/Pt	0.6	700	/	0.77	140	4.6	[73]
Ti/Al/TiN	0.62	/	/	/	/	/	[74]
Ti/Al/NiV	0.13	210	/	2.3	60	/	[76]
Ti/Al/Ti/W	0.41	350	/	/	/	7	[78]
Ti <sub>x</sub> Al <sub>y</sub>	0.063	/	/	/	/	/	[79]
Ti/Al/Ni/Ti	/	400	15.6	6.39	/	7.9	[80]

### 3.2. Low-Temperature Au-Free Ohmic Contact Technology

The benchmark of  $R_C$  values against annealing temperatures of state-of-the-art Au-free ohmic contacts for the AlGaIn/GaN HEMT can be seen in Figure 10, including recess and non-recess schemes [33,69–82]. It can be seen that low  $R_C$  values (<0.3  $\Omega$ ·mm) always occur

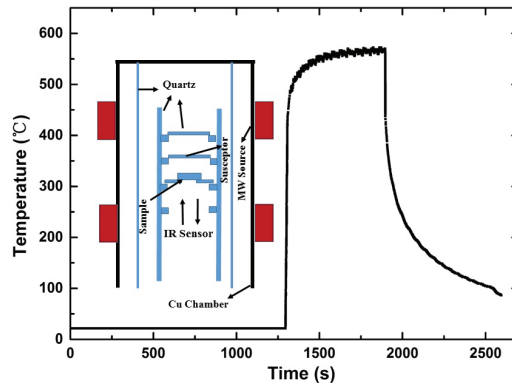
with high annealing temperature ( $>600$  °C) conditions. Only a few methods meet the low  $R_C$  and low annealing temperature requirements. Thermal budget is another issue that should be considered in AlGaIn/GaN HEMT source/drain ohmic contact formation.



**Figure 10.** Comparison of  $R_C$  as a function of annealing temperature of different Au-free ohmic contact to AlGaIn/GaN HEMT from various publications.

A high-temperature atmosphere will lead to the oxidation of AlGaIn surfaces and create N defects [34], degrading the dynamic performance of AlGaIn/GaN-based HEMTs. Also, TiN protrusions of random sizes take shape during the high-temperature annealing process [35]. Rough surface morphology and unideal ohmic metal edge sharpness can be observed, easily forming short contact between the source/drain metal stack and gate metal electrode [36]. This phenomenon will be more severe for the Q band and Ka band small-sized AlGaIn/GaN HEMT. In addition, the high-temperature process is incompatible with the gate-first fabrication technique [37]. Thus, the Au-free low-temperature ohmic contact technique should be investigated and proposed for AlGaIn/GaN HEMT. Au-free ohmic contact with AlGaIn/GaN HEMT always needs a high temperature for contact formation using traditional RTA. With the existing optimized Au-free metal schemes, the annealing method might be another element which affects the ohmic contact quality. Therefore, the novel annealing technique should be introduced for low-temperature Au-free ohmic contact to AlGaIn/GaN HEMT. A novel annealing technique may be employed and investigated for AlGaIn/GaN HEMT ohmic contact formation: microwave annealing (MWA) and laser annealing (LA), etc.

**MWA:** as a novel annealing technique, MWA has special characteristics (including selective heating of specific materials, rapid heating rates and temperature gradients, the elimination of wall effects, and the superheating of solvents) and non-thermal effects [87]. Ohmic metals and 2DEG have strong ability to absorb microwaves. Thus, MWA can be an alternative to AlGaIn/GaN HEMT source/drain ohmic contact formation. Using an Au-contained Ti/Al/Ni/Au metal stack, Zhang et al. [88] demonstrated that a low temperature of approximately 600 °C can be used to achieve good quality of ohmic contact ( $R_C = 0.6 \Omega\text{-mm}$ ) with an MWA power of 4200 W and heating time of 20min, as shown in Figure 11 [89]. High-resolution atomic force microscope (AFM) results show that the MWA-HEMT source/drain ohmic metal surface, after annealing process, is relatively flat compared to the RTA one.  $R_C$  values and root mean square (RMS) surface roughness characteristics for various MWA conditions are compared with the RTA method and shown in Table 3 [90].

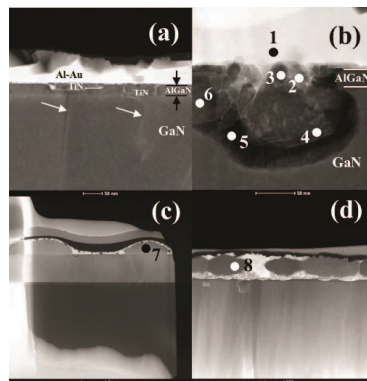


**Figure 11.** The schematic diagrams of MWA equipment. Reprinted with permission from Ref. [89]. Copyright 2017, IEEE.

**Table 3.** Comparisons of peak temperature,  $R_C$ , and RMS characteristics for various annealing conditions. Reprinted with permission from Ref. [90]. Copyright 2016, IEEE.

