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<td>Author(s)</td>
<td>Ravikiran, L.; Dharmarasu, N.; Radhakrishnan, K.; Agrawal, M.; Yiding, Lin; Arulkumaran, S.; Vicknesh, S.; Ng, G. I.</td>
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L. Ravikiran, N. Dharmaraju, K. Radhakrishnan, M. Agrawal, Lin Yiding,
S. Arulkumaran, S. Vicknesh, and G. I. Ng

Prior to the growth, single heterojunction HEMT (SH-HEMT) and DH-HEMT heterostructures were grown using ammonia-MBE on 100-mm Si substrate. The AlGaN/GaN HEMT heterostructures were successfully grown using ammonia-MBE on 100-mm Si substrate. The high two-dimensional electron gas (2DEG) density obtained in the channel increases due to the combined effect of positive polarization charge that develops at the top AlGaN/GaN interface and the negative polarization charges at the bottom GaN/AlGaN interface. This increase in the electric field further improves the confinement of the 2DEG.

The AlGaN/GaN HEMT heterostructures were successfully demonstrated on 100-mm silicon substrate by ammonia-molecular beam epitaxy (ammonia-MBE). The high two-dimensional electron gas (2DEG) density obtained in the HEMT heterostructures may spill over from the quantum well to the GaN buffer during the high voltage operation of the devices and result in the reduction of peak currents and RF power densities. Thus, improvement of carrier confinement in the channel is essential to achieve high power performances. Higher electrical field in the GaN channel provides uphill barrier for 2DEG to spill into the GaN channel and hence improves its confinement in the quantum well. In the case of a single heterojunction AlGaN/GaN HEMT (SH-HEMT) heterostructure, the electric field in the channel is mainly controlled by the presence of positive polarization charges at the AlGaN/GaN heterojunction interface. However, in an AlGaN/GaN/AlGaN double heterojunction HEMT (DH-HEMT) heterostructure, the electric field in the channel increases due to the combined effect of positive polarization charge that develops at the top AlGaN/GaN interface and the negative polarization charges at the bottom GaN/AlGaN interface. This increase in the electric field further improves the confinement of the 2DEG.

I. INTRODUCTION

AlGaN/GaN high electron mobility transistors (AlGaN/GaN HEMTs) are promising for high frequency power amplification and high voltage power switching applications. The AlGaN/GaN HEMT heterostructures were successfully grown using ammonia-MBE on 100-mm Si substrate. The high two-dimensional electron gas (2DEG) density obtained in the HEMT heterostructures may spill over from the quantum well to the GaN buffer during the high voltage operation of the devices and result in the reduction of peak currents and RF power densities. Thus, improvement of carrier confinement in the channel is essential to achieve high power performances. Higher electrical field in the GaN channel provides uphill barrier for 2DEG to spill into the GaN channel and hence improves its confinement in the quantum well. In the case of a single heterojunction AlGaN/GaN HEMT (SH-HEMT) heterostructure, the electric field in the channel is mainly controlled by the presence of positive polarization charges at the AlGaN/GaN heterojunction interface. However, in an AlGaN/GaN/AlGaN double heterojunction HEMT (DH-HEMT) heterostructure, the electric field in the channel increases due to the combined effect of positive polarization charge that develops at the top AlGaN/GaN interface and the negative polarization charges at the bottom GaN/AlGaN interface. This increase in the electric field further improves the confinement of the 2DEG.

AlGaN/GaN/AlGaN DH-HEMT heterostructures have been well studied using MOCVD growth techniques. However, only a few reports are available employing MBE growth technique. Using ammonia-MBE growth process, DH-HEMT heterostructure growth was demonstrated on 50-mm diameter Si substrate. MBE growth technique offers distinctive advantages such as in-situ growth monitoring, low impurity incorporation and the capability to produce atomically sharp interfaces. In particular, ammonia-MBE is advantageous due to easy cracking of ammonia molecules to produce abundant active nitrogen leading to the nitrogen rich growth conditions. The nitrogen rich growth condition offers wider growth window, higher growth rate, and droplet-free growth surface and lower buffer leakage currents. In this work, aluminum (Al) mole fraction of the AlGaN buffer in the DH-HEMT heterostructure was designed based on Poisson-Schrödinger simulations and grown on 100-mm Si substrate using ammonia-MBE growth process. A comparative study with SH-HEMT is presented and detailed analysis of the surface, structural, and electrical characteristics is discussed.

