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2DEG properties of AlScN/GaN and AlYN/GaN HEMTs determined by terahertz optical Hall effect

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We present a contactless determination of the two-dimensional electron gas (2DEG) properties in AlScN/GaN and AlYN/GaN high electron mobility transistor (HEMT) structures using the terahertz optical Hall effect (OHE) over a temperature range of 20 K–360 K. The structures are grown on sapphire or 4H-SiC substrates by metalorganic chemical vapor deposition (MOCVD) and feature ~10-nm thick barrier layers with Sc and Y contents ranging from 4.6% to 17.3% and 3.3% to 8.2%, respectively. The temperature dependencies of the 2DEG density and mobility parameters are analyzed and discussed in a comparative manner. Additionally, conclusions are drawn regarding the predominant scattering mechanisms at both low and room temperatures. Furthermore, the 2DEG effective mass parameter m^* in AlScN/GaN and AlYN/GaN is determined for the first time. At low temperatures m^* is found to be in the range $0.20 - 0.27m_0$, close to the value of $0.23m_0$ for bulk GaN. As temperature increases above 100 K, m^* gradually rises reaching $0.33 - 0.39m_0$ at room temperature, consistent with findings for AlGaIn/GaN HEMTs. The underlying causes of this temperature-dependent increase in effective mass are discussed, with a possible explanation linked to polaron effects and deviations from the classical Drude model.

KEYWORDS

HEMT, 2DEG, ellipsometry, AlScN, AlYN, effective mass, optical Hall effect

1 Introduction

In recent decades, GaN-based technology has not only revolutionized solid-state lighting and optoelectronics but has also emerged as a key enabler of a more sustainable future, driving the development of high-efficiency radio-frequency and high-power electronic devices (Amano et al., 2018). Achieving this potential relies on the advancement of high-power transistors capable of switching large currents at high frequencies and across wide bandwidths. In this context, AlGaIn/GaN high-electron-mobility transistors (HEMTs) have proven particularly promising, with commercially available devices already meeting these demanding performance requirements (Quay et al., 2017; Ture et al., 2019; Cwiklinski et al., 2019; 2020; Meneghini et al., 2021; Roccaforte et al., 2018; Krause et al., 2023).

In AlGaIn/GaN HEMTs, electrons accumulate at the interface between the GaN channel layer and the AlGaIn barrier due to the different bandgap energies as well as the spontaneous

and piezoelectric polarizations inherent to these wurtzite nitride layers (Ambacher et al., 1999; Ture et al., 2019; Cwiklinski et al., 2019; 2020; Thome et al., 2022; Fichtner et al., 2024). These electrons are confined close to the interface, forming a two-dimensional electron gas (2DEG) with very high electron mobilities. The higher the 2DEG density n_s , the higher the current and output power of the HEMT. In conventional AlGaIn/GaN HEMTs with an Al content of 25%–30%, n_s up to approximately 10^{13} cm^{-2} is attained. Higher n_s can be achieved in AlN/GaN HEMTs (Cwiklinski et al., 2019; Manz et al., 2021; Papamichail et al., 2024), but the barrier thickness is limited to $\sim 5 \text{ nm}$ due to the significant lattice mismatch between AlN and GaN. As a result, AlN/GaN HEMTs are prone to short-channel effects, degraded device performance, shorter lifetimes, and reduced reliability (Storm et al., 2013; del Alamo and Lee, 2019).

One approach to improve the performance of GaN-based HEMTs is to use the novel nitride semiconductors AlScN and AlYN as barrier layers. These materials have large bandgaps and intrinsically high spontaneous polarization, which allows for an enhanced n_s in the mid 10^{13} cm^{-2} range (Žukauskaitė et al., 2012; Sedrine et al., 2013; Hardy et al., 2017; Kazior et al., 2019; Ambacher et al., 2021). For Sc and Y concentrations below 30% and 50%, respectively, these materials crystallize in wurtzite lattice. Furthermore, for compositions of ~ 7 –11% their a lattice parameter matches that of GaN (Dinh et al., 2023; Nguyen et al., 2024; Streicher et al., 2024b) thus overcoming the critical thickness limitations of AlN and allows for the growth of unstrained, thicker barrier layers (Zhang et al., 2013).

AlScN/GaN and AlYN/GaN heterostructure grown by molecular beam epitaxy (MBE) exhibit characteristics superior to those of conventional low-Al content AlGaIn/GaN heterostructures (Hardy et al., 2017; Frei et al., 2019; Elias et al., 2023; Wang et al., 2023a,c,b; Hasan et al., 2024) and demonstrated the viability of utilizing AlScN and AlYN as barrier layers in GaN-based HEMTs. However, MOCVD is the preferred growth technique in industry because of its higher throughput, lower cost, and faster growth processes. On the other hand, the growth of AlScN and AlYN by MOCVD is challenging due to the low vapor pressure of available Sc and Y precursors. A heated gas mixing system was recently demonstrated at Fraunhofer IAF, enabling MOCVD growth with precursors that have extremely low vapor pressures. This advancement facilitated the successful growth of the first AlScN (Leone et al., 2020) and AlYN (Leone et al., 2023) by MOCVD, as well as AlScN/GaN (Streicher et al., 2023a; Leone et al., 2020; Ligl et al., 2020; Manz et al., 2021; Streicher et al., 2023b; 2024a) and AlYN/GaN (Streicher et al., 2024b) heterostructures with the presence of a 2DEG.