Methods	Peak Temperature (°C)	$R_C$ ( $\Omega$ -mm)	RMS (nm)
MWA, 3500 W, 20 min	579.6	1.16	37.7
MWA, 4200 W, 5 min	579.6	4.57	37.5
MWA, 4200 W, 10 min	594	4.02	35.8
MWA, 4200 W, 15 min	597.6	1.44	49.6
MWA, 4200 W, 20 min	597.6	0.6	63.5
RTA, 840 °C, 35 s	840	0.4	101

TEM and EDS analysis are employed to learn the ohmic contact formation mechanism and reasons for surface roughness [88]. From the TEM and EDS results, as shown in Figure 12a,b, a direct current path is also formed in MWA-HEMT, which facilitates the flow of electrons in both directions, indicating that the spike mechanism is still the major mechanism of forming carrier conduction paths. From the EDS results as shown in Table 4, we deduce that less Ni-Au blocks were formed under a low-temperature atmosphere, which accounts for the superior surface morphology formation.



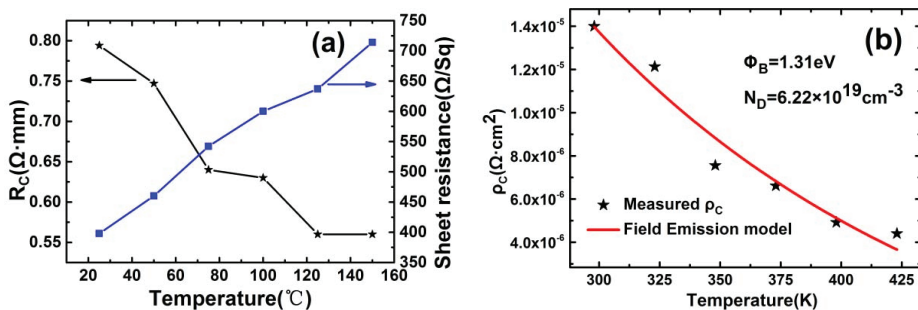
**Figure 12.** (a) TEM image of the post-annealing structure by MWA where the arrows markings indicate dislocations. (b) Magnified image of the interface. (c) TEM image of bulge area of the alloyed ohmic contact treated by RTA. (d) TEM image of bulge area of the alloyed ohmic contact treated by MWA. Reprinted with permission from Ref. [88]. Copyright 2015, IEEE.



**Table 4.** EDS Composition (at. %) from the points labeled in Figure 12. Reprinted with permission from Ref. [88]. Copyright 2015, IEEE.

	N	Al	Ti	Ni	Ga	Au
1		26.37		2.76		70.87
2		9.95	57.37	7.10	3.42	22.16
3			89.30	2.47		8.23
4		8.96	83.24	1.63		6.16
5		97.81	1.59			0.60
6	19.53	20.27	23.75		35.20	1.26
7		48.77		45.49	5.75	
8		51.35		48.65		

The MWA-HEMT also exhibits good gate leakage and output current characteristics as compared to RTA-HEMT. The maximum drain current value reaches 850 mA/mm. The MWA method was also employed to form ohmic contact to AlN/GaN HEMT [89] and InAlN/GaN HEMT [91]. For InAlN/GaN HEMT, Chou et al. [91] fabricated an MWA-HEMT, which exhibits better  $R_{ON}$ , subthreshold swing (SS), RF performance, and current gate leakage characteristics than the RTA one. Furthermore, MWA-HEMT ohmic contact has a much smoother surface morphology, which results in high reliability. For AlN/HEMT [89], MWA also delivers better surface morphology and a lower gate leakage current. The ohmic contact formation mechanism was also studied. The experimental results fit well with the field emission (FE) model, as shown in Figure 13.

**Figure 13.** (a) Temperature–dependent characteristics of the  $R_{SH}$  and  $R_C$  of MWA–HEMT. (b) Measured (symbols) and modeled (lines)  $\rho_C$  of MWA–HEMT as a function of temperature. Reprinted with permission from Ref. [89]. Copyright 2017, IEEE.