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II. POISSON-SCHRÖDINGER SIMULATION

Theoretical simulations using self-consistent one-dimensional Poisson-Schrödinger solver were performed to understand the behavior of the 2DEG and its confinement in the quantum well for the SH-HEMT and DH-HEMT heterostructures with increasing “Al” composition in the AlGaN buffer. In the case of SH-HEMT heterostructure, the GaN buffer was assumed to be an AlGaN buffer with “Al” mole fraction of 0%. The self-consistent one dimensional Poisson-Schrödinger simulation program that was used in this work has been developed by Snider et al.,17 which is capable of working with non-uniform mesh sizes.18 The maximum number of mesh points for Poisson solution is 5000, while it is 500 for Schrödinger solution. In the Poisson solution, the mesh size was kept at 0.5 nm for the thicker (Al)GaN buffer of (DH)SH-HEMTs. However, the mesh size was kept at 0.3 nm for the Schrödinger solution, which was solved between top 0 to 150 nm of both heterostructures. For the simulations, all the epilayers in the heterostructures were considered to be undoped. Polarization values for the ternary nitride compounds were obtained from their respective binary compounds. The required mechanical and polarization constants of binary compounds, AlN and GaN were obtained from Ref. 19 and are listed in Table I. Both the spontaneous and piezoelectric polarizations were considered for the AlGaN barrier, GaN channel, and cap layers. However, in the case of buffer GaN (SH-HEMT) and AlGaN (DH-HEMT) epilayers, only spontaneous polarization was considered in the simulation as these buffer layers were assumed to be relaxed.

“Al” composition and thickness of AlGaN barrier for all the HEMT heterostructures were maintained at 32% and 27 nm, respectively. Figure 1(a) shows the simulated conduction band profile of GaN (cap)/AlGaN (barrier)/GaN (channel)/AlGaN (buffer) of HEMT heterostructures and their 2DEG distribution with “Al” mole fraction in the buffer layer varying from 0 to 20%. Figure 1(b) is the zoom-in image of conduction band profile near AlGaN/GaN heterostructure interface. Figure 2 shows the simulated 2DEG carrier concentration as a function of “Al” mole fraction of AlGaN buffer. However, for the simulation, it is assumed that there are no holes in these layers of the heterostructure.

The electric field in the GaN channel region increases with the increase of “Al” mole fraction of the buffer layer, which leads to the improved triangular shape of the quantum well as shown in Fig. 1(b). It can also be seen from the figure that higher electric field together with the improvement of the triangular shape of the quantum well enhances the confinement of 2DEG leading to its reduced spreading in the interface. However, for the simulation, it is assumed that there are no holes in these layers of the heterostructure.

TABLE I. The mechanical and polarization constants of AlN and GaN used in the simulation.

<table>
<thead>
<tr>
<th>Elastic constants (GPa)</th>
<th>AlN</th>
<th>GaN</th>
</tr>
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<tr>
<td>C13</td>
<td>108</td>
<td>103</td>
</tr>
<tr>
<td>C33</td>
<td>373</td>
<td>405</td>
</tr>
<tr>
<td>Polarization parameters (C m⁻²)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Psp</td>
<td>−0.081</td>
<td>−0.029</td>
</tr>
<tr>
<td>e33</td>
<td>1.46</td>
<td>0.73</td>
</tr>
<tr>
<td>e31</td>
<td>−0.60</td>
<td>−0.49</td>
</tr>
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</table>

FIG. 1. Poisson-Schrödinger simulation of (a) AlGaN/GaN/AlGaN DH-HEMT heterostructures showing conduction band profile and 2DEG distribution with variable “Al” mole fraction of the AlGaN buffer (b) zoom-in image of conduction band profile near AlGaN/GaN interface.

