Towards E-mode AlGaN/GaN HEMTs with ferroelectrics

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Abstract

By using the polarization effects induced by a ferroelectric layer, a normally off AlGaN/GaN HEMT is achieved in simulations, with minimal leakage current and a high current capability.

1. Introduction

When it comes to the AlGaN/GaN HEMT, polarization plays a key role in its functioning. This is because the polarization effects at the AlGaN/GaN interface causes a two-dimensional electron gas (2DEG) to form just below the interface in the gallium-nitride. GaN-based HEMTs are interesting for their high speed and high-power handling capabilities. This is due to the high electron mobility, which is caused by the 2DEG, hence the name high electron mobility transistor (HEMT). The one downside is that a conventional version is normally-on due to the strong polarization at the AlGaN/GaN interface. This makes them less practical due to the need of a more complex driver circuit and potential hazards.

There are already multiple methods of achieving a normally off GaN HEMT, each with their own up and downsides. Some methods have been studied more than others, these are the cascode configuration, p-GaN, doping under the gate and recessed gate (1). Another method is by using a ferroelectric in the gate stack. This method makes use of the polarization properties of a ferroelectric material to counteract the polarization already present at the AlGaN/GaN interface, therefore depleting the 2DEG. By depleting the 2DEG the high-power capacity of the HEMT stays relatively unchanged. This is opposed to destroying the 2DEG, which happens with for example the recessed gate. This destruction creates a gap in the 2DEG, which results in a higher channel resistance, thus making this less suitable for high power applications.

In this paper, a feasibility study of adopting a ferroelectric material in the gate stack to obtain a normally off/enhanced mode (e-mode) AlGaN/GaN HEMT has been carried out. This study has been carried out by performing

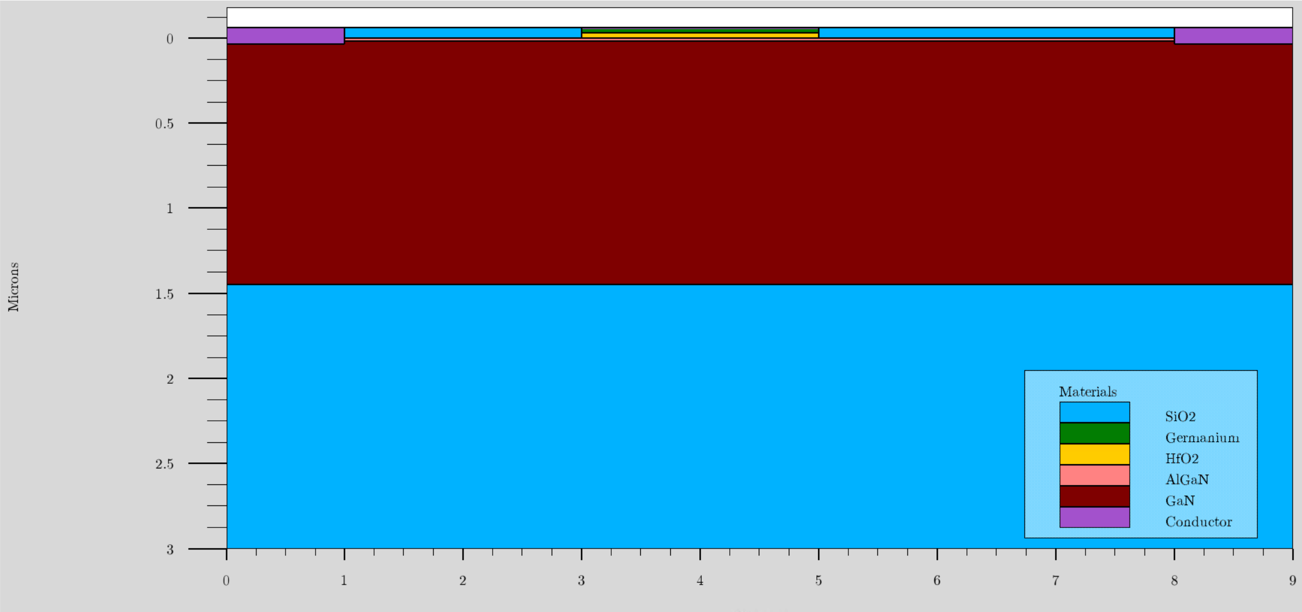


Figure 1: Structure of the final design.

computer (FEM) simulations with a commercial two-dimensional device simulation tool, Atlas (2). The device optimization process will be explored in the following section, followed by the obtained results, a discussion of these results, and finally the conclusion with some future recommendations.

2. Design optimization process

The design process was carried out in Silvaco Atlas, which is a two-dimensional device simulator. The final design can be found in figure 1. The gate stack can be seen in more detail in figure 2. The gate stack consists of two layers on top of the AlGaN, the PZT, which is the ferroelectric, and underneath that is a layer of hafnium dioxide. This layer of hafnium dioxide is chosen as a charge trapping layer (3). The rest of the structure is the same as a conventional AlGaN/GaN HEMT, an AlGaN layer on top of a GaN layer, with an insulating oxide layer at the bottom. In the simulations the source and drain are recessed so they reach into the GaN and therefore connect to the 2DEG, and the gate electrode rests on top of the gate stack, on the PZT. The thicknesses of the layers are $30nm$ for the PZT and hafnium oxide, $20nm$ for the AlGaN, and $1.5\mu m$ for the GaN. The length of the whole HEMT is $9\mu m$, with a channel length of $7\mu m$. The gate length L_G and drift length L_D are $2\mu m$ and $3\mu m$ respectively.

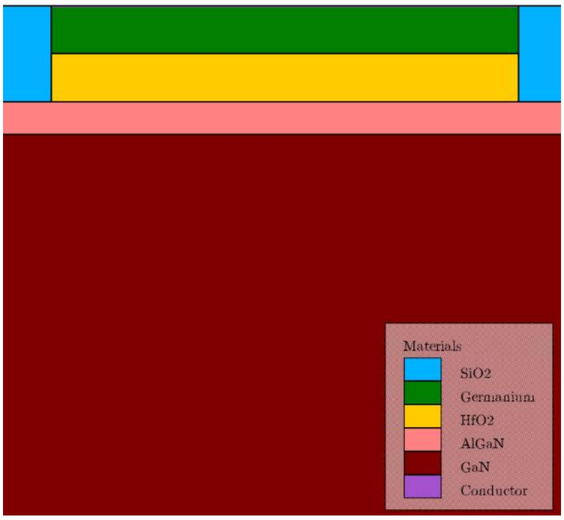


Figure 2: Gate stack of the final design.