Optimization and further improvement of AlScN/GaN and AlYN/GaN HEMTs require accurate assessment of 2DEG properties and scattering mechanisms. Traditionally, charge carrier mobility μ and density n can be obtained with electrical Hall measurements at variable temperatures. The effective mass parameter m^* , however, can be directly determined using cyclotron resonance measurements only at very low temperatures (LT) (4–10 K). At higher temperatures this method becomes impractical due to significant broadening of the energy levels.

Hence, a combination of mid-infrared and electrical Hall measurements (e.g., Perlin et al., 1996; Kasic et al., 2000; Feneberg et al., 2013) is typically used to estimate the effective mass indirectly. The development of the optical Hall effect (OHE)—which applies generalized spectroscopic ellipsometry at long wavelengths in the presence of magnetic fields—has enabled the determination of electron effective mass, its anisotropy from low to room temperature (and beyond), as well as carrier density and mobility, all without requiring additional electrical measurements (Schubert et al., 2016).

In this work we report a study of the temperature-dependent 2DEG properties in MOCVD grown AlScN/GaN and AlYN/GaN HEMT structures by using the contactless THz OHE.

2 Materials and methods

2.1 Samples

The AlScN/GaN and AlYN/GaN heterostructures were grown by MOCVD as described in Streicher et al. (2024a) and Streicher et al. (2024b). Thick GaN channel layers (~ 2 – $3 \mu\text{m}$) were grown on either GaN template on sapphire or on semi-insulating 4H-SiC substrates, followed by ~ 10 -nm thick barrier layers with Sc and Y content of 4.6%–17.3% and 3.3%–8.2%, respectively. For improved cost and energy efficiency, GaN/sapphire templates were simultaneously grown on multiple wafers in a multi-wafer reactor. This approach allowed for economical development and optimization of growth conditions and parameter tuning. The HEMTs grown on GaN/sapphire templates have a regrowth surface between the template and the GaN channel layer. The templates and HEMTs were grown in different reactors, and the regrowth surface was exposed to air. It is well documented that this leads to Si atoms being trapped on the regrowth surface (Fu et al., 2021; 2018; Xing et al., 2005; Noshin et al., 2022). The heterostructures on 4H-SiC were grown in one reactor and do not have a regrowth surface. The structures were capped with a thin SiN_x layer. A 0.5 nm thin AlN interlayer was inserted between the channel and barrier layers for all structures. AlN interlayers are reported to eliminate alloy scattering in both AlGaIn/GaN (Shen et al., 2001) and AlScN/GaN heterostructures (Casamento et al., 2022), and reduce interface roughness scattering (Dogmus et al., 2016). Furthermore, they are used to increase the abruptness of the interface and can act as diffusion barriers (Cai et al., 2013). In these works the effect of these interlayers is investigated in detail by HRTEM and electrical measurements.

2.2 OHE measurements

OHE measurements were carried out at the terahertz (THz) wavelength range to study the 2DEG properties in the AlScN/GaN and AlYN/GaN HEMT structures. The OHE describes the magnetic field-induced optical birefringence generated by free charge carriers under the influence of the Lorentz force and can be measured by Mueller matrix spectroscopic ellipsometry (Schubert et al., 2016). The Mueller matrix, M , is defined by arranging incident and exiting Stokes vectors into matrix form