FIG. 2. 2DEG density n_s as a function of “Al” mole fraction of AlGaN buffer obtained using Poisson-Schrödinger simulations.
GaN channel. Moreover, the 2DEG concentration is also found to decrease with the increase of “Al” mole fraction of the buffer as shown in Fig. 2. The decrease in the 2DEG concentration can be attributed to the increase in the negative polarization that develops at the bottom GaN/AlGaN interface. Hence, overall, increase in the “Al” mole fraction of the AlGaN buffer improves the confinement of the 2DEG but simultaneously decreases its carrier concentration. Furthermore, “Al” mole fraction beyond 15% was found to have increased the possibility of the formation of hole gas at the bottom GaN/AlGaN interface due to movement of the Fermi level into the valence band at this interface. Degradation of the crystalline quality with increase in the “Al” mole fraction of the AlGaN was also reported. Moreover, due to the increased alloy scattering, thermal conductivity becomes very poor for the AlGaN buffer with “Al” mole fraction beyond 10%. In order to minimize these issues, “Al” mole fraction of 10% was considered for the growth of DH-HEMT heterostructure, which resulted in a simulated 2DEG concentration of $1.085 \times 10^{13} \text{cm}^{-2}$, with the Fermi level position above the quantum well of the valence band at bottom GaN/AlGaN interface.

III. EXPERIMENTAL

Figures 3(a) and 3(b) show the cross sectional view of typical epilayers of AlGaN/GaN SH-HEMT and DH-HEMT heterostructures, respectively. These epilayers were grown on 100-mm Si substrate using ammonia-MBE growth technique. The growth process was initiated with thermal cleaning of Si substrate at 750 °C for 30 min to obtain a clean Si (111) surface, which was confirmed by the observation of Si (7 × 7) reflection high-energy electron diffraction (RHEED) pattern. This was followed by the intentional nitridation of Si surface using ammonia, as the unintentional nitridation is unavoidable in ammonia-MBE growth process. The intentional nitridation resulted in a (8 × 8) RHEED surface reconstruction pattern. Subsequently, predeposition of a few monolayers of aluminum followed by ramping up of the substrate to AlN growth temperature resulted in the formation of AlN nucleation layer on Si surface. A 50 nm thick 1st AlN layer was then grown on the AlN nucleation layer for both SH- and DH- HEMT heterostructures. In both heterostructures, AlN/GaN stress mitigation layers (SMLs) were used to mitigate the stress to obtain 1 µm thick crack free (Al) GaN buffer. The AlN and GaN epilayers in the heterostructure were grown at 920 and 800 °C, respectively. The growth rate of (Al) GaN buffer in both the heterostructures was maintained at ~0.3 Å/µh with a V/III ratio (beam equivalent pressure ratio) of ~2070. Based on the Poisson-Schrodinger simulations, “Al” composition of AlGaN buffer was kept at 10% in the DH-HEMT heterostructure. A thin layer of GaN (40 nm) acts as channel in the DH-HEMT heterostructure. Typical chamber pressure attained during the entire epilayer growth was ~$10^{-5}$ Torr. “Al” composition and the thickness of the barrier layer are 31.7% and 27 nm and 32.5% and 28.5 nm for the SH-HEMT and DH-HEMT, respectively.

IV. RESULTS AND DISCUSSION

A. Structural characterization

Room temperature ex-situ bow measurements on as-grown SH-HEMT and DH-HEMT heterostructures on 100-mm Si substrate revealed mutually opposite bowing, which are shown in Figs. 4(a) and 4(b), respectively. The SH-HEMT heterostructure showed a concave (tensile) bow of ~44 µm, while the DH-HEMT heterostructure showed a convex (compressive) bow of +120 µm. In spite of completely opposite bowing observed for the SH-HEMT and DH-HEMT heterostructures, the microscopic investigation revealed crack free surfaces for both of these heterostructures on 100-mm Si substrate. From these results, it is clear that the growth of AlGaN buffer instead of GaN buffer in the
DH-HEMT heterostructure should be the reason for its high convex bowing. Based on the observations from nitride heterostructures grown with AlGaN/AlN/GaN SMLs, the lower rate of compressive stress relaxation due to reduced lattice mismatch at AlGaN/2nd AlN interface and the mitigation of stress at AlGaN/2nd AlN interface could be the reason for the observed higher convex bow of the wafer. The achieved high convex bowing further indicates the feasibility of growing even thicker buffer layers or expanding the growth process to larger diameter Si substrates.