Multiple design choices were made based on existing research or remained unchanged from the template one of my supervisors provided me. No modifications have been made to the width of any of the regions or the total HEMT, and nothing was changed at all underneath the AlGaN layer. The position of the gate stack was not experimented with either. When it comes to the ferroelectric material, no material changes were made. The PZT that was already present in the template is a material that is known and proven to work in this role, therefore changing it was not a priority (4). Layer thicknesses were experimented with, and from the simulation exercise the same conclusion can be drawn as the literature, thinner layers work better (3) (4) (5). The thinner layers resulted higher threshold voltages, yet still negative, and steeper current curves at the threshold voltage. Therefore, the minimum thickness that Atlas would allow at this point before running into issues was chosen.

Another design choice that is based on existing research is the use of a trapping layer between the ferroelectric and the AlGaN (3). Hafnium dioxide was picked as the material for the trapping layer since this was used with success in one of the papers (3). The decision to stick with this material and not experiment with other materials was made due to time constraints and because this material has been proven to work already. Most of the time went into finding the optimal polarization by varying the sheet charge densities. The final sheet charge values that were set are $8 \times 10^{13} cm^{-2}$ for the PZT, which is located at the bottom of the PZT, and $-2.7 \times 10^{13} cm^{-2}$ and $0.8 \times 10^{13} cm^{-2}$ at the top and bottom of the AlGaN respectively. The polarization in the PZT can be achieved by poling the material. The AlGaN values can be varied by adjusting the aluminium gallium composition, which is 0.16 to 0.84 in the final design. Table 1 shows an overview of the device parameters.

Although the only significant difference in the gate stack between the template that was handed over and this final design is an additional hafnium dioxide layer in the gate stack, more things were experimented with during the design process. After integrating the hafnium dioxide layer into the gate stack, the next step was experimenting with a recessed gate. According to the research a greater recess depth should result in a higher threshold voltage yet lower drain current. The impact of the recess was limited, this may have been due to the persistent problems with the meshing caused by misaligned layers. Although the voltage was shifted slightly, the amount was not significant enough to shift it to a positive voltage, and therefore dropped to save on time, avoid more problems, and avoid the decrease in drain current caused by it.

Table 1: Design parameters

	Final design	Antiparallel design	conventional
Device length (µm)	9	9	9
Channel length (µm)	7	7	7
Gate length (µm)	2	2	2
Drift length (µm)	3	3	3
PZT layer thickness (nm)	30	30	-
HfO2 layer thickness (nm)	30	30	-
AlGaN layer thickness (nm)	20	20	20
GaN layer thickness (µm)	1.5	1.5	1.5
Aluminium/Gallium composition	0.16/0.84	0.16/0.84	0.16/0.84
Sheet charge PZT/HfO2 (cm^{-2})	8×10^{13}	-8×10^{13}	-
Sheet charge HfO2/AlGaN (cm^{-2})	-2.7×10^{13}	-2.7×10^{13}	-
Sheet charge AlGaN/GaN (cm^{-2})	0.8×10^{13}	0.8×10^{13}	0.8×10^{13}

After reverting back to the unrecessed gate with the PZT/hafnium dioxide gate stack, some more exercises was done with it. It is here where a threshold voltage that approached 0 was achieved, which was achieved with unrealistically high polarization values. Getting past the 0 volts was the difficult part. In the following struggle to achieve a positive threshold voltage some things were tried that go against the theory. One thing that was tried and oddly enough yielded a positive threshold voltage, therefore achieving a normally off HEMT. This thing was changing the polarization of the PZT layer from antiparallel to parallel with the polarization at the AlGaN/GaN interface. This is illogical because an antiparallel raises the conduction band while a parallel one lowers it, a comparison of this can be seen in figure 3 and 4. The band bending is the strongest near the gate electrode, which is on the left, and the difference becomes significantly less at the 2DEG, where the conduction bands of the parallel and antiparallel are $0.507eV$ and $0.536eV$ respectively. Note that these figures are with the final values, which can be found in table 1, where final design is the parallel polarization and antiparallel design is with the antiparallel polarization. At this point the next task was to bring the polarization values back down to realistic values, which resulted in the final design described above.

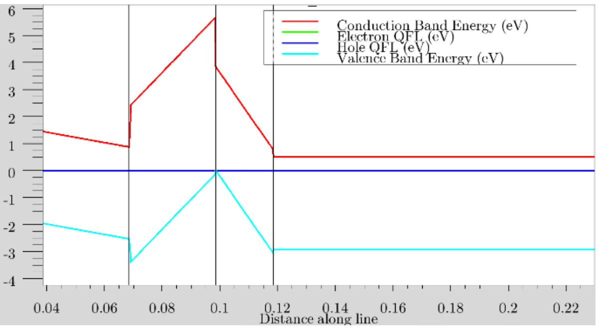


Figure 3: Band diagram with parallel polarization $(0V_{Gate})$.

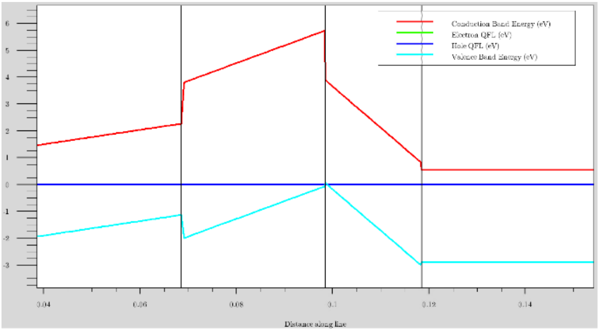


Figure 4: Band diagram with antiparallel polarization $(0V_{Gate})$.

The structure indicate that the ferroelectric layer is germanium, but this is not the case. The material properties are the ones from PZT, the only reason it is named germanium is for atlas to treat is at a semiconductor, which is needed for it to work.