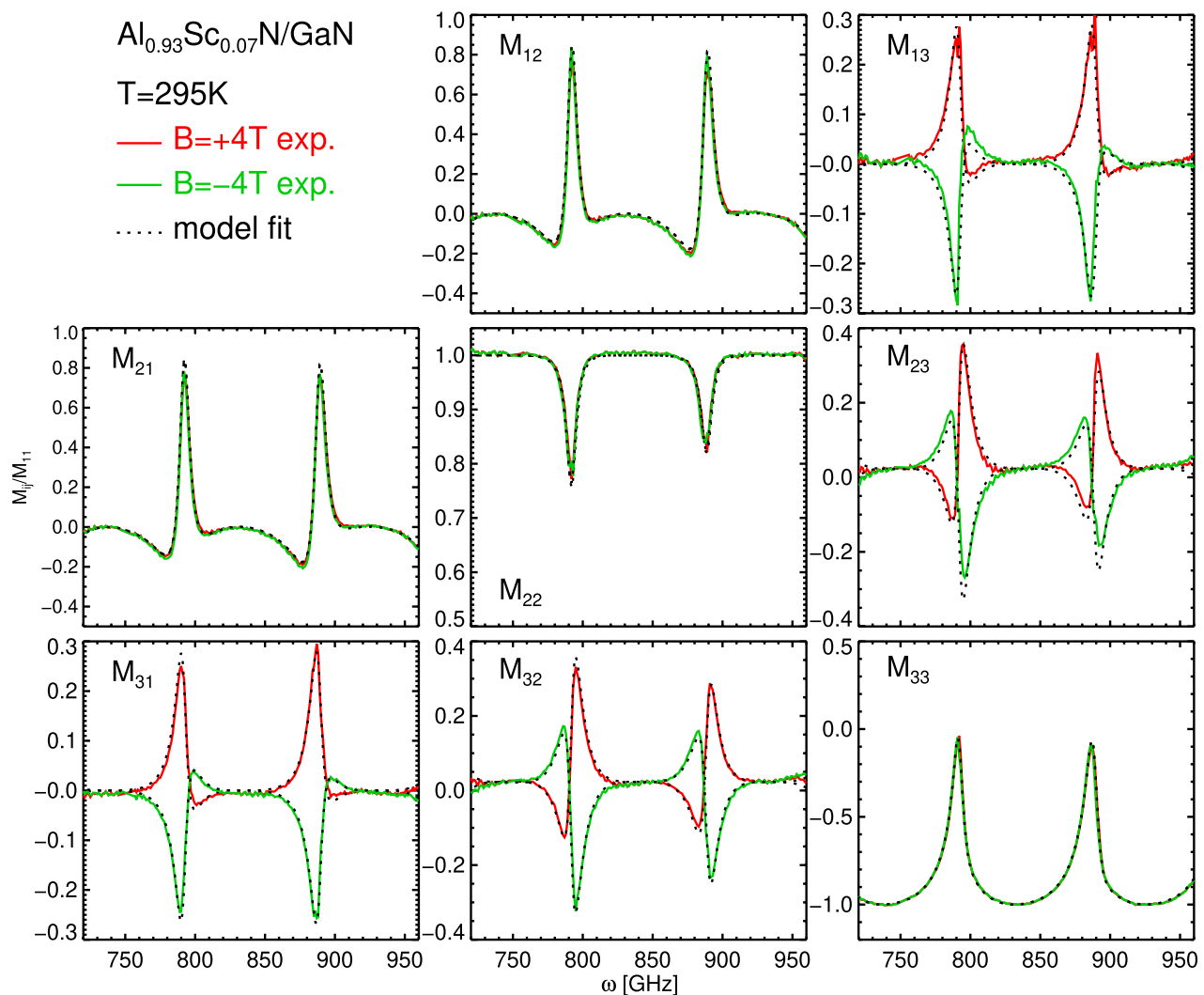


FIGURE 1
Representative THz OHE Mueller Matrix spectra measured at magnetic field $B = +4$ T (red line) and $B = -4$ T (green line) and at temperature of 295 K, along with the best-fit model (dashed line) for an $\text{Al}_{0.93}\text{Sc}_{0.07}\text{N}/\text{GaN}/4\text{H-SiC}$ HEMT structure.

$$\begin{pmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \end{pmatrix}_{\text{output}} = \begin{pmatrix} M_{11} & M_{12} & M_{13} & M_{14} \\ M_{12} & M_{22} & M_{23} & M_{24} \\ M_{13} & M_{32} & M_{33} & M_{34} \\ M_{14} & M_{42} & M_{43} & M_{44} \end{pmatrix} \begin{pmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \end{pmatrix}_{\text{input}},$$

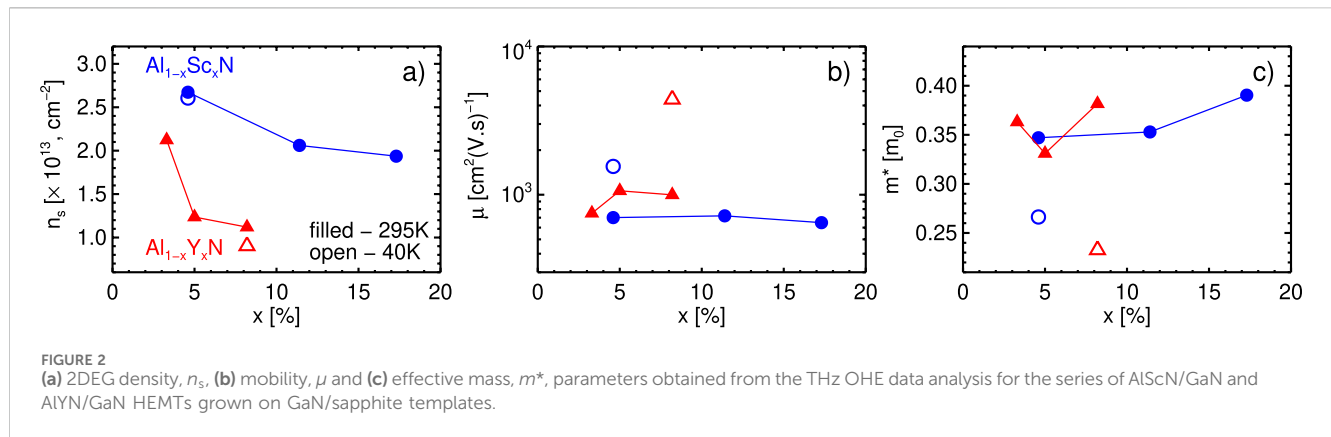
with $S_0 = I_p + I_s$, $S_1 = I_p - I_s$, $S_2 = I_{45} - I_{-45}$, $S_3 = I_{\sigma+} - I_{\sigma-}$, where I_p , I_s , I_{45} , I_{-45} , $I_{\sigma+}$, and $I_{\sigma-}$ denote the intensities for the p -, s -, $+45^\circ$, -45° , right-, and left-handed circularly polarized light components, respectively (Fujiwara, 2007). The OHE is thus a noninvasive, contactless method. Another significant advantage of OHE is its ability to independently determine the free charge carrier mobility μ , density n , effective mass m^* , and sign at arbitrary temperature.