Surface morphology of the SH-HEMT and DH-HEMT heterostructures was investigated by AFM (atomic force microscope) and the corresponding images are shown in Figs. 5(a) and 5(b), respectively. Mound type surface morphology was observed for both the heterostructures. However, the mound features appeared to be larger in the lateral direction for the DH-HEMT compared to SH-HEMT heterostructure. While an RMS roughness value of 2.2 nm was obtained for the DH-HEMT, it was 2.9 nm for the SH-HEMT heterostructure for a scan area of \(10 \times 10 \mu \text{m}^2\). Streaky RHEED patterns observed during the growth of different epilayers of SH-HEMT and DH-HEMT heterostructures indicate that the growth proceeded through two dimensional growth mode in both the heterostructures. However, the larger mound size and lower RMS roughness indicate that the lateral growth is enhanced in the buffer of DH-HEMT heterostructure. Similar observation has also been reported by Cordier et al. with lower RMS roughness for the DH-HEMT compared to the SH-HEMT heterostructure.

Enhancement of the lateral growth and the consequent improvement in the surface morphology of nitride epilayers in the ammonia-MBE growth process can primarily be attributed to two parameters. They are the enhanced surface diffusion of metallic adatoms and the increased ammonia cracking, leading to improved incorporation of metal and nitrogen atoms at the step edges. In the case of a DH-HEMT, the reduced lattice mismatch between 2nd AlN and Al\(_{0.10}\)Ga\(_{0.90}\)N buffer might have led to lower relaxation and higher residual compression in the AlGaN buffer. This higher residual compression enhances the surface diffusion of adatoms. Moreover, additional metal flux available in the form of aluminum during the growth of AlGaN buffer might have also contributed in the cracking of more ammonia at the step edges leading to the replenishment of the adsorption sites to incorporate more atoms into the lattice. Thus, the combined effect of increased adatom diffusion followed by the improved incorporation of metal atoms at the step edges might possibly have enhanced the 2D growth mode and resulted in larger mound features with smoother surface morphology for the DH-HEMT heterostructure.

Structural properties of both the HEMT heterostructures were investigated by HR-XRD technique. In order to investigate the strain states and relaxation properties of different epilayers, reciprocal space mapping (RSM) was performed along GaN \(\langle 10\overline{1}0\rangle\) plane. The results are presented in Figs. 6(a) and 6(b) for the SH-HEMT and DH-HEMT samples, respectively. While 2nd AlN, AlGaN barrier and 2nd GaN are clearly observed in the RSM of SH-HEMT heterostructure, AlGaN buffer and GaN channel, instead of 2nd GaN are observed in the case of DH-HEMT sample. GaN channel (40 nm thick) in the DH-HEMT was found to be under high residual compressive stress with only a parallel mismatch of 1334 ppm with respect to Al\(_{0.10}\)Ga\(_{0.90}\)N buffer. However, AlGaN barrier was found to have grown coherently with GaN buffer for the SH-HEMT and GaN channel for the DH-HEMT. Coherent growth ensures the development of piezoelectric polarization \(P_{\text{PE}}\) to induce 2DEG in the quantum well at the heterojunction interfaces.

In order to investigate the crystal quality, XRD rocking curve scans were performed along \((0002),(1012)\) and \((0001)\) planes.
planes of GaN and AlGaN buffers of SH-HEMT and DH-HEMT heterostructures, respectively. The corresponding full width at half maxima (FWHM) values are listed in Table II. The FWHM of (0002) plane indicates slight degradation in the screw type dislocation density in the DH-HEMT buffer compared to the GaN buffer in the SH-HEMT. However, the FWHM of (3032) plane shows improvement in the edge type dislocation density for the buffer in the DH-HEMT compared to that of SH-HEMT heterostructure. The overall dislocation density as observed from the FWHM of (1012) scan is almost similar in both the heterostructures. This further signifies the fact that the growth of Al0.10Ga0.90N buffer in the DH-HEMT did not contribute to any overall degradation in the crystal quality.

B. Electrical characterization

Electrical characteristics of SH-HEMT and DH-HEMT heterostructures were measured using Van der Pauw Hall measurement and mercury probe capacitance-voltage (C-V) techniques. The obtained electrical properties of both the heterostructures are listed in Table III.