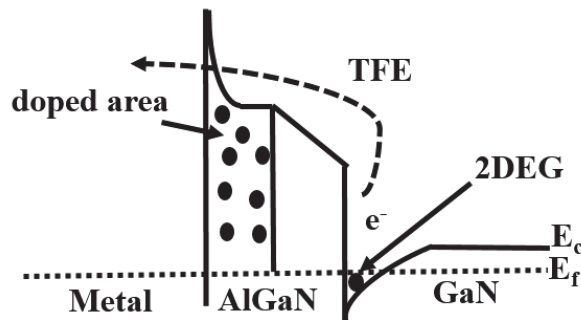
The MWA GaN-based HEMTs devices' electrical characteristics compared to the RTA ones can be summarized in Table 5 as follows: the results show that MWA-HEMT exhibits comparable  $R_C$ , output current,  $G_M$  characteristics, and better  $R_{ON}$  and surface morphology. Thus, considering the excellent advantages of MWA, combined with Ti/Al-based, Ta-based, and Ti<sub>x</sub>Al<sub>y</sub> metal stack schemes, the MWA method is promising to realize low-temperature Au-free ohmic contact formation to AlGaN/GaN HEMT instead of pursuing an optimized record-low temperature for the RTA method.

LA: Tzou A J et al. [92] demonstrated the incorporation of a Si implantation in the GaN HEMTs and non-alloyed ohmic contact process by using the LA method. The surface morphology, contact resistance, on-resistance, and surface trap density can be improved by LA instead of the RTA technique. Ferreyra R A et al. [93] achieved a non-alloy ohmic contact using a Hf/Al/Ti metal stack with the picosecond LA method, featuring the  $R_C$  of 0.17  $\Omega$ ·mm. Without source/drain n<sup>+</sup> GaN regrowth, Sheng's group proposed a laser annealing (LA) for AlGaN/GaN HEMT ohmic contact formation with a Ti/Al/Ni/Au metal stack [94]. The fabricated LA-HEMT exhibits smooth morphology, low contact resistance, high breakdown voltage and low dynamic on-resistance. The wafer is not

damaged during the LA period due to the larger energy bandgap of GaN than LA photon energy. By applying a wavelength of 532 nm, 20 ns of a pulse duration, 100 kHz of pulse frequency, and energy density up to 2.99 J/cm<sup>2</sup>, the achieved  $R_C$  is 2.18  $\Omega\cdot\text{mm}$  [95]. The ohmic contact formation mechanism by LA has been studied and proposed. The experiment's data fit the thermionic field emission (TFE) model closely. From their results they deduce that the current transport mechanism of the LA sample is dominated by thermionic field emission (TFE). The energy band diagram for the contacts annealed by LA can be seen in Figure 14.

**Table 5.** GaN-based HEMTs devices' electrical characteristics: MWA vs. RTA [88–91].

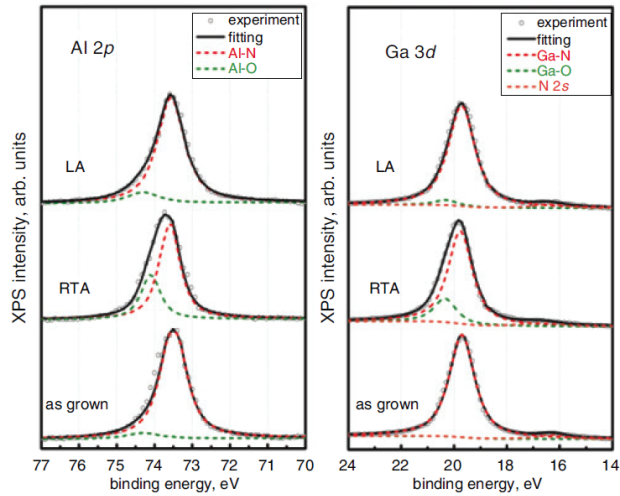
Material	Methods	Temperature (°C)	$R_C$ ( $\Omega\cdot\text{mm}$ )	$\rho_c$ ( $\times 10^{-5}\Omega/\text{cm}^2$ )	RMS (nm)	$I_{dmax}$ (mA/mm)	$R_{ON}$ ( $\Omega\cdot\text{mm}$ )	$G_m$ (mS/mm)
AlGaIn/GaN	MWA	579.6	0.6	/	63.5	850	/	/
AlGaIn/GaN	RTA	840	0.4	/	101	800	/	/
AlN/GaN	MWA	572.4	0.65	/	29.3	1400	/	270
AlN/GaN	RTA	750	0.4	/	56.5	1320	/	267
InAlN/GaN	MWA	/	/	4.29	6.79	/	4.9	/
InAlN/GaN	RTA	875	/	4.02	115	/	6.1	/



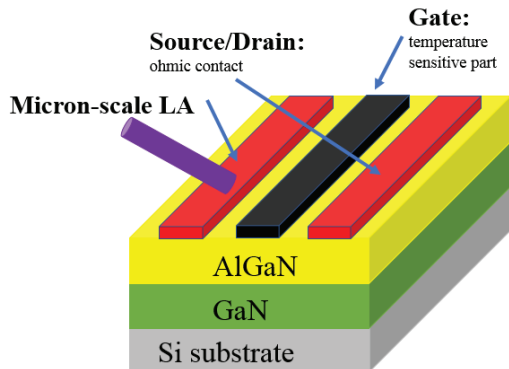
**Figure 14.** The schematic energy band diagram for the contacts annealed by LA.

