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Impact of growth conditions on AlN/GaN heterostructures with in-situ SiN capping layer

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Abstract

In this work we have studied the growth of AlN barriers on GaN channels by Metal-Organic Vapor Phase Epitaxy (MOVPE). We have shown that an SiN in-situ capping layer is critical on AlN barrier layers. In addition, we have shown that an extreme reduction of NH₃ partial pressure results in gallium incorporation into the layers around 22%. However, we have shown that lesser reductions of NH₃ partial pressure allow us to achieve thin (3 nm) AlN layers capped with SiN which have a high quality crack free surface and state of the art Rsheet values < 330 Ohm/sq for such thin layers.

Keywords : AlN, SiN, Rsheet, GaN, MOVPE

1. Introduction

In High Electron Mobility Transistor (HEMT) architectures AlGa_N barriers have been widely used [1] [2] [3]. However, to improve device performance, and especially to reduce the barrier thickness for very high frequency switching, different approaches using AlN barriers have been explored both by Molecular Beam Epitaxy (MBE) [4] [5] [6] and Metal-Organic Vapor Phase Epitaxy (MOVPE) [7] [8]. In this work we investigate the effect of growth conditions of AlN barrier layers with SiN in-situ passivation to achieve AlN/GaN heterostructures grown by MOCVD with low resistivity 2-dimensional electron gas (2DEG) and very good surface morphology for barrier layers < 4 nm thick.

2. Experimental details

The growth was performed on a fully automatic AIXTRON CRIUS-R close coupled showerhead reactor, on single 200 mm diameter silicon 1 mm thick (1-1-1) oriented wafers with a resistivity of 3-20 Ohm.cm. The precursors for the growth of AlN and GaN were: Tri-methylaluminum (TMAI), Ti-methylgallium (TMGa), and ammonia (NH₃) for aluminum, gallium and nitrogen respectively, with H₂ as carrier gas. The growth structures use an AlN nucleation layer, AlGa_N transition layers (600nm at 50% Al and 900nm at 25% Al) and 1.6 μm of GaN. The last 200 nm of GaN are non-intentionally doped, in order to produce a high quality channel layer, with the initial 1.4μm of GaN intrinsically carbon doped. The structures grown in this study were nominally identical with only the AlN barrier varied. Where included, the SiN layer is grown with SiH₄ and NH₃ as precursors using a V/IV ratio of 10000 at 1030°C. The thickness of the AlN and SiN layers were measured by X-Ray Reflectivity (XRR) using a Bruker D8Fabline, and analysed using Bruker software. Atomic Force Microscopy (AFM) was performed using a Bruker Fastscan, and High Resolution X-ray Diffraction (HR-

XRD) 2theta/omega scans and Reciprocal Space Maps (RSM) were performed on a Bruker – Delta X diffractometer. Sheet resistivity values have been measured using a 4-point probe technique especially developed at LETI for GaN HEMT structures [9]. The sheet electron density (ns) and mobility (μ) have been measured using Hall Effect, also specially adapted to GaN at LETI [10]. These Hall Effect measurements were performed on 1 x 1 cm square isolated structures, with contacts at each corner. ns calculations were performed using a Poisson-Fermi formalism based on an analogy with MOS physics [11].

3. Results and discussion

This study was composed of three types of structure, as shown in Figure 1. One structure without SiN was grown with a very thin AlN layer. Several structures with AlN layers between 1 and 5nm with SiN capping were grown for electrical and morphological characterization, and finally 2 structures with thicker (20-30 nm) AlN layers were grown for easier physical-chemical analysis.

In previous work focused on AlGa_N/GaN heterostructures, [12] it has been demonstrated that in-situ SiN capping layers give a strong improvement to the surface quality. The SiN capping layer grown on top of the AlGa_N barrier layer acts as a protection from surface degradation and stabilizes the layer underneath. This capping layer drastically reduced emerging dislocations and improved the surface morphology. Based on these results, we compared a very thin AlN barrier layer on GaN buffer with and without SiN capping layer and a second identical structure with the addition of an in-situ SiN capping layer on top of the AlN. All SiN layers in this study are grown under identical conditions.