The DH-HEMT heterostructure shows lower \( n_s \) compared to SH-HEMT. However, the room temperature mobility of 2DEG in the DH-HEMT heterostructure is considerably higher compared to that of SH-HEMT heterostructure. Hall measurements were also performed as a function of temperature from 400 to 90 K. Figure 7 shows the product of the carrier concentration and the mobility \( (n_s \times \mu_H) \) as a function of temperature for both SH-HEMT and DH-HEMT heterostructures. The \( (n_s \times \mu_H) \) product yields almost close values for both heterostructures. This may indicate that the current driving capabilities are similar. However, the slight deviation obtained in the product at lower temperatures is due to the saturation of mobility in the DH-HEMT heterostructure, which can possibly be attributed to slightly higher alloy scattering due to increased “Al” composition in the barrier and lesser screening effect due to lower 2DEG carrier concentration.

Figures 8(a) and 8(b) show the C–V measurements obtained on the SH-HEMT and the DH-HEMT heterostructures, respectively. Nearly flat plateaus of capacitance followed by a sharp pinch off characteristic indicates the improved confinement of 2DEG in the DH-HEMT compared to the SH-HEMT heterostructure. The pinch off characteristics of the capacitance were further analyzed by taking the derivative of C–V data (dC/dV) as shown in Figs. 8(a) and 8(b). The sharp dC/dV profile with lower FWHM shows the improvement in the confinement of 2DEG in DH-HEMT heterostructure compared to SH-HEMT heterostructure. Further, the integration of capacitance as a function of voltage \( \int C \, dV \) from zero bias to pinch off is also plotted in the figure in order to estimate the 2DEG carrier concentration in the heterostructures. Here, A and q are the area of the mercury probe contact and charge of an electron, respectively. The values of \( n_s \) estimated are \( 1.04 \times 10^{13} \) cm\(^{-2}\) and \( 0.97 \times 10^{13} \) cm\(^{-2}\) for SH-HEMT and DH-HEMT heterostructures.

![Reciprocal space mapping](image)

**FIG. 6.** Reciprocal space mapping along (1015) plane for (a) SH-HEMT and (b) DH-HEMT heterostructures.

**TABLE II.** FWHM of XRD rocking curves along different planes of buffers in SH- and DH-HEMT heterostructures.

<table>
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<th>Buffer</th>
<th>(0002)</th>
<th>(1012)</th>
<th>(3032)</th>
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<tr>
<td>GaN (SH-HEMT)</td>
<td>1003</td>
<td>1652</td>
<td>2540</td>
</tr>
<tr>
<td>AlGaN (DH-HEMT)</td>
<td>1185</td>
<td>1640</td>
<td>2376</td>
</tr>
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</table>

![Electrical properties](image)

**FIG. 7.** \( (n_s \times \mu_H) \) product of SH- and DH-HEMT heterostructures as a function of temperature.

**TABLE III.** Electrical properties SH- and DH-HEMT heterostructures obtained using Hall, C-V, and Poisson-Schrödinger simulation.

<table>
<thead>
<tr>
<th>Heterostructure</th>
<th>( R_s ) (Ω/sq.)</th>
<th>( \mu_H ) (cm(^2)/V.s)</th>
<th>( n_s ) ( \times 10^{13} ) cm(^{-2})</th>
<th>C-V Simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>SH-HEMT</td>
<td>434</td>
<td>1310</td>
<td>1.09</td>
<td>1.04</td>
</tr>
<tr>
<td>DH-HEMT</td>
<td>421</td>
<td>1510</td>
<td>0.97</td>
<td>0.97</td>
</tr>
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</table>
heterostructures, respectively. These data are closer to the $n_s$ values obtained from Hall measurements. It was also observed that the capacitance in the sub-threshold region was lower for the DH-HEMT heterostructure, indicative of lower background carrier concentration compared to SH-HEMT heterostructure. Thus, the electrical characterization overall indicates that the DH-HEMT heterostructure provides improved confinement of 2DEG with slight reduction in carrier concentration. However, the mobility of 2DEG is improved for the DH-HEMT heterostructure.