In this study, we used the THz cavity-enhanced optical Hall effect (CE-OHE) technique, where a fully reflective aluminum surface is placed behind the sample with a small gap of about 100 μm in between. This allowed for multiple interaction between the THz radiation and the carriers, greatly enhancing the OHE signal (Knight et al., 2020). Measurements were performed using

custom-built ellipsometry instrumentation at the THz Materials Analysis Center (Kühne et al., 2018) equipped with a superconducting magnet, which allows measurements at magnetic fields up to ± 8 T and sample temperature between 4.2 K and 400 K. The measurements were carried out in the temperature 20–360 K and at an angle of incidence of 45° . The measurements were performed at magnetic fields $B = -4$ T, 0 T and $+4$ T, with the magnetic field oriented parallel to the incoming beam, resulting in a magnetic field strength $B_c = B/\sqrt{2}$ along the sample normal. Note that in the OHE experiments the entire sample area was probed.

2.3 OHE data analysis

The THz ellipsometer is of rotating analyzer type, which allows one to measure only the upper left 3×3 part of the Mueller matrix (Kühne et al., 2018). The measured data was analyzed using a stratified optical model with parameterized model dielectric



functions (MDFs) assigned to each layer, following the methodology described in Schubert et al. (2016). The model consists of a perfect mirror, air gap, 4H-SiC or sapphire substrate, GaN channel, 2DEG, barrier layer and SiN_x layer. The MDFs of 4H-SiC, sapphire and GaN, which are independent on the magnetic field, were determined from measurements of bare substrates. These MDFs were kept fixed during the analysis and only the thicknesses of the corresponding layers were treated as free parameters. The barrier and SiN_x layers are much thinner than the wavelength of THz radiation and do not make measurable contribution.

The 2DEG is described as a thin layer of Drude-type carriers in the presence of a magnetic field (Schubert et al., 2016; Kühne et al., 2018). The parameters describing the properties of the 2DEG, the carrier mobility μ , sheet density n_s and effective mass m^* were determined by non-linear least-squares fit of the calculated Mueller matrix data to the experimental data. The data analysis was carried out using the WVase32™ software (J.A. Woollam Co. Inc.). Further details of the analysis can be found in Stanishev et al. (2021).

Figure 1 shows an example of CE-OHE measurements performed at room temperature and magnetic fields $B = \pm 4$ T, with the dashed line showing the best-fit model. Note that the block-off-diagonal Mueller matrix elements M_{13} , M_{31} , M_{23} and M_{32} are proportional to the cyclotron frequency and provide the most sensitivity to the effective mass parameter. Without in-plane crystal structure anisotropy, OHE induces symmetric off-diagonal block elements ($M_{ij} = M_{ji}$ with $ij = 13, 23$ and $ji = 31, 32$). Any difference in the off-diagonal block elements from zero represents the magnetic-field-induced OHE signatures. Non-conductive samples reveal no OHE signatures. In the case of a zero magnetic field, all off-diagonal block elements are zero within the measurement error. The block-off-diagonal elements flip around the zero upon changing the magnetic field polarity, which allows to distinction between electrons and holes. Meanwhile, the on-diagonal block elements (M_{ij} , $ij = 12, 21, 22, 33$) are mainly determined by the plasma frequency and broadening parameters.

