

Title	Barrier-channel intermixing and 2-dimensional electron gas degradation in Al-rich Al(Ga)N/AlGaN high electron mobility transistor heterostructures
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Publication date	2026-07-01
Original Citation	Pampili, P, Zubialevich, V Z, Mondal, B, Mukherjee, J, Schulz, S, Moran, D A J & Parbrook, P J 2026, 'Barrier-channel intermixing and 2-dimensional electron gas degradation in Al-rich Al(Ga)N/AlGaN high electron mobility transistor heterostructures', Applied Physics Letters, vol. 128, no. 26, 262108, pp. 1-6. https://doi.org/10.1063/5.0325471
Type of publication	Article (peer-reviewed)
Link to publisher's version	https://www.scopus.com/pages/publications/105043980007 - 10.1063/5.0325471
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Download date	2026-10-24 14:51:52
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Barrier–channel intermixing and 2-dimensional electron gas degradation in Al-rich Al(Ga)N/AlGaN high electron mobility transistor heterostructures

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Appl. Phys. Lett. 128, 262108 (2026)

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Cite as: Appl. Phys. Lett. **128**, 262108 (2026); doi: [10.1063/5.0325471](https://doi.org/10.1063/5.0325471)

Submitted: 30 January 2026 · Accepted: 8 June 2026 ·

Published Online: 1 July 2026



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Note: This paper is part of the Special Topic on Frontiers in Nitride Semiconductors Research.

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ABSTRACT

In this work, we report on recent results in understanding and addressing the issue of interface smearing in high-aluminum content AlGa_{0.75}N/AlGa_{0.25}N heterostructures. On the one hand, the growth of high-crystal quality AlGa_{0.75}N by metal-organic vapor phase epitaxy requires the use of high temperatures, but, on the other hand, this may lead to alloy intermixing between barrier and channel layers, which smoothens out the polarization contrast and severely degrades or even completely destroys the 2-dimensional electron gas (2DEG). We show that x-ray diffraction analysis can be used as a nondestructive way to assess the sharpness of the interface, and that improved growth schemes can be successfully used to achieve high-quality 2DEG, as confirmed by contactless resistivity measurements. In particular, sheet resistivities around 2500 Ω/□ were demonstrated for AlN/Al_{0.75}Ga_{0.25}N, consistent with the best-reported values in the literature.

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AlGa_{0.75}N/GaN high electron mobility transistors (HEMTs) have emerged as one of the most successful electronic devices for high-frequency and high-power-density applications, owing to the exceptional mobility and high carrier density of the characteristic 2-dimensional electron gas (2DEG) formed at the AlGa_{0.75}N/GaN interface. Despite the success of these devices, it has become challenging to keep up with industry demands for increased high voltage and high-power operation, as the technology is fast approaching material limits.

An approach that has attracted significant interest is the replacement of GaN with Al-rich AlGa_{0.75}N as the channel material, in order to exploit the advantages of ultra-wide bandgap semiconductors.^{1–3} However, such AlGa_{0.75}N/AlGa_{0.25}N HEMTs are still at an early stage of development, and several challenges remain to be addressed. In this study, we report about a new understanding of the impact of barrier-channel intermixing on the conductivity of the 2DEG as well as a growth and characterization strategy to overcome this issue.

The samples discussed in this study were grown by metal-organic vapor phase epitaxy (MOVPE) using an AIXTRON CCS 3 × 2" showerhead reactor, with trimethylgallium (TMGa), trimethylaluminum (TMAI), and ammonia (NH₃) as precursors for Ga, Al, and N, respectively. Before the growth of the actual HEMT heterostructures, a number of AlN templates were grown on sapphire wafers using an approach previously reported elsewhere.⁴ The template thickness was set in the range 2.0–2.5 μm, which was sufficient to ensure good crystal quality, with a threading dislocation density on the order of low 10⁹ cm^{−2}, while simultaneously avoiding excessive tensile strain and suppressing crack formation, a known issue in thick AlN templates grown on sapphire.⁵ To ensure a fair comparison, only templates with similar crystal quality were used to overgrow the HEMT structures for this study.