The observed improvement in the confinement of 2DEG in the DH-HEMT heterostructure from the CV measurements can be attributed to the enhanced electric field in the GaN channel and the improved quantum well of the DH-HEMT heterostructure as observed from Poisson-Schrödinger simulations shown in Fig. 1(b). The 2DEG concentration values obtained from the simulation are also tabulated in Table III. The simulated values were found to be slightly higher compared to measured values. The slight deviation might be due to the variation in values of different physical constants considered for the simulation. As described earlier, the decrease in the 2DEG concentration (both measured and simulated) in the DH-HEMT heterostructure can be attributed to the negative polarization that develops at the bottom GaN/AlGaN interface. Further, the increase in the electron mobility of the 2DEG as observed from the Hall measurements can be attributed to the increased confinement of 2DEG.

C. AlGaN/GaN/AlGaN DH-HEMT devices

HEMT devices with submicron gate were fabricated on the DH-HEMT heterostructure using a T-gate with a gate metal stack of Ni/Au with thicknesses of 50/400 nm. The length and width of the gate was kept at ~0.27 and (2 x 150) µm, respectively. $I_{DS}$-$V_{DS}$ characteristics (Fig. 9) of the HEMT device exhibited a maximum drain current of 806 mA/mm at $V_g$ = +1 V and an extrinsic transconductance of 178 mS/mm. The devices exhibited good pinch off characteristics with a threshold voltage of ~ 5.1 V.

The current carrying capability of the DH-HEMT is similar to that of similarly grown SH-HEMT devices. However, the DH-HEMT heterostructure exhibited 3 times higher buffer breakdown voltage at a current compliance of 0.2 mA/mm (see Fig. 10). The higher value obtained can be attributed to the use of wide-band gap AlGaN buffer ($E_g$ = 3.69 eV) in the DH-HEMT heterostructure. The AlGaN buffer in the DH-HEMT prevents the punch through effects and result in lower leakage current and higher breakdown voltage. This is consistent with the observed lower capacitance in the sub-threshold region in the CV measurements of the DH-HEMT heterostructure.

Hence, DH-HEMT heterostructure may be a better option overall for the development of AlGaN/GaN HEMTs in the application of high power switching devices due to its improved 2DEG-confinement and higher breakdown voltages but with similar current driving capabilities as that of SH-HEMT. Small-signal RF characteristics of the fabricated DH-HEMTs were obtained as illustrated in Fig. 11. To the best of our knowledge, these are the first demonstration of small-signal RF characteristics for the ammonia-MBE grown DH-HEMT on Si substrate. The best unity current-gain cut-off
frequency ($f_T$) and maximum oscillation frequency ($f_{\text{max}}$) obtained for the DH-HEMTs are 22 and 25 GHz, respectively.

V. CONCLUSION

AlGaN/GaN/AlGaN DH-HEMT heterostructure was designed using Poisson-Schrödinger simulations in order to improve the confinement of the 2DEG in AlGaN/GaN based HEMTs, with $n_s$ at a reasonably higher level of $\sim 10^{13}$ cm$^{-2}$. AlGaN barrier and buffer with “Al” composition of 32% and 10%, respectively, showed both improved confinement and higher 2DEG in the DH-HEMT. AlGaN/GaN/AlGaN DH-HEMT heterostructure grown on 100-mm Si(111) substrate using ammonia-MBE growth showed higher compressive wafer bow and smoother surface morphology compared to SH-HEMT. HR-XRD measurements revealed that the buffers of both SH-HEMT and DH-HEMT heterostructures are of similar crystal quality. Hall measurements on DH-HEMT heterostructure showed a room temperature mobility of 1510 cm$^2$/V.s and $n_s$ of 0.97 $\times\ $10^{13} $\text{cm}^{-2}$. The mobility value is found higher, but the 2DEG concentration is lower compared to SH-HEMT heterostructure. Capacitance-voltage measurements revealed better confinement of 2DEG and hence the higher channel mobility in DH-HEMT heterostructure compared to SH-HEMT. Moreover, the buffer breakdown voltage of DH-HEMT structure exhibited three times higher than that of SH-HEMT structure. The sub-micron gate DH-HEMT exhibited maximum drain current density of 806 mA/mm and maximum extrinsic transconductance of 178 mS/mm. This is the first demonstration of DH-HEMT on 100-mm Si substrate using ammonia-MBE growth.


$^{17}$See http://www.nd.edu/~demand for 1D Poisson Program, by G. Snider, University of Notre Dame.