3 Results and discussion

Figure 2 shows the results of a series of three Al_{1-x}Sc_xN/GaN and Al_{1-x}Y_xN/GaN structures with Sc and Y content in the ranges $x = 4.6 - 17.3\%$ and $x = 3.3 - 8.2\%$, respectively, grown on GaN/

sapphire templates. The room temperature (RT) $T = 295$ K OHE results reveal high 2DEG densities of $n_s = 2 - 3 \times 10^{13} \text{ cm}^{-2}$ for all Sc contents and mobility parameters of $\mu = 640 - 700 \text{ cm}^2 (\text{V.s})^{-1}$. For the Al_xY_{1-x}N/GaN HEMT structures the mobility was found to be higher $\mu = 730 - 1000 \text{ cm}^2 (\text{V.s})^{-1}$, but for a slightly lower 2DEG density in the range of $n_s = 1.2 - 2.2 \times 10^{13} \text{ cm}^{-2}$. This is in line with theoretical calculations, which predict that AlScN and AlYN barriers should provide 2DEG densities higher than low-Al content AlGaN. Note also the trend of increasing 2DEG density with decreasing Sc and Y content, indicating that pure AlN barrier should indeed provide even higher density. For all samples on sapphire substrates, the 2DEG effective mass parameters at RT were determined to be in the range $m^* = 0.33 - 0.39m_0$. These values are higher than the commonly accepted value of $m^* = 0.23m_0$ for bulk GaN (Armakavicius et al., 2024a). The larger 2DEG effective mass observed here aligns with previous findings for AlGaN/GaN HEMTs (Kühne et al., 2018; Knight et al., 2023; Armakavicius et al., 2024b; Hofmann et al., 2012; Armakavicius et al., 2016; Pashnev et al., 2020; Adamov et al., 2021; Pashnev et al., 2022), where $m^* > 0.23m_0$ was reported at room temperature.

For two of the HEMTs on sapphire, one AlScN/GaN and one AlYN/GaN, OHE measurements at $T = 40$ K were also obtained. The analysis of these measurements shows that the carrier density changed little as expected for 2DEG. However, the mobility and the effective mass change considerably. The mobility increased to $\mu = 1530 \text{ cm}^2 (\text{V.s})^{-1}$ and $\mu = 4400 \text{ cm}^2 (\text{V.s})^{-1}$ for AlScN/GaN and AlYN/GaN, respectively. The effective mass decreased to $m^* = 0.27m_0$ and $m^* = 0.23m_0$ for AlScN/GaN and AlYN/GaN, respectively.

To further study the dependence of the 2DEG parameters on temperature, two HEMT samples grown on 4H-SiC substrates with 7% Sc and 5% Y in the barrier layers were selected. Figure 3 shows the 2DEG density n_s , mobility μ and effective mass parameter m^* as a function of temperature extracted from the analysis of the THz OHE measurements. The AlScN/GaN heterostructure has approximately twice the 2DEG sheet density as compared to the AlYN/GaN (Figure 3a). A slight increase in 2DEG density with temperature is also observed in both samples, which is unexpected for a pure 2DEG system. Streicher et al. (2024a) reported a similar behavior in AlScN/GaN structures and attributed it to 2DEG electrons being trapped in shallow acceptor states, likely caused by carbon impurities in the GaN channel, or to the presence of a

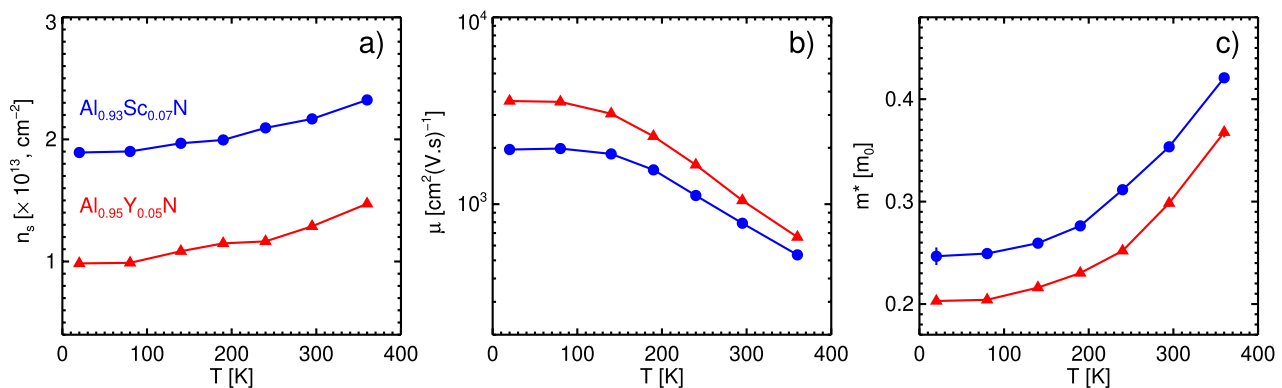


FIGURE 3
(a) 2DEG density n_s , (b) mobility μ and (c) effective mass parameter m^* as a function of temperature extracted from the analysis of the THz OHE measurements for the $\text{Al}_{0.93}\text{Sc}_{0.07}\text{N}/\text{GaN}$ and $\text{Al}_{0.95}\text{Y}_{0.05}\text{N}/\text{GaN}$ HEMT structures grown on 4H-SiC.