At the start of each run, the templates were initially heated in an ammonia atmosphere (500 sccm) and baked for 5 min at a temperature of 1120 °C and a pressure of 100 mbar, followed by the growth of

a 200 nm AlN connecting layer, prepared under the same conditions used for the templates. Subsequently, a 600-nm thick AlGaIn channel of different compositions was grown, followed by an Al(Ga)N barrier with higher Al content than in the channel, and a thickness of 50 nm (unless otherwise specified). Both barrier and channel were grown at a pressure of 50 mbar, V/III ratio of 1000, and a total gas flow of 8 slm, which resulted in a growth rate of approximately 0.58 nm/s. The relatively high V/III ratio was selected based on the results of a previous study,⁶ in which it led to smoother AlGaIn surface morphologies compared with those obtained under standard AlGaIn growth conditions, which typically use V/III ratios in the range of 50–100. The growth temperature was kept at 1160 °C for the channel but was varied in the range 850–1160 °C for the barrier, as will be discussed in more detail later. The growth temperatures here reported were measured using an *in situ* Laytec EpiCurve TT pyrometer system, which uses corrected infrared emissivity at 950 nm.

After growth, the samples were analyzed for crystal quality, composition, and strain-relaxation by x-ray diffraction (XRD), using a Malvern Panalytical X'Pert Pro diffractometer equipped with a 2-bounce hybrid monochromator and a PIXcell solid-state 2D detector. The crystal quality was estimated by the full-width at half maximum (FWHM) of the ω -scans of symmetric 002 and skew-symmetric 101 reflections, which led to peak broadening below 300 and 650 arc sec, respectively.

For analysis purposes, in addition to the above-mentioned AlN templates optimized for crystal quality, bufferless auxiliary substrates were co-loaded in almost all growth runs. These substrates were commercially sourced templates, in which a thin AlN nucleation layer of approximately 25 nm was sputtered on sapphire wafers. The HEMT structures overgrown on these bufferless substrates consistently exhibited FWHM values of the order of 2400 arc sec for the 101 reflection of the AlGaIn channel. This is more than three times larger than those measured in HEMT structures grown on AlN templates with thick buffers and corresponds to roughly an order of magnitude increase in edge dislocations. The formation of a very high dislocation density in these samples was intentional, in order to promote relaxation in the channel through dislocation bending⁷ and to enable separation of the AlN XRD reflections of the barrier from those of the buffer, as discussed later.

To determine composition and relaxation state of the different samples, reciprocal space maps (RSMs) of the asymmetric 105 reflection were collected. To compensate for alignment errors that produce random ω offsets among different samples, $\bar{1}05$ reflections (i.e., the reflections with opposite ω - θ offsets) were also measured, and the RSMs were rotated by the angle necessary to align both reflections at the same Q_z while maintaining opposite Q_x . Composition and degree of relaxation were calculated using the lattice constants and elastic properties reported in Ref. 8 and references therein. Processing and analysis of the RSM data were done using our in-house developed open-access *xrddy* Python package.⁹ The thicknesses of the barrier layers were measured, when possible, by x-ray reflectivity (XRR).

In the first sample of this study, a pure AlN barrier was grown immediately after the channel at a temperature of 1160 °C. The sample was generally smooth, with only a few cracks visible by optical Nomarski microscopy, mostly at the wafer edges, caused by a somewhat thicker AlN buffer; this issue was corrected in the subsequent samples.

As shown in Fig. 1(a), two main peaks are apparent in the RSMs, which correspond to AlN (barrier and buffer) and AlGaIn (channel). The vertical alignment of the two peaks indicates that barrier and channel remained coherently strained to the buffer, and a channel composition of 80% AlN was calculated. A particularly interesting feature of this RSM is the presence of a high-intensity streak connecting the two peaks, consistent with a relatively thick graded interface. This interpretation is further supported by the absence of Kiessig fringes in the XRR measurements.¹⁰

Although sharp heterointerfaces also produce characteristic streaks called crystal truncation rods (CTRs),¹¹ their intensity typically follows a power-law decay with increasing Q_z distance from the main Bragg peaks, which is not observed in our samples. Instead, the nearly constant intensity of the streak connecting the AlN and AlGaIn peaks suggests the presence of a graded layer with an approximately linear variation in composition.