3. Results

The final design with the parallel polarization at the bottom of the PZT yielded a threshold voltage of $1.1V$ and an $I_{D,max}$ of $6.9 \times 10^{-5} A/\mu m$ with a drain voltage of $0.25V$. The leakage current with this design is $1.9 \times 10^{-10} A/\mu m$, therefore negligible compared to the on-current. This can be seen in figure 5. This design compares favourably to a conventional HEMT with the same polarization between the AlGaN and the GaN. The conventional HEMT yields a lower $I_{D,max}$ of $5.6 \times 10^{-5} A/\mu m$ with a threshold voltage of $-2.4V$, which can be seen in figure 6.

When looking at the drain voltage with the same gate overdrive voltage however, the conventional HEMT and the final design yield the same drain current. Take a gate overdrive voltage of $2V$, here both the final design and the conventional HEMT have a drain current of $4.6 \times 10^{-5} A/\mu m$, which indicates that the design has a minimal if any impact on the drain current. This indicates that Note that the current collapses around the $1V$ point, which is due to gate leakage (6). The parameters can be found in table 1.

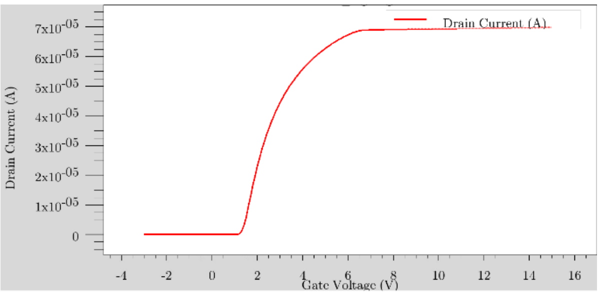


Figure 5: Drain current of the final design.

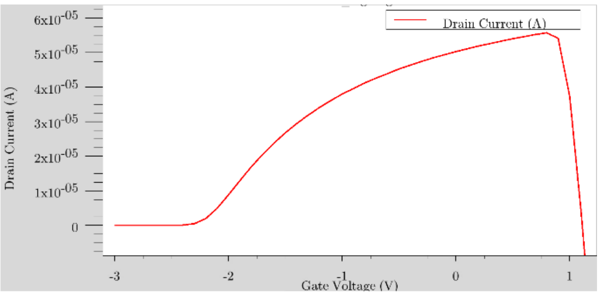


Figure 6: Drain current of a conventional AlGaN/GaN HEMT.

When looking at the band diagram, it is clearly visible that the conduction band is raised above the electron QFL (quasi Fermi level), meaning that the 2DEG is depleted. When the gate voltage is increased to past the threshold voltage, the conduction band dips below the electron QFL just below the AlGaN/GaN interface, therefore restoring the 2DEG under the gate. This can be seen in figure 7, while the state at $0V$ can be seen above in figure 3. The location of the 2DEG is just after the last black line in both figures. The electron and hole QFLs are (almost) equal, and therefore lay on top of each other. It is visible that the conduction band (red) dips below the electron QFL (green, but it is the same as the blue line) at the on state, but the conduction band is well above the Fermi level at the $0V$ state.

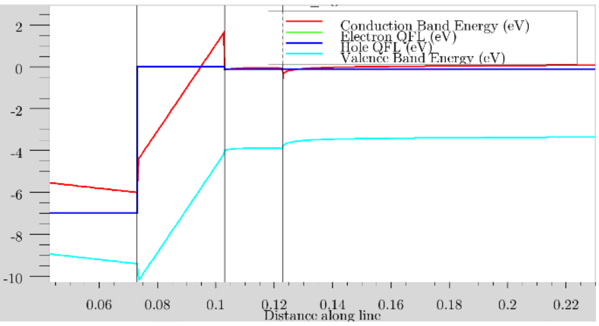


Figure 7: Band diagram when conducting $(7V_{Gate})$.

4. Discussion

The final design has a few caveats, this is because the polarization direction of the PZT layer seems to have a limited impact. The impact that it does have is a trade-off, a higher sheet charge, means a lower threshold voltage, but also a lower drain leakage current. Parallel polarization lowers the conduction band, therefore lowering the threshold voltage, which is the logical part of this trade-off. The band diagram of the antiparallel polarization can be seen in figure 4, which can be compared to the band diagram with parallel polarization in figure 3. To fully suppress the leakage current, a high enough parallel polarization is needed, this is because when this is high enough, the electron concentration in the AlGaN and GaN get forced out of the region under the gate stack significantly more than when there is a leakage current present, see figure 8. On the left side the electron concentration under the gate is significantly reduced, while this is not the case on the right. The resulting drain current with antiparallel polarization can be seen in figure 9. It is visible that the threshold voltage is significantly higher than with parallel polarization, and so is the leakage current. The device parameters of these two can be found in table 1.

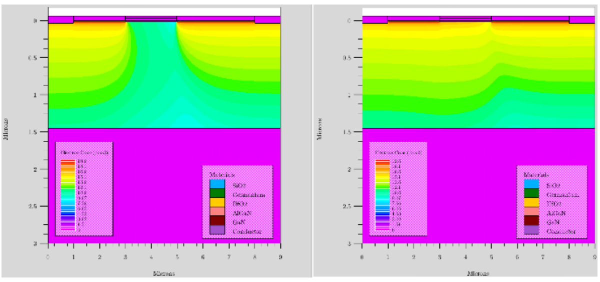


Figure 8: Electron concentration at $0V_{Gate}$, with parallel (left) and antiparallel (right) polarization.

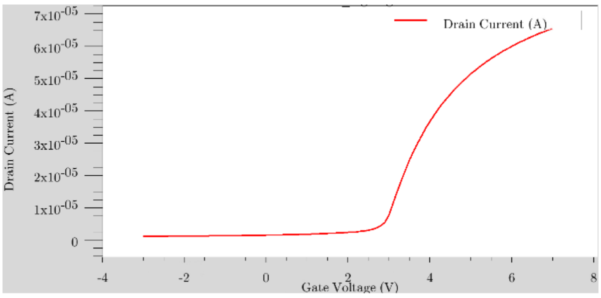


Figure 9: Drain current with antiparallel polarization.