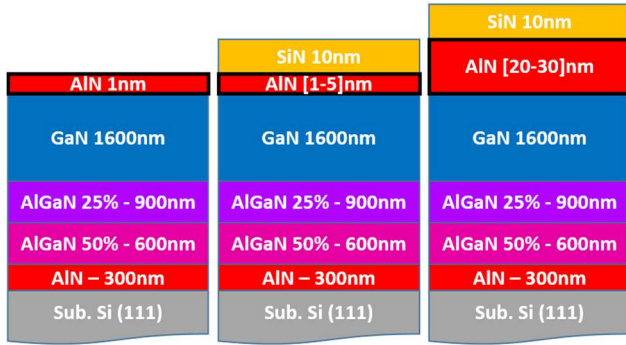


Figure 1: Structure with and without SiN cap

The AFM image on Figure 2.a shows that even with a very thin AlN layer we see a very high surface degradation and dislocation opening without SiN capping. Figure 2.b shows, the AFM scan from a structure with a 10 nm in-situ SiN capping layer show a very good surface morphology. The SiN appears to be extremely conformal, and should be amorphous as previously seen in [12]. The AlN surface morphology is transferred to the SiN. Hence the SiN surface is representative of the underlying AlN surface quality. This confirms that there is a very strong impact of the in-situ SiN on AlN layers, even stronger than that for AlGaIn layers [12] and so this protection layer is maintained for all of the following layers. It is notable that for the layer without SiN, the holes in the AlN are much deeper than the layer itself, and so degrade the GaN layer beneath as well.

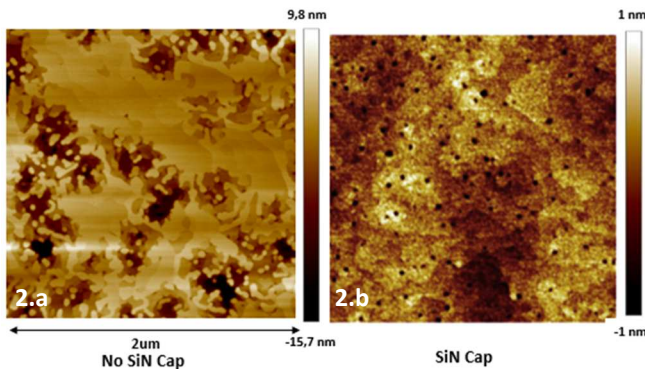


Figure 2: AFM scans ($2 \times 2 \mu\text{m}$) of 1 nm thick AlN layers without SiN capping layer (2.a) and with 10 nm SiN (2.b)

For the second part of the study, we focused on process conditions, in particular the NH_3 partial pressure and its impact on the layers grown. As discussed above, we kept an identical 10 nm in-situ SiN capping layer for all samples. We grew a variety of AlN layers at thickness from 1 to 5 nm in order to study the impact of the thickness on the layer quality, and at the same time, we varied the partial pressure of NH_3 from 1.7 to 50 mbar. As shown in Figure 3, AlN and SiN thicknesses are determined using X-Ray Reflectivity.

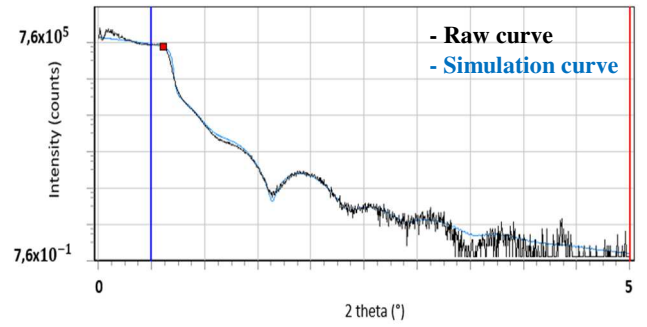


Figure 3: XRR scan of AlN + SiN cap layer

Because of the large lattice mismatch between AlN and GaN (2.4%), and according to work by Matthew Blakelee [13] we expect that growing an AlN layer on GaN above the critical thickness will lead to emerging dislocations and relaxation through crack formation which we can expect to result in degradation of the electrical properties especially a reduction of the carrier mobility due to increased interface roughness. In Figure 4, we show the surface morphology of AlN layers with thickness variation from 1 to 5 nm grown with a partial pressure of NH_3 of 50 mbar. As expected, increasing the thickness of the AlN layer leads to the opening of dislocations from 2 nm thickness. For increased thicknesses, we see increasing crack formation due to the high lattice mismatch between AlN and GaN, and for the 4 nm and 5 nm thick AlN layers, the surface is extremely cracked, despite the SiN capping layer. We chose to work with a 3 nm structure to vary the NH_3 partial pressure on the AlN layer as these were the thickest layers without serious crack formation. In Figure 5, we see that reducing the NH_3 partial pressure from 50 mbar to 17 mbar gives a big improvement in morphology for 3 nm thick layers, and there is further improvement of the morphology as the NH_3 partial pressure is reduced.