The LA method results in a much smoother surface morphology due to less metal diffusion and alloy aggregation for the ultra-short LA time. They also studied the surface damage condition by LA and compared it with the RTA method [96]. The X-ray photoelectron spectroscopy (XPS) results, as shown in Figure 15, show that the oxidation reaction with a high-temperature atmosphere can be eliminated by the LA method. Also, Au-free ohmic contact using an Au-free Ti/Al/Ni/W metal stack combined with the LA annealing technique was proposed and studied. The LA-HEMT exhibits better isolation leakage current, low-density surface states, and suppressed  $R_{ON}$  [97].

Instead of a whole device region under a high-power laser pulse, Liu et al. [98] proposed a micro-scale LA approach to form ohmic contact to AlGaIn/GaN HEMT. The schematic illustration of the micron-scale laser annealing is shown in Figure 16. Due to the selective source/drain region heating by LA, the gate electrode, which is temperature sensitive, is not thermally affected. Therefore, gate-first devices are realized using this micro-scale LA technique. The extracted  $R_C$  is as low as 0.3  $\Omega\cdot\text{mm}$  when the laser power setting is 0.9 W. The high heating rate tends to form a thicker TiN layer, leaving a high density of N vacancy in AlGaIn which makes tunneling much easier. In addition, the LA-HEMT shows better output current and smaller gate leakage.



**Figure 15.** XPS core-level spectra of AlGaIn surface as grown, after RTA and after the LA method. Reprinted with permission from Ref. [96]. Copyright 2019, Wiley.



**Figure 16.** The schematic diagrams of micron-scale LA.

The LA GaN-based HEMTs devices' electrical characteristics compared to the RTA ones can be summarized in Table 6 as follows: from the testing results [94], the laser annealing reveals smooth morphology, low contact resistance, high breakdown voltage, and low dynamic on-resistance for the fabricated devices combined with the existing Au-free metal stack technique; this method is beneficial for gate-first technology and Si-CMOS compatible GaN HEMT technique.

**Table 6.** GaN-based HEMTs devices' electrical characteristics: LA vs. RTA.

Methods	$R_C$ ( $\Omega$ -mm)	RMS (nm)	$I_{dmax}$ (mA/mm)	$R_{ON}$ ( $\Omega$ -mm)	$G_m$ (mS/mm)	Ref.
LA	2.18	16.5	329	14.4	/	[94]
RTA	0.85	/	330	14.3	/	[94]

#### 4. Conclusions

In this work, the conventional AlGaIn/GaN HEMT Ti/Al/Ni/Au Au-contained ohmic contact technique was discussed comprehensively, including the selected metal stack, the metal thickness, ohmic recessing the AlGaIn layer, surface pre-treatment prior to

ohmic metallization, annealing time and temperature, n-type doped in the semiconductor, etc. After that, the existing Au-free ohmic contact was briefly introduced. In addition, to lower the thermal budget for the annealing process, novel MWA and LA annealing techniques were proposed for low-temperature Au-free ohmic contact to AlGaN/GaN HEMT, which is beneficial for gate-first technology and Si-CMOS compatible GaN HEMT technique realization.

**Author Contributions:** L.-Q.Z.; writing—original draft, investigation, data curation, conceptualization. X.-L.W., W.-Q.M., Z.-Y.W.; writing—original draft, investigation, data curation, conceptualization. Q.X., P.-F.W.; writing—review & editing, visualization, validation. All authors have read and agreed to the published version of the manuscript.

**Funding:** This work was supported in part by the Doctoral Scientific Research Start-Up Foundation of Henan Normal University under Grant 5101239170008, Henan Province Natural Science Foundation of Youth Fund No. 212300410185, Key scientific research projects of higher education institutions in Henan Province No. 21A510005, 22B510009 and in part by Key Laboratory of Optoelectronic Sensing Integrated Application of Hennan Province.

**Institutional Review Board Statement:** Not applicable.

**Informed Consent Statement:** Not applicable.

**Data Availability Statement:** Not applicable.

**Conflicts of Interest:** The authors declare no conflict of interest.

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ISBN 978-3-0365-8625-0