The hypothesis why this is the case is that due to the antiparallel polarization, the hole concentration under the hafnium dioxide/AlGaN interface is increased. This increased hole concentration screens the 2DEG from the effects of the gate stack. The result is that the 2DEG is not fully depleted. Therefore, there is still a significant current flowing when the gate voltage is lower than the threshold voltage. Figure 10 shows the difference in hole concentration in the top of AlGaN, figure 11 shows the electron concentration at the gate region, and figure 12 shows the current flowlines, demonstrating that the current does indeed flow through the 2DEG and not deeper in the GaN. Note that the scale in this figure is on a relative scale, which means that the red area on the left does not have the same current flow as the same red on the right. One should only focus on the current flow in the GaN layer.

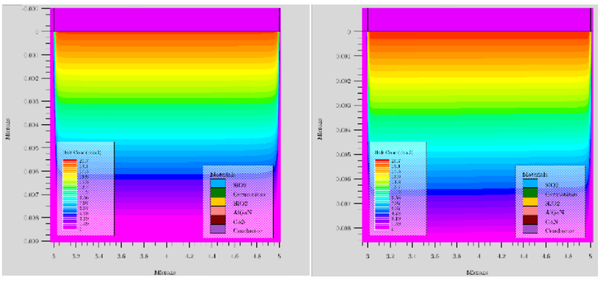


Figure 10: Hole concentration in the top of the AlGaN, with parallel (left) and antiparallel (right) polarization.

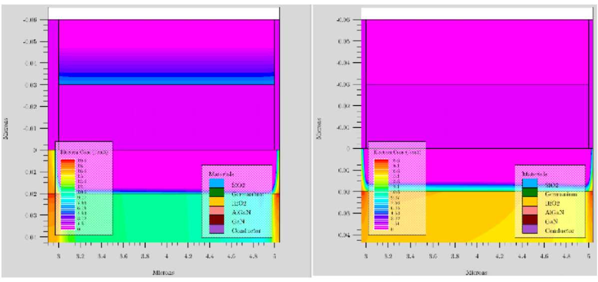


Figure 11: Electron concentration at the gate region, with parallel (left) and antiparallel (right) polarization.

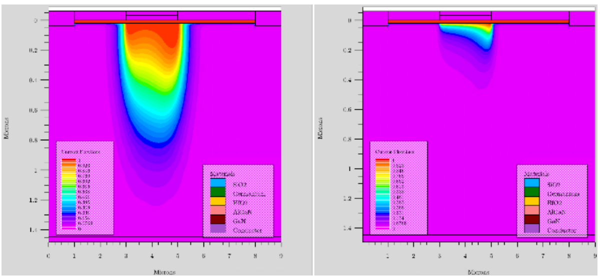


Figure 12: Current flowlines with a relative scale, with parallel (left) and antiparallel (right) polarization.

When the leakage current is fully supressed, and there is the possibility to further increase the parallel polarization underneath the PZT, there is the option to increase the polarization at the AlGaN/GaN interface by increasing the aluminium content. This increase in polarization will increase the maximal drain current and makes it more difficult to deplete the 2DEG.

Although there is still room to increase the drain current by increasing the polarization at the AlGaN/GaN interface, it was decided not to do this. This model has simplifications and approximations in it, and therefore will deviate from reality, where there will always be a leakage current, however small it may be. When there is more leakage current suppression due to a weaker 2DEG than may have worked without any leakage current in the model, the leakage current should be less in a real version as well. Another positive consequence of not going right to the edge of what works is leaving some wiggle room to adjust most if not all parameters to mitigate unforeseen flaws that may come up when less simplifications or for the reality.

One of the significant simplifications is that the silicon oxide is an ideal isolator in the model, which is obviously not the case in real life, meaning that this has an impact on the functioning of the design.

One peculiarity with the simulations is that the hafnium dioxide layer seems to act like an isolator instead of its intended use as a charge trapping layer. Despite this, the design still seems to work. If this is a quirk from Atlas, then there is a chance this design will not work as intended, if this behaviour carries over to the real world, then this design should still work. As mentioned above, changing only the name of a material could result in a different result because Atlas treats it differently. This was also tried with the hafnium oxide, by changing it to silicon, which Atlas treats as a semiconductor. This did not yield any different results, however.

5. Conclusions and recommendations

To conclude, the device simulation predict that the design offers normally off behaviour, with the caveat of the model simplifications and atlas peculiarities that may influence the outcome significantly. At $1.1V$, the threshold voltage shifted well into the positive range, resulting in a normally off AlGaN/GaN HEMT. The simulated leakage current is less than 0.001% of what the $I_{D,max}$ is, therefore more than enough of a difference for this to be used in high power applications.

Although this design works, there is still plenty of room for improvements and optimizations. Some applications may prefer for example a higher threshold voltage, higher drain current, or an even lower drain current. Replacing the PZT and/or hafnium dioxide could be one way to reach the desired alteration. Another aspect where there is still room to further enhance the design is by optimizing the layer thicknesses, which is something that was done in the beginning, but that was before a normally off result was achieved, thus there is still room for optimization there as well. Reintroducing a partially recessed gate is also an option to increase the threshold voltage, although this will negatively affect the drain current (3).

6. References

1. Kok, Frank. *Literature study normally off AlGaN/GaN HEMTs.* 2020. p. 18.

2. *Atlas User's Manual.* Santa Clara, CA : Silvaco, Inc, 2016.

3. *High Vth enhancement mode GaN power devices with high ID, max using hybrid ferroelectric charge trap gate stack.* Wu, C. H., et al. Kyoto : s.n., 2017. Symposium on VLSI Technology. pp. 60-61.