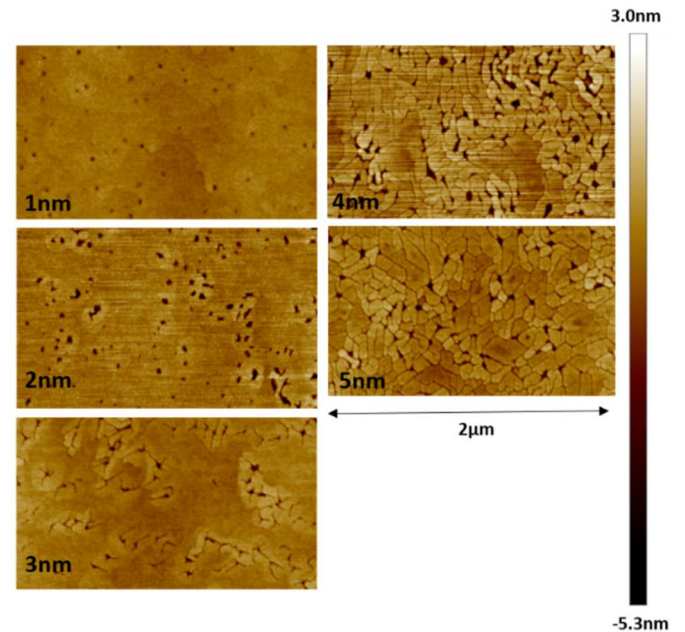


Figure 4: AFM scans ($2 \times 1.2 \mu\text{m}$) with AlN thickness variation from 1 to 5 nm with NH_3 partial pressure of 50 mbar

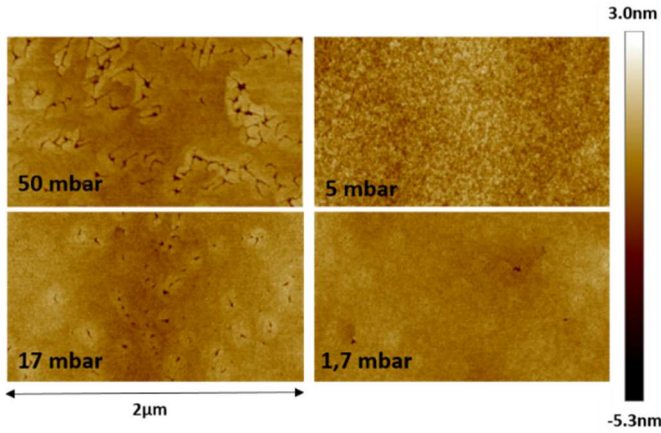


Figure 5: AFM scans ($2 \times 1.1 \mu\text{m}$) of 3 nm thick AlN layers with NH_3 partial pressure variation from 50 mbar to 1.7 mbar. All layers are capped with 10 nm of SiN

The sample grown at 5 mbar does not seem well resolved, but the layer is very flat. For the layer grown at 1.7 mbar partial pressure, the AlN layer does not have open dislocation pits, and nor does the thickest layer have cracks, and so we consider that these two samples exhibit a good surface morphology in contrast to the high NH_3 partial pressure samples.

We measured the sheet resistance of the AlN layers with SiN capping described above, and the results are shown in Figure 6 [8]. The layers grown with high ammonia partial pressure have poor R_{sheet} values, perhaps linked to the poor surface morphology seen in Figure 5 and consequent reduced mobility. Due to their high values, these samples were not measured by Hall Effect. Also, we can see that when the thickness is too low, there is a higher sheet resistance, likely due to a reduction in the N_s due to field effects. Equally, when the thickness is increased too much, we see that the surface is degraded, which would likely increase scattering at the AlN/GaN interface, and thus reduce the mobility. Thus the 3 nm thickness appears to be an optimum for these conditions.