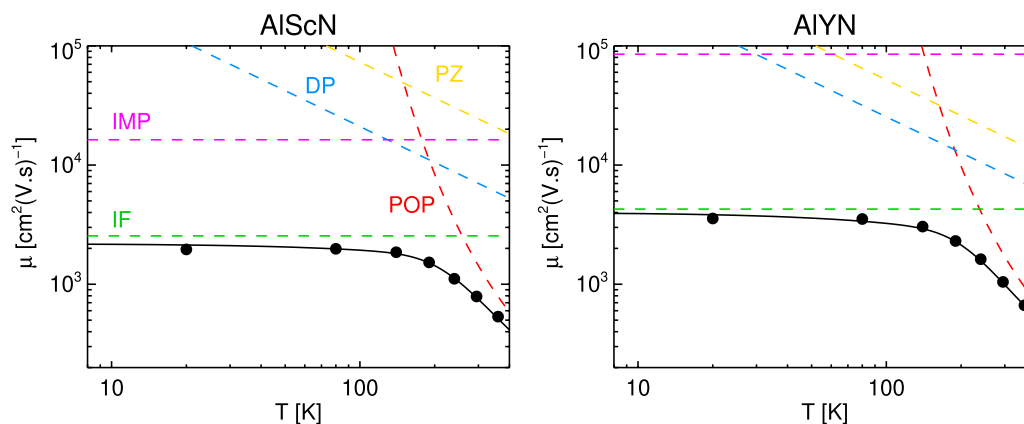
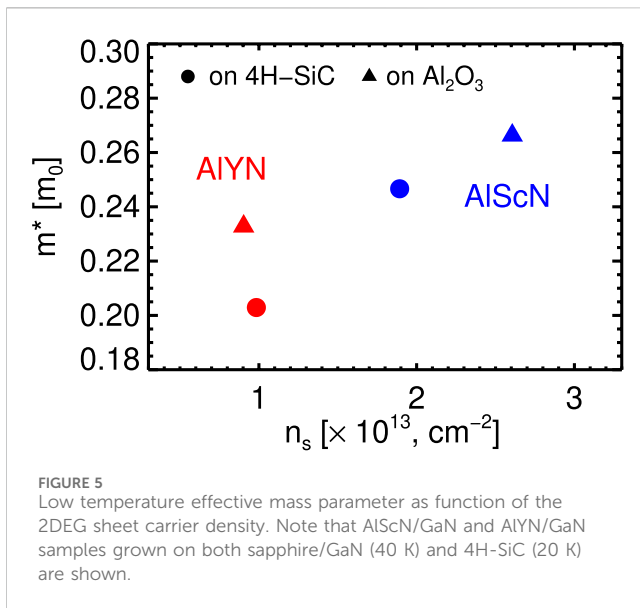


FIGURE 4
Best fits to the mobility data vs. temperature for $\text{Al}_{0.93}\text{Sc}_{0.07}\text{N}/\text{GaN}$ (left panel) and $\text{Al}_{0.95}\text{Y}_{0.05}\text{N}/\text{GaN}$ (right panel) HEMT structures grown on 4H-SiC. The contributions from individual scattering mechanisms (IF - interface roughness, IMP - residual impurities, DP - deformation potential, POP - polar optical phonons, PZ - polarization) are shown with dashed lines of different colors and the combined effect of all scattering mechanisms is depicted with solid lines.

small number of bulk donors that freeze out at low temperatures. In addition, strain-induced variations in piezoelectric polarization with temperature could also potentially contribute to the observed increase in 2DEG density.

The mobility parameter exhibits a typical trend, increasing as temperature decreases before saturating below 100 K (Figure 3b). For all temperatures, the 2DEG mobility in AlYN/GaN remains higher than in AlScN/GaN, reaching $\mu = 3600 \text{ cm}^2(\text{V.s})^{-1}$ and $\mu = 2000 \text{ cm}^2(\text{V.s})^{-1}$, respectively, at low temperatures. The temperature dependence of the mobility parameter was modeled by taking into account the contributions of different scattering mechanisms using the equations for Fang–Howard variational wave function described in Ref. Jena (2022). We considered temperature-dependent scattering mechanisms, including polar optical phonon (POP), acoustic deformation potential (DP), and piezoelectric (PZ) scattering, alongside temperature-independent scattering from background residual impurities (IMP) and interface roughness (IF). In our

calculations, 2DEG density and effective mass, and background impurity concentration are set to their measured values, with interface scattering parameters, i.e., correlation length and roughness, being the only adjustable variables. Due to the strong correlation between these two parameters, the correlation length was fixed at 3.5 nm, while roughness was varied to achieve the best fit. Figure 4 shows the individual contributions and the total mobility calculated according to the Matthiessen rule. At low temperature, the dominating mechanism is the interface roughness scattering. The best fits indicate similar interface roughness for the two samples, $\sim 0.9 \text{ nm}$ and $\sim 0.8 \text{ nm}$ for the AlScN/GaN and AlYN/GaN heterostructures, respectively. At high temperatures, scattering from polar optical phonons dominates. All other scattering mechanisms make only small contribution. Therefore, at both low temperatures and room temperature, the higher 2DEG mobility in AlYN/GaN compared to AlScN/GaN is likely due to its lower 2DEG density.