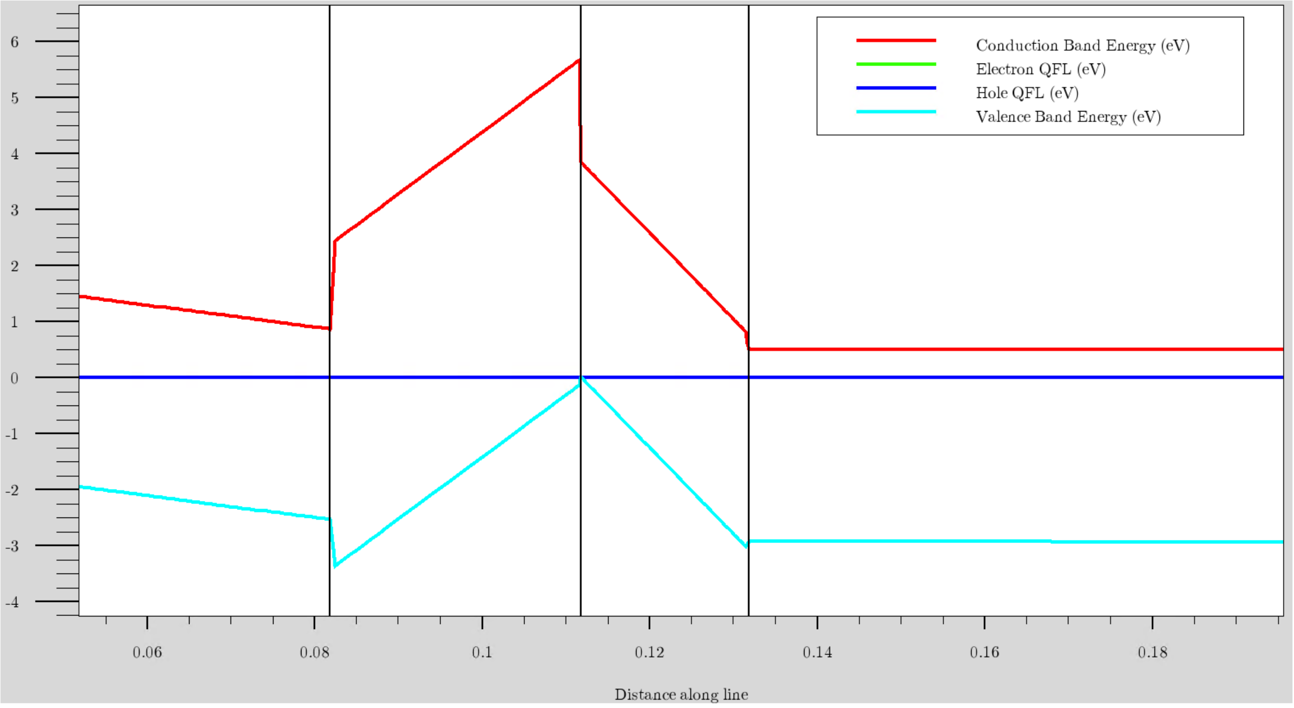
4. *Ferroelectric Gate AlGaN/GaN E-Mode HEMTs With High Transport and Sub-Threshold Performance.* Zhu, Jiejie, et al. 1, 2018, IEEE Electron Device Letters, Vol. 39, pp. 79-82.

5. *Polarization effects in ferroelectric gate AlGaN/GaN High Electron Mobility Transistors.* Zhou, R, et al. 2020, Accepted for IEEE International Symposium for Power Semiconductor Devices & IC's (ISPSD).

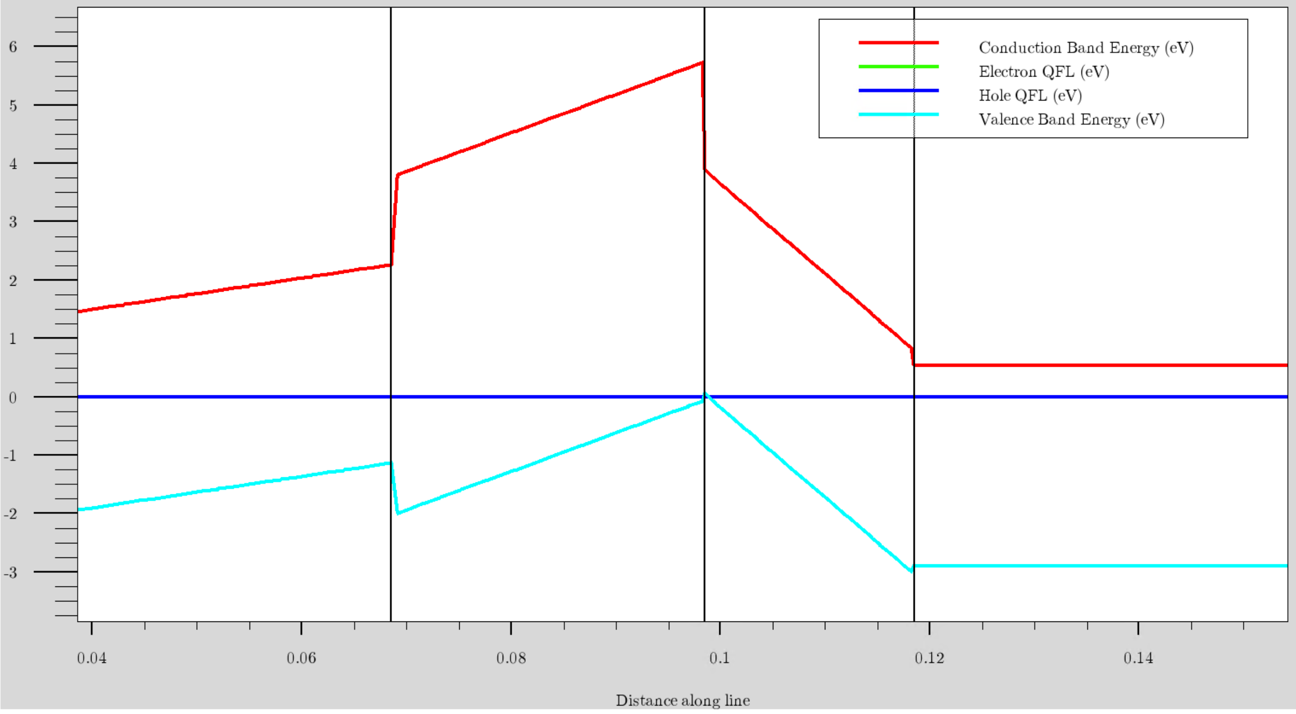
6. *Gate leakage mechanisms in AlGaN/GaN and AlInN/GaN HEMTs: Comparison and modeling.* Turuvekere, Sreenidhi, et al. 60, 10 2013, Electron Devices, IEEE Transactions on, pp. 3157-3165.