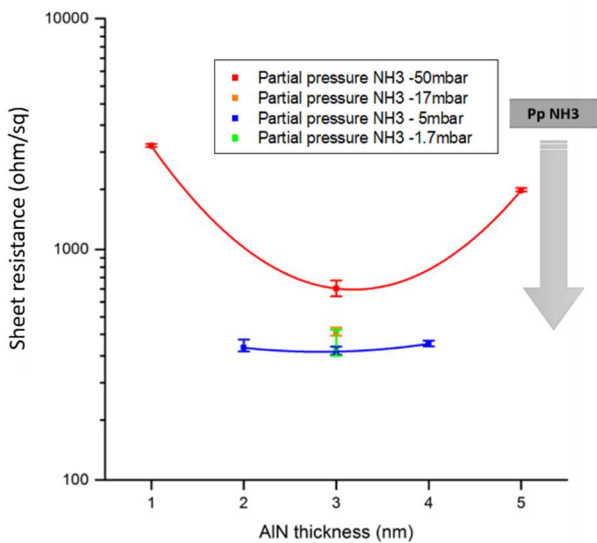


Figure 6: Sheet resistance as function of AlN thickness for AlN layers grown with different NH_3 partial pressures. All layers have a 10 nm SiN cap

As the NH_3 partial pressure is reduced, the sheet resistance is improved, as would be expected from the improved surface morphology. However, for further reduction in NH_3 partial pressure there was no significant improvement in surface morphology, and there is a small increase in sheet resistance. We performed Hall Effect measurements on these 3 nm thick layers with various NH_3 partial pressures to determine both sheet electron density (N_s) and mobility (μ), as shown in Figure 7. We see that decreasing the NH_3 partial pressure leads to an increase in mobility, with a particularly strong increase at 1.7 mbar resulting in a sheet resistance increase as described above. The sheet electron density is roughly constant for the highest partial pressures, but the layer grown at 1.7 mbar NH_3 partial pressure shows a significant drop from around $2 \times 10^{13} \text{ cm}^{-2}$ to $8 \times 10^{12} \text{ cm}^{-2}$. Both N_s and μ for these conditions are therefore closer to those expected from AlGaN barrier structures, which suggests that there may be gallium incorporation in these layers, as will be investigated below.

The impact of AlN layer thickness on electrical characteristics is shown in Figure 8 for growth at NH_3 partial pressure of 5 mbar. We confirm that growing thicker layers leads to higher charge density, while the mobility is reduced.

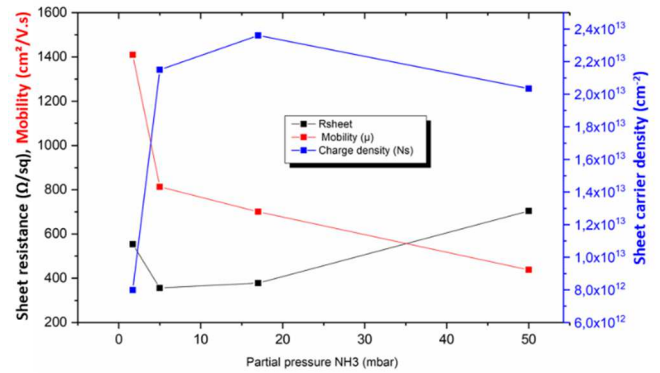


Figure 7: N_s , mobility and R_{sheet} for 3 nm thick AlN layers with various partial pressures of NH_3 for the growth. All layers also have a 10 nm SiN cap.

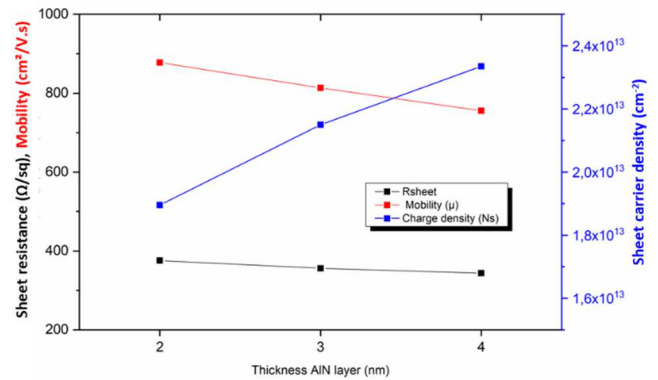


Figure 8: N_s , mobility and R_{sheet} for different AlN thicknesses grown with 5 mbar NH_3 partial pressure. All layers also have a 10 nm SiN cap.