To rule out any effect due to the relatively high V/III ratio, the same nominal structure was grown also with the AlN barrier deposited at a V/III ratio of 50. No detectable differences were observed compared with the sample in which the entire HEMT structure was grown at a V/III ratio of 1000.

In order to understand if the interface grading observed in the RSM was at the channel–buffer, barrier–channel, or at both interfaces, the co-loaded sample grown on the bufferless auxiliary template was also analyzed, and the results are shown in Fig. 1(b). As highlighted by the two arrows, the interface between the AlN connecting layer and the channel does not show any streak (green arrow), which is consistent with a rather sharp interface. However, the barrier/channel interface shows the same high-intensity streak (red arrow) already observed in the strained sample.

One possible explanation for this behavior, namely, the formation of a sharp interface when the TMGa source is opened and a graded interface when it is closed, is an anomalously long residence time of the Ga precursor due to gas recirculation within the growth chamber. To test this hypothesis, the same structure was grown again, with the introduction of a 5-min pause between the end of the channel and the start of the barrier growth. The growth pause was implemented by switching off both TMGa and TMAI sources while keeping the supply of ammonia on. Despite this growth pause being many orders of magnitude longer than the typical residence time of the species in the reactor, usually considered to be of the order of a few tenths of a second,¹² no detectable improvement was found.

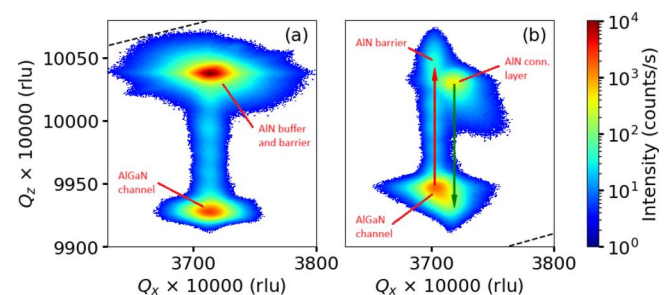


FIG. 1. Reciprocal space maps of the AlN/Al_{0.8}Ga_{0.2}N HEMT structures grown on (a) standard and (b) auxiliary templates, with a nominal barrier thickness of 50 nm. Arrows explained in the text.

Although there are currently limited data on intermixing in AlGaIn/AlGaIn heterostructures for electronic applications, this issue is already well known in the field of UV lasers, where degradation of waveguide confinement due to smeared interfaces has been reported.^{13,14} Theoretical mechanisms have also been proposed to explain this behavior.¹⁵ Both experimental observations and theoretical considerations suggest that low-temperature growth can be used to overcome this issue. For this reason, the growth was repeated using the same heterostructure, but with the barrier grown also at 1000 °C and at 850 °C. While the sample with a barrier temperature of 1000 °C showed an RSM indistinguishable from the sample entirely grown at 1160 °C, the RSM of the sample with the barrier grown at 850 °C does not present the high-intensity streak, but only much lower intensity truncation tails, as shown in Fig. 2.

We note that this approach also proved to be an effective solution for devices with thinner barriers and different compositions, as shown in the RSMs of Fig. 3, where high-intensity streaks are not present. Clear XRR Kiessig fringes were also observed (not shown) confirming sharp interfaces.

To further prove that the absence of a streak in the RSM is associated with a much sharper interface, we sourced high-resolution secondary ion mass spectroscopy (SIMS) measurements for samples grown on auxiliary substrates with different barrier temperatures. The SIMS profiles of the samples at both ends of the temperature range are shown in Figs. 4(a) and 4(b). A graded composition transition layer is apparent in both; however, while its thickness is about 35 nm in the sample entirely grown at 1160 °C, it reduces to only about 5 nm when the barrier is grown at 850 °C. To better estimate the temperature dependence of the transition layer thickness, the SIMS data of all samples were fitted with a Boltzmann sigmoidal function:

$$y(x) = A_2 + (A_1 - A_2) \frac{1}{1 + e^{\frac{x-x_0}{d}}}, \quad (1)$$

where y is the SIMS signal for either Al or Ga compositions, as a function of the depth x (centered at x_0), A_1 and A_2 the signal intensities of the two plateaus, and d the broadening parameter, which is proportional to the graded layer thickness.

As shown in Fig. 4(c), we found that the thickness of the graded layer increases almost linearly with temperature.