7. Appendix

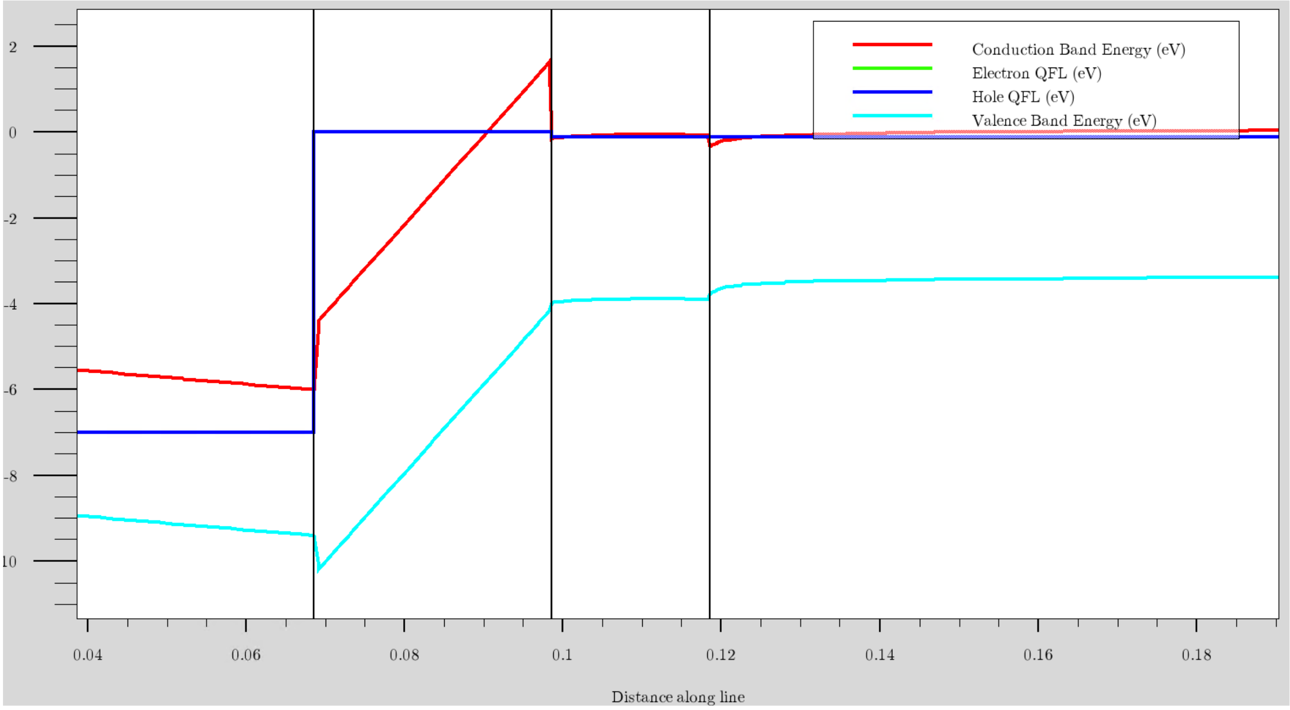
Larger figures



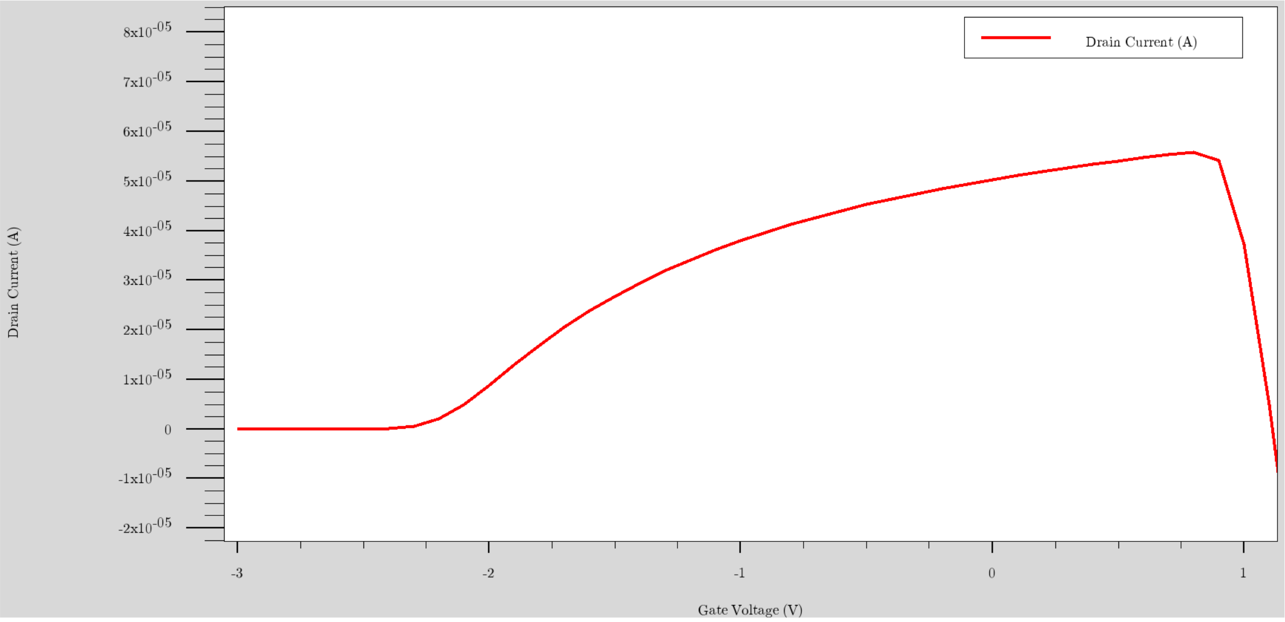
Band diagram with parallel polarization (figure 3).