In order to better understand the Hall Effect measurements, we calculated the expected 2DEG sheet carrier density as shown in Figure 9. The calculations are based on a Poisson-Fermi formalism developed based on MOS physics [11]. As expected, for pseudomorphic growth of the AlN barrier, higher N_s values are obtained as the contribution from piezoelectric polarization charges is higher. Equally, as we increase the layer thickness, the N_s should increase which can be understood in terms of field effect.

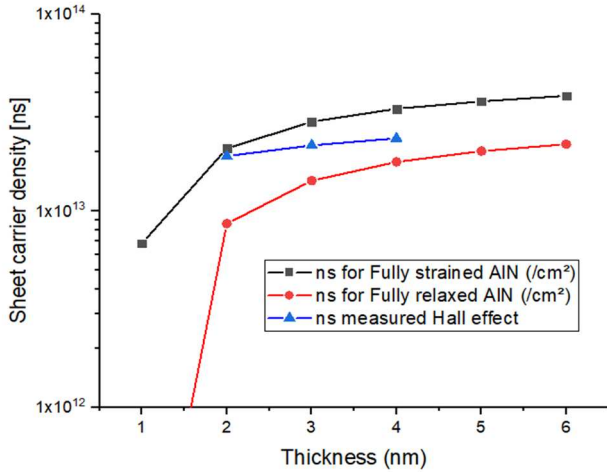


Figure 9: N_s calculation for AlN barrier, with strained and unstrained values shown. Measured points are shown in blue

We have also plotted the values of N_s seen with ammonia partial pressure of 5 mbar in Figure 9. These experimental points are found to be close to the fully strained AlN values for 2 nm thickness, while falling between strained and relaxed values for 4 nm thickness. This shows that our results are coherent with theoretical calculations. The surface morphology was unchanged across the 3 samples (not shown here), so the reduction in mobility is unlikely to be due to increased scattering due to a rougher AlN-SiN interface. In addition, the increased distance between the AlN-SiN interface and the 2DEG would be likely to improve the transport properties for thicker layers if this interface was defective. As the 2DEG sheet density increases, the electrons move closer to the AlN/GaN interface. This would increase the scattering due to any interface roughness, and this may explain the reduced mobility [14].

Gallium pollution has previously been seen for InAlN layers grown using showerhead reactors [15] and this could explain the high mobility and low N_s for the AlN layers with the lowest NH_3 partial pressure, as well as the improved surface morphology. We thus performed SIMS analysis of the two extreme NH_3 condition on the study: 50 mbar and 1.7 mbar. These were thicker layers grown for easier characterization, as described in Figure 1. Comparing SIMS profiles shown in Figure 10 between the two samples with higher and lower partial pressure of NH_3 gave us a

relative difference of the presence of gallium in the AlN but these measurements are very hard to interpret. Both layers appear to show a gradient of gallium into the AlN layers, but the profile is sharper for the layer with the higher NH_3 partial pressure, suggesting less gallium incorporation. However, due to cracks in the samples, it is difficult to quantify the gallium in each sample.

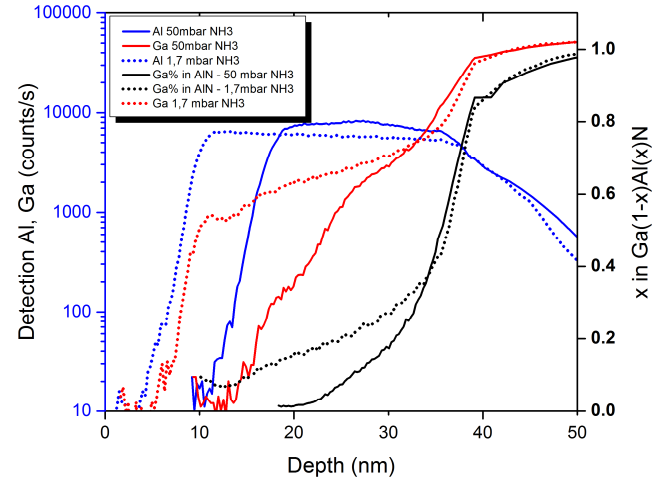


Figure 10: SIMS profiles of Ga (red), Al (blue) and xGa (%) in $Al_{(1-x)}Ga_xN$ (black) for a 23 nm thick layer with 50 mbar NH_3 partial pressure during growth and for a 1.7 mbar 27 nm thick layer with 1.7 mbar NH_3 partial pressure during growth.