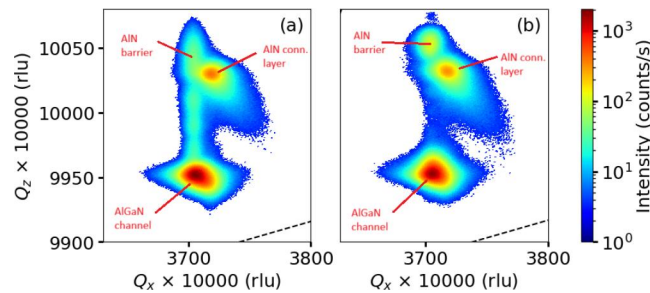


FIG. 2. Reciprocal space maps of the AlIn/Al_{0.8}Ga_{0.2}N HEMT structures grown on the auxiliary substrate, with barriers grown at (a) 1160 and (b) 850 °C, with a nominal thickness of 50 nm. To ensure a fair comparison, sample (a) underwent a growth pause equal in duration to the time required to cool from 1160 to 850 °C during the growth of sample (b).

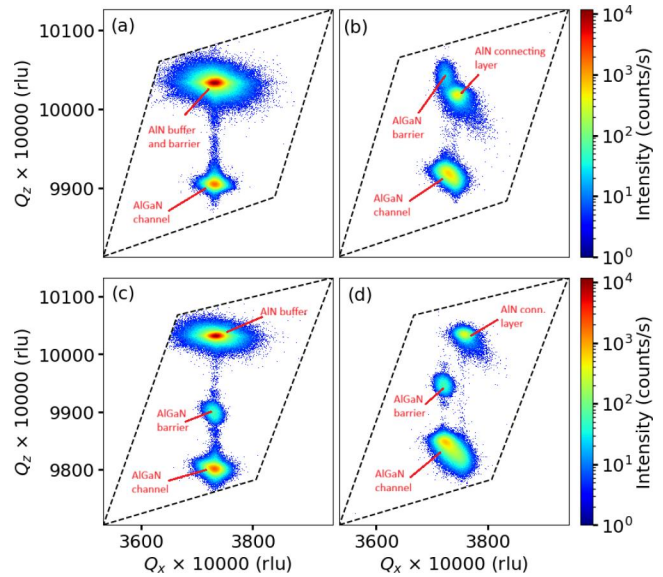


FIG. 3. Reciprocal space maps of different HEMT structures with barriers grown at 850 °C, and with a nominal barrier thickness of 30 nm: AlIn/Al_{0.75}Ga_{0.25}N on (a) standard and (b) auxiliary templates; Al_{0.75}Ga_{0.25}N/Al_{0.55}Ga_{0.45}N on (c) standard and (d) auxiliary templates.

Although low-temperature growth proved to be essential for achieving sharp heterointerfaces, there is concern that this may favor the incorporation of unwanted point defects. However, as shown by the SIMS data in Fig. 4(d), the concentrations of carbon and oxygen impurities did not increase detectably with the decrease in barrier growth temperature. Carbon levels remained constant around $4.0 \times 10^{16} \text{ cm}^{-3}$; oxygen levels remained constant around $1.0 \times 10^{17} \text{ cm}^{-3}$ in the channel

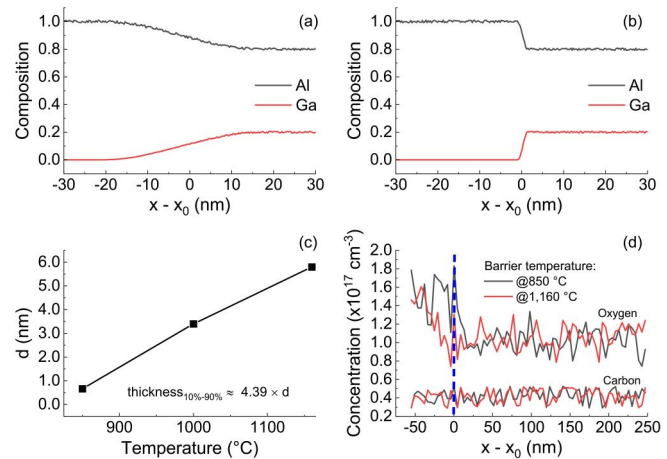


FIG. 4. High-resolution SIMS scans of the barrier/channel heterointerface for the AlIn/Al_{0.8}Ga_{0.2}N HEMT heterostructure grown at (a) 1160 °C and (b) 850 °C; (c) estimation of the temperature dependence of the broadening parameter d of the graded layer; (d) standard resolution SIMS scans of oxygen and carbon impurities, the vertical dashed line (blue) indicates the position of the AlIn/AlGaIn interface.