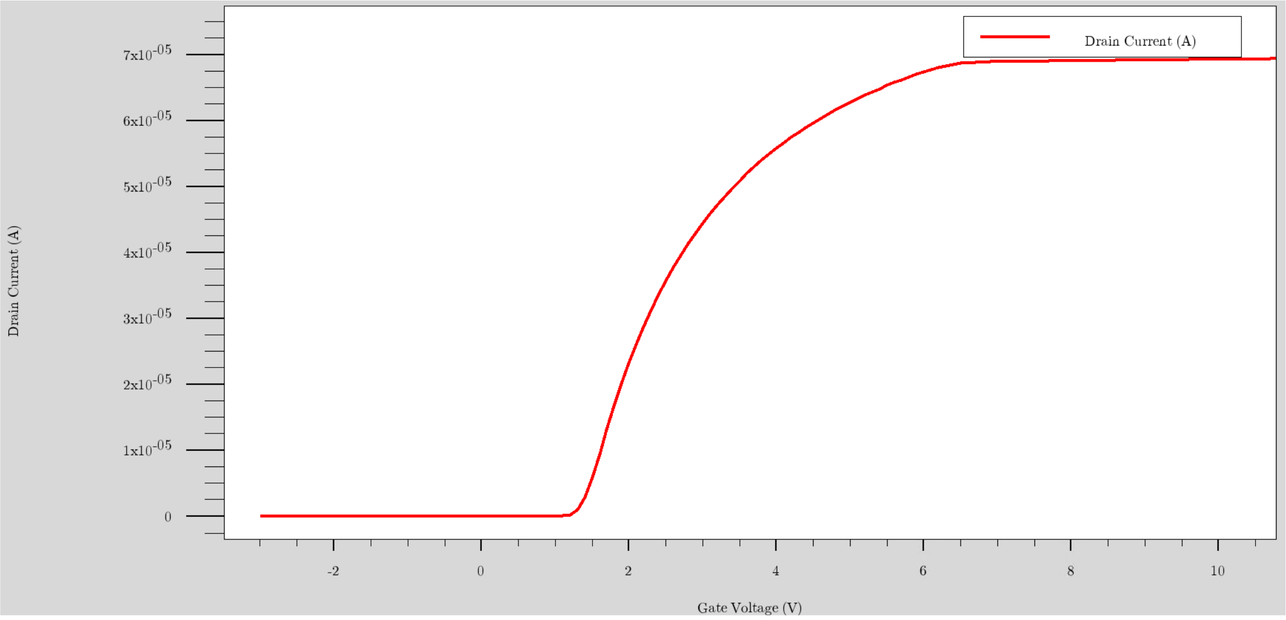
Band diagram with anitparallel polarization (figure 4).



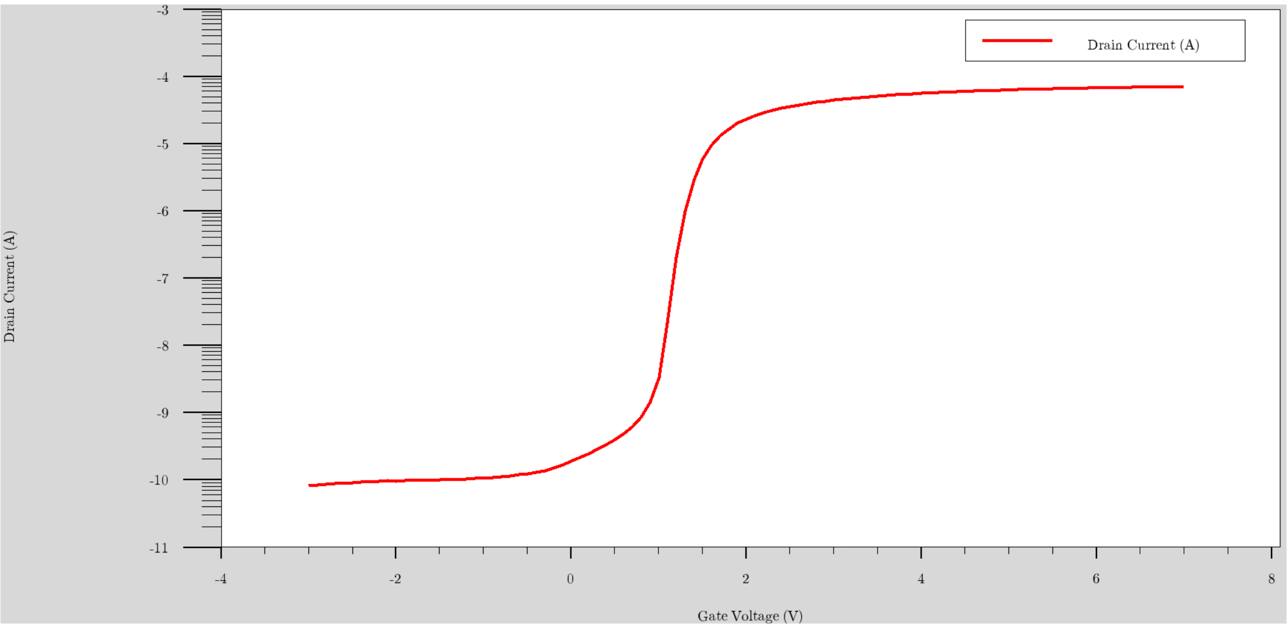
Band diagram with parallel polarization at $7V_{Gate}$ (figure 7).



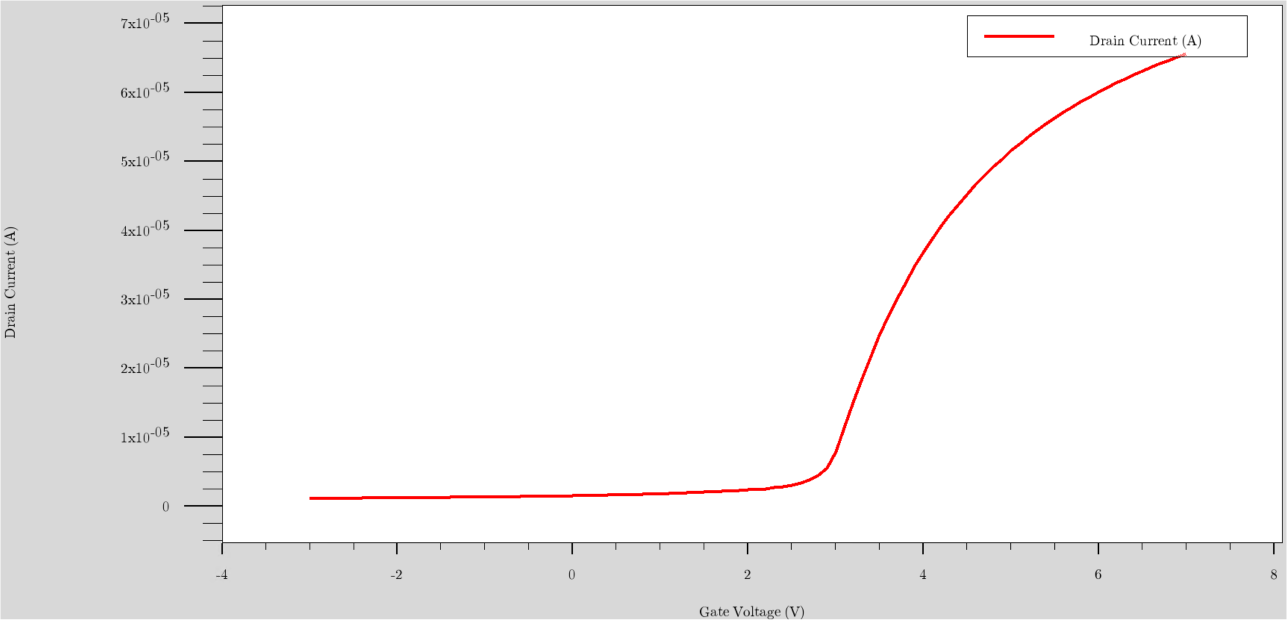
Drain current conventional HEMT (figure 6).