Figures 2c, 3c show that at low temperatures (below $T = 100$ K) the effective mass parameter is close to the widely accepted value of $m^* = 0.23m_0$ for bulk GaN (Armakavicius et al., 2024a), being 0.20–0.23 m_0 for AlYN/GaN and 0.25–0.27 m_0 for AlScN/GaN. Figure 5 shows the relationship between 2DEG effective mass and 2DEG density in different AlScN/GaN and AlYN/GaN structures (also including the samples grown on sapphire) measured at low temperatures (20 K–40 K). There is a trend of increasing low-temperature effective mass with the density, suggesting that the observed variation might be driven by band nonparabolicity effects (Syed et al., 2003; Spencer et al., 2016). According to the model proposed by Syed et al. (2003) and assuming a band-edge effective mass of $m^* = 0.21m_0$, the effective mass increase due to non-parabolicity effects should range from 27% to 66% for the 2DEG densities of $n_s = 0.9 - 2.6 \times 10^{13} \text{ cm}^{-2}$ determined for our samples (Figure 5). Our results indicate that the low-temperature effective mass is enhanced by approximately half the predicted value. Note that if the 2DEG density remains constant with temperature, the increase in effective mass due to non-parabolicity effects should exhibit only a very slight temperature dependence (1%–2%) following the variations of band gap energy. In contrast, Figure 3c shows a strong temperature-dependent increase in the effective mass parameter. Until $T = 100$ K it is nearly constant, but it gradually increases afterwards and at RT reaches $m^* = 0.30m_0$ for AlYN/GaN and $m^* = 0.35m_0$ for the AlScN/GaN. At 360 K it increases even further to 0.37 m_0 and 0.42 m_0 (Figure 3c), i.e., 70% and 80% increase with respect to low temperature. Such an increase of the effective mass parameter in other GaN-based heterostructures have previously been reported (Kühne et al., 2018; Knight et al., 2023; Armakavicius et al., 2024b; Hofmann et al., 2012; Pashnev et al., 2020), as well as in bulk GaN and in thick GaN epilayers (Armakavicius et al., 2024a). The fact that this behavior is observed in different GaN structures and barrier materials hints at a common mechanism at play. However, such a large increase of the effective mass parameter with temperature is not easy to explain with the conventional mechanisms typically invoked, e.g.,

conduction band non-parabolicity and polaronic effects. In addition to the 1%–2% increase resulting from band gap energy variations with temperature, non-parabolicity effects may also arise if the 2DEG density changes with temperature. Considering the observed increase in 2DEG density Figure 3a (i.e., assuming it is entirely due to the detrapping of electrons from shallow acceptor states) and using the equations in Syed et al. (2003), we estimate an increase of 12% between $T = 20$ K and $T = 360$ K for the effective mass. Note that this increase also takes into account the GaN bandgap change with temperature (e.g., Zubrilov et al., 1995).

Another cause of effective mass increase could be associated with the polaronic effect. The quasiparticle polaron is used to describe the interaction (coupling) of free charge carriers with the lattice vibrations, phonons. The formation of polarons decreases the carriers mobility and increases their effective mass. As the phonon population increases with increasing temperature, the polaronic effect is expected to be enhanced at RT and higher. This process is responsible for the reduction of carrier mobility at high temperatures (Figure 4). In the case of 2DEG weakly interacting with phonons in the surrounding 3D media, the relation between the effective mass of the polaron m_p^* and the band-edge effective mass m^* of the free electrons is often described with the equation:

$$m_p^* = m^* \left(1 + \frac{\pi}{8} \alpha + 0.1272348 \alpha^2 \right), \quad (1)$$

where α is the Fröhlich coupling constant $\alpha = 0.49$ in GaN. In this case, the polaronic effect should lead to ~22% increase in the effective mass independent of the temperature. However, Equation 1 is a simplification and previous theoretical studies have shown that polaron effective mass should explicitly depend on the temperature in a rather complex way (e.g., Fedyanin and Rodriguez, 1982a,b; Smilga, 1991; Peeters and Devreese, 1982), but in general should increase up to temperatures of the order of few hundreds Kelvin. From the relations presented in these works, we estimate effective mass enhancement of up to ~12–15% at $T = 360$ K, which can only partially explain our results. These relations are valid for polarons in 3D. In 2D the coupling should be stronger, however this may be compensated by screening effects (Peeters and Devreese, 1987; Devreese and Peeters, 1987). Fedyanin and Rodriguez (1982a) also noted that the coupling constant α and other parameters in the Pakar-Fröhlich Hamiltonian, which is used to describe polarons, should also be temperature-dependent.

Armakavicius et al. (2024a) discussed the possibility that the free-electron behavior deviates from the classical Drude model. One set of models introduces the so-called memory functions (Götze and Wölfle, 1972; Zwanzig, 1961; Mori, 1965). In some implementations of this model, the effective mass parameter becomes a function of both frequency and temperature (Rukelj, 2020; Kumari and Singh, 2020; Kupčić, 2017), and could potentially explain our results. However, analytical expressions for semiconductors have not been developed, and quantitative evaluation of these models is currently not straightforward.