and increased to about $1.8 \times 10^{17} \text{ cm}^{-3}$ in the barrier due to the higher Al content in both samples, regardless of the temperature. While these results suggest no dramatic increase in C and O impurities, further work is still needed to determine optimal growth conditions that limit interface smearing while minimizing point defect incorporation.

The presence of a residual ($\sim 5 \text{ nm}$) graded layer in the top heterointerface of the low-temperature sample is also confirmed by cross-sectional transmission electron microscopy (TEM), as reported in Fig. 5 for the $\text{AlN}/\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$ HEMT structure. It should be noted that the bottom heterointerface is much sharper despite the fact that it was grown at the standard temperature of 1160°C , which is consistent with the lack of streak along the green arrow already mentioned in the discussion of Fig. 1(b).

Having established the temperature-dependent origin of the composition gradient at the barrier-channel interface, we next investigated its impact on the 2DEG conductivity, a key determinant of HEMT performance. We used the Semilab LEI-88 non-contact sheet resistivity measurement system to characterize the 2DEG conductivity, which has a nominal calibration range of $16\text{--}3600 \Omega/\square$ but is capable of measuring up to $20 \text{ k}\Omega/\square$, although with a reduced precision characterized by a standard deviation of 17%. We note that while Hall measurements provide a more accurate quantitative insight into the 2DEG properties (density and mobility), the fabrication of reliable Ohmic contacts on Al-rich materials remains challenging to date.² Therefore, to gain initial insight, we report the electrical characterization based on this contactless technique.

The contactless measurements revealed that despite the good surface morphology (RMS roughness $< 5 \text{ nm}$) and low C and O densities of $\sim 10^{17} \text{ cm}^{-3}$, as shown in Fig. 4(d), none of the HEMT structures with barriers grown at 1160°C exhibited measurable conductivity (sheet resistivity above detection limit). However, all HEMTs with barriers grown at 850°C showed clear 2DEG conductivity. In particular, R_{sh} of about 2500 and $5500 \Omega/\square$ was obtained for the $\text{AlN}/\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$ and $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.55}\text{Ga}_{0.45}\text{N}$ HEMT structures, respectively. These R_{sh} values are among the best reported for HEMTs with comparable composition contrasts and barrier thicknesses.²

To understand the connection between the interface composition gradient and the observed 2DEG conductivity degradation, we next performed one-dimensional Schrödinger-Poisson simulations. Details of the simulation methodology and parameters are provided in the [supplementary material](#) (Secs. S1–S3).^{8,16–19}

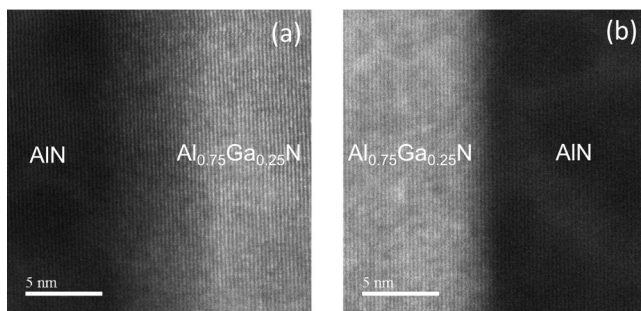


FIG. 5. Cross-sectional TEM of the top (barrier-channel) and bottom (channel-buffer) heterointerfaces for the $\text{AlN}/\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$ HEMT structure: (a) top interface grown at 850°C and (b) bottom interface grown at 1160°C .