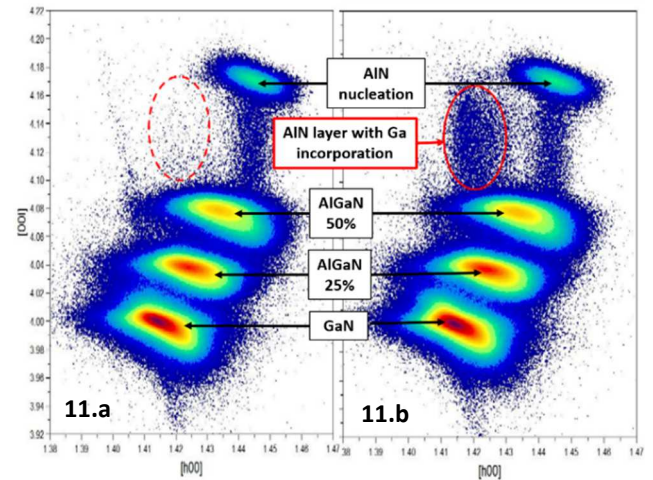


Figure 11: RSM (114) of structure with AlN/SiN grown with 50 mbar NH_3 partial pressure (11.a) vs 1.7 mbar NH_3 partial pressure (11.b)

Following the SIMS analysis, we measured these samples by HR-XRD, performing RSM scans on the (114) asymmetrical peak. Figure 11 shows that the layer grown at higher NH_3 (11.a) has only the peaks corresponding to the AlN nucleation layer, the AlGaIn buffer layers and the GaN layer. However, for the layer grown with 1.7 mbar of NH_3 (11.b), we have an additional peak. This additional peak is very broad with a c-lattice parameter changing for a given a-lattice. If we take the center of this broad peak in the RSM, we find a composition of 78 % Al. This is similar to the

average value seen in SIMS, and shows clearly that for the low NH_3 sample has gallium pollution, which confirms our hypothesis. However, it is difficult to conclude whether there is any gallium in the layer with 50 mbar partial pressure of NH_3 . If there is no gallium, it is likely that the layer would not be seen in the RSM as it would be hidden by the peak from the AlN nucleation layer. This could be confirmed with further measurements such as High Resolution Transmission Electron Microscopy (HRTEM) with Energy Dispersive X-ray composition analysis (EDX).

4. Conclusion

We have shown that growth of thin AlN layers without a SiN cap under our growth conditions is very difficult without resulting in a poor surface morphology. We have also shown that reducing the ammonia partial pressure of AlN layers leads to an improvement in surface morphology and a reduction in sheet resistance, which is predominantly due to an increase in mobility. In addition, as expected by theoretical calculations, we see that increasing the thickness of AlN layers leads to an increase in N_s , despite a decreasing mobility which may be due to a degradation in the surface morphology. We found that for the lowest NH_3 partial pressure, there was a significant increase in mobility, and a drop in N_s , which we attribute to a gallium contamination in the layers. This pollution was confirmed with the growth of thicker AlN layers which were estimated by XRD to contain around 22% gallium for the lowest NH_3 partial pressure growth.

From our study, the optimum growth conditions of an AlN barrier layer with a 10 nm SiN cap is a 3 nm layer at 5 mbar of NH_3 partial pressure. A 3 nm layer allows us to keep a high sheet electron density while staying below the critical thickness for crack formation. This also avoids a rough AlN-SiN interface to maintain a high mobility. Using 5 mbar NH_3 partial pressure for the growth gives both improved surface morphology and mobility to achieve the lowest sheet resistance values. Even if surface morphology is still good at the lowest NH_3 partial pressure (1.7mbar), this has a strong drop in sheet electron density due to high Ga incorporation.

By varying the ammonia partial pressure, we have achieved state of the art R_{sheet} values $< 330 \text{ Ohm/sq}$ for 3 nm thick AlN barrier layers with SiN capping, creating layers which should be compatible with high frequency RF operation.

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