Recently, Koroteyev et al. (2022) proposed that deviations from the classical Drude model—arising from thermally activated inelastic electron scattering processes—could qualitatively explain the increase in the effective mass parameter with temperature in AlGaIn/GaN with grating couplers as reported by Pashnev et al. (2020). According to Koroteyev et al. (2022), their model, which accounts for inelastic

scattering, requires only an 18% enhancement of the effective mass at room temperature to fit the experimental data of Pashnev et al. (2020), in contrast to the ~55% enhancement needed when using the classical Drude model. Such deviations from the Drude model could also explain the observed increase in the 2DEG effective mass in AlN/GaN and AlN/GaN, which exceeds the enhancement predicted by nonparabolicity and polaron effects alone (Figure 3c). As the temperature increases, the contribution from polar optical phonon (POP) scattering, an inelastic process, also becomes more significant (see Figure 4), further enhancing the deviation from Drude-like behavior.

Finally, it should be noted that some earlier works on thick GaN layers, have reported effective mass at room temperature $m^* \approx 0.23m_0$. All these estimates involve measurements in the mid-infrared (MIR) – a combination of MIR reflectivity or ellipsometry and electrical measurements (Perlin et al., 1996; Kasic et al., 2000; Feneberg et al., 2013) and MIR OHE (Armakavicius et al., 2024a) – which led to the suggestion of possible frequency and temperature dependent deviations from the classic Drude model by Armakavicius et al. (2024a). However, a possible explanation for these results could be the relatively high doping levels in these samples, with a carrier concentration exceeding $4 \times 10^{18} \text{ cm}^{-3}$. As Feneberg et al. (2013) pointed out, at such high concentrations the polaronic effects should be significantly reduced by screening and that non-parabolicity effects should also be small. Consequently, the effective mass was estimated to be $m^* \approx 0.23m_0$.

Because the effective mass can be most easily directly measured through cyclotron resonance at low temperatures, the polaronic, non-parabolicity, and other effects on the effective mass parameters at high temperature are not well studied experimentally and thus the existing theoretical models have not been rigorously tested. The recent development of the OHE made it possible for the first time to directly access the effective mass parameter at temperatures above RT and evidence for the increase of the effective mass parameter with temperature in GaN based materials has begun to emerge. We have discussed several possible mechanisms that could partially explain this. While we are currently not in a position to conclusively identify quantitatively the process (or a combination of processes) responsible for the strong dependence of the effective mass parameter on temperature, we hope that our findings will stimulate further theoretical and experimental investigations on this subject. It would also be interesting to perform similar studies on other materials that are not GaN-based.

4 Conclusion

The 2DEG density, mobility, and effective mass parameters in AlScN/GaN and AlYN/GaN HEMTs have been determined using THz optical Hall effect measurements over a temperature range of 20 K–360 K. At room temperature, the AlScN heterostructures exhibit a 2DEG sheet density $n_s = 2.0 - 2.7 \times 10^{13} \text{ cm}^{-2}$ and mobility $\mu = 640 - 790 \text{ cm}^2 (\text{V.s})^{-1}$. For the AlYN heterostructures, the RT values are $n_s = 1.2 - 2.2 \times 10^{13} \text{ cm}^{-2}$ and $\mu = 750 - 1050 \text{ cm}^2 (\text{V.s})^{-1}$. At low temperatures, the

mobility increases, reaching $\mu = 4400 \text{ cm}^2 (\text{V.s})^{-1}$ for AlYN/GaN and $\mu = 2000 \text{ cm}^2 (\text{V.s})^{-1}$ for AlScN/GaN. In this regime, mobility is primarily limited by interface roughness scattering. At low temperatures ($T = 20 - 130 \text{ K}$) the effective mass is determined to be in the range $0.20 - 0.27 m_0$. These values correlate with the 2DEG density and their variation is attributed to conduction band nonparabolicity effects. Above 130 K, the effective mass parameter in both AlScN/GaN and AlYN/GaN HEMTs increases strongly with temperature in agreement with previous results for AlGaIn/GaN HEMTs. We suggest that the observed increase in effective mass may be explained by a combination of temperature-dependent polaronic and nonparabolicity effect. Other factors, such as potential deviations from the classical Drude model caused by inelastic scattering or frequency-dependent scattering, could also play an important role. Further theoretical and experimental studies are necessary to establish a comprehensive understanding of the underlying mechanisms.

Data availability statement

The raw data supporting the conclusions of this article will be made available by the authors, without undue reservation.

Author contributions

VS: Visualization, Writing – review and editing, Formal Analysis, Writing – original draft, Investigation, Conceptualization. IS: Writing – review and editing, Investigation, Resources. AP: Investigation, Writing – review and editing. VR: Writing – review and editing, Investigation. PP: Writing – review and editing, Investigation. SL: Supervision, Investigation, Resources, Writing – review and editing. VD: Supervision, Funding acquisition, Resources, Conceptualization, Writing – review and editing.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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