Figure 6(a) shows the variation of total carrier density, n_{es} , as a function of the composition gradient length, Δ_L , introduced at the barrier-channel interface for a representative $\text{AlN}(50 \text{ nm})/\text{Al}_{0.8}\text{Ga}_{0.2}\text{N}$ HEMT structure. Following our experimental observations in Figs. 4 and 5, a linear composition grading was incorporated within the AlN barrier in the simulated structures, see Fig. 6(a), bottom-right schematic. In this case, n_{es} decreased with increasing Δ_L (black circles), as the composition grading within the barrier reduces the “effective” barrier thickness.

From the carrier density distribution profiles, Fig. 6(b), we further found that the composition grading caused the carrier density to spatially spread out. This can affect the carrier transport: as the carrier density extends toward the binary AlN barrier within the graded region, alloy disorder related effects are reduced. An increase in the overall carrier mobility, μ , is thus expected with increasing Δ_L .^{19–21} Although a quantitative evaluation of μ is beyond the scope of this work, prior studies on comparable systems, such as in polarization field-effect transistors (in which composition gradients are introduced

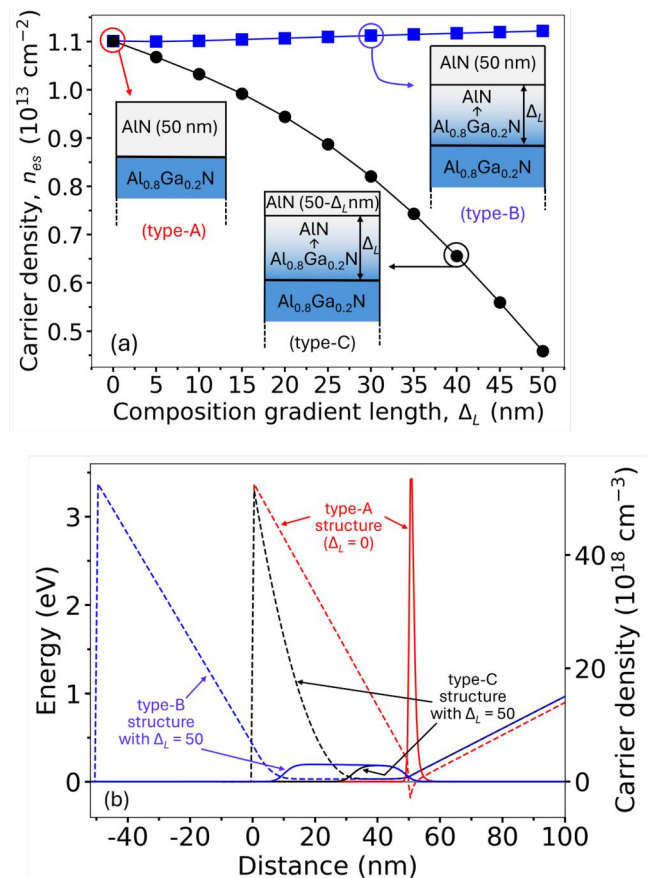


FIG. 6. (a) Total carrier density, n_{es} , as a function of the composition grading length, Δ_L , in an $\text{AlN}(50 \text{ nm})/\text{Al}_{0.8}\text{Ga}_{0.2}\text{N}$ HEMT. $\text{AlN} \leftarrow \text{Al}_{0.8}\text{Ga}_{0.2}\text{N}$ denotes linear grading of the Al-composition from $\text{Al}_{0.8}\text{Ga}_{0.2}\text{N}$ to AlN; $\Delta_L = 0$ corresponds to a sharp barrier-channel interface. (b) Conduction band (dashed lines) and volumetric carrier density profiles (solid lines) for three representative structures (type-A, type-B, and type-C) with different Δ_L and barrier thicknesses from (a).

intentionally), have reported mobility enhancements up to $\sim 1.5\times$ at maximum.^{19,20}

With increasing Δ_L , n_{es} , in our case, decreased by a factor of ~ 2.5 , Fig. 6(a), whereas μ is expected to increase by only a factor of ≤ 1.5 . We thus conclude that conductivity degradation, or equivalently the increase in R_{sh} [$\propto 1/(n_{es}\mu)$], in an unintentional compositionally graded HEMT can strongly be driven by the reduction in n_{es} . While this is consistent with trends observed in our experiments, it cannot quantitatively explain the findings. Further studies, including the mobility measurements and calculations, are required to fully elucidate the origin of the observed collapse of the conductivity.

Additionally, our simulation showed that employing a thick AlN barrier can mitigate the adverse effect of unintentional composition grading on n_{es} [blue squares in Fig. 6(a)]. In these simulations, the composition grading was introduced as an additional transition layer with the AlN barrier thickness kept fixed at 50 nm [Fig. 6(a), top-right schematic]. Here, we found that n_{es} remained nearly constant with Δ_L . The graded region only modified the carrier distribution, transitioning it from a 2- to a 3-dimensional profile [Fig. 6(b)], without affecting the integrated free carrier density. This suggests that by extending the growth of the barrier, in principle, the reduction of the total carrier density can be prevented. However, since thick barriers would again pose challenges to realizing reliable Ohmic contacts, this approach may not be optimal from a device-implementation perspective.

In conclusion, we observed that standard growth of Al(Ga)N barriers at high temperatures leads to smeared barrier-channel interfaces and 2DEG collapse. Low-temperature growth at 850 °C prevents the intermixing and restores 2DEG. With the implementation of this growth strategy, we successfully demonstrated AlN/Al_{0.75}Ga_{0.25}N and Al_{0.75}Ga_{0.25}N/Al_{0.55}Ga_{0.45}N HEMT structures with 2DEG sheet resistivity of about 2500 and 5500 $\Omega/\square$, respectively. While the results were confirmed by both high-resolution SIMS and cross-sectional TEM, we demonstrated that the presence of an intermixed layer can also be detected with nondestructive XRD analysis. In particular, the presence of high-intensity streaks in RSMs correlates with interface grading. We showed that unintentional composition grading at the barrier-channel interface is detrimental to HEMT devices and should thus be avoided. Our proposed low-temperature barrier growth strategy therefore proved to be a critical approach for realizing high-quality, high-performance Al-rich AlGaN/AlGaN HEMTs.

See the [supplementary material](#) (Secs. S1–S3) for a detailed description of the simulation methodology.

We thank Dr. Paweł Michałowski from Łukasiewicz—Institute of Microelectronics and Photonics in Warsaw, Poland, for the high-resolution SIMS, and Dr. Donald MacLaren from the School of Physics, University of Glasgow, UK, for the cross-sectional TEM. This research is jointly supported by Taighde Éireann—Research Ireland, formerly Science Foundation Ireland (SFI) under Grant No. 23/EPSC/3888 and by EPSRC under Grant No. EP/X036901/1. Part of this research was also supported by Research Ireland under the Grant Nos. 21/FFP-A/9014 and 12/RC/2276_P2. Open-access publication of this article was supported by the IREL consortium.

AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

P. Pampili: Conceptualization (equal); Data curation (equal); Formal analysis (equal); Investigation (lead); Methodology (lead); Software (supporting); Validation (equal); Visualization (equal); Writing – original draft (lead); Writing – review & editing (equal). **V. Z. Zubialeich:** Conceptualization (supporting); Formal analysis (supporting); Validation (supporting); Writing – review & editing (equal). **B. Mondal:** Conceptualization (supporting); Data curation (equal); Formal analysis (equal); Investigation (supporting); Methodology (supporting); Software (lead); Validation (equal); Visualization (equal); Writing – original draft (supporting); Writing – review & editing (equal). **J. Mukherjee:** Conceptualization (supporting); Formal analysis (supporting); Investigation (supporting); Methodology (supporting); Validation (supporting); Visualization (equal); Writing – original draft (supporting); Writing – review & editing (equal). **S. Schulz:** Conceptualization (equal); Formal analysis (supporting); Funding acquisition (equal); Methodology (supporting); Project administration (equal); Resources (equal); Supervision (equal); Validation (equal); Writing – review & editing (equal). **D. A. J. Moran:** Conceptualization (equal); Formal analysis (supporting); Funding acquisition (equal); Methodology (supporting); Project administration (equal); Resources (equal); Supervision (equal); Validation (supporting); Writing – review & editing (equal). **P. J. Parbrook:** Conceptualization (equal); Formal analysis (supporting); Funding acquisition (equal); Methodology (supporting); Project administration (equal); Resources (equal); Supervision (equal); Validation (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are openly available in Zenodo at <https://doi.org/10.5281/zenodo.20042244>, Ref. 22 and are also available from the corresponding author upon reasonable request.

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