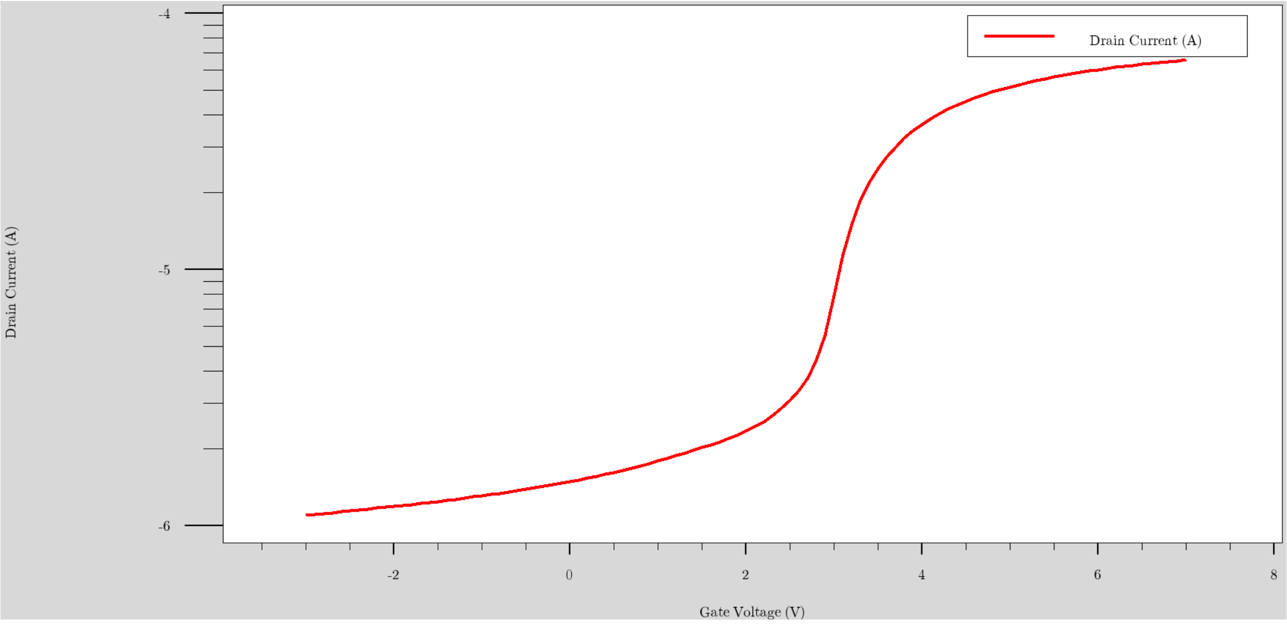
Drain current final design (figure 5).



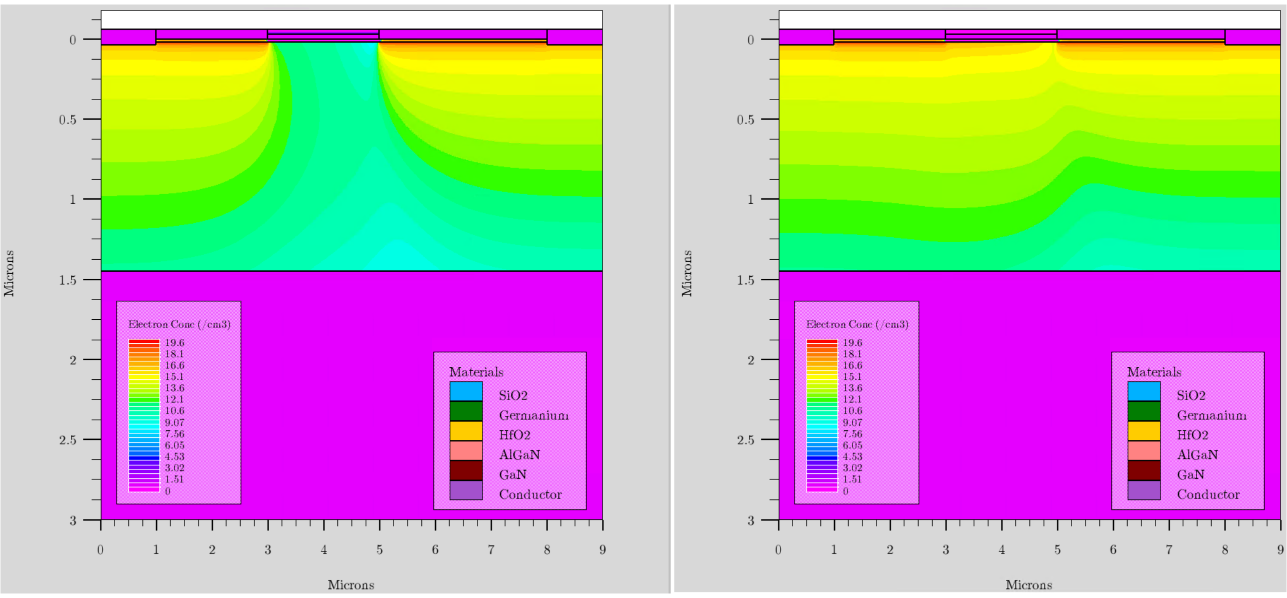
Drain current final design (figure 5), logarithmic y-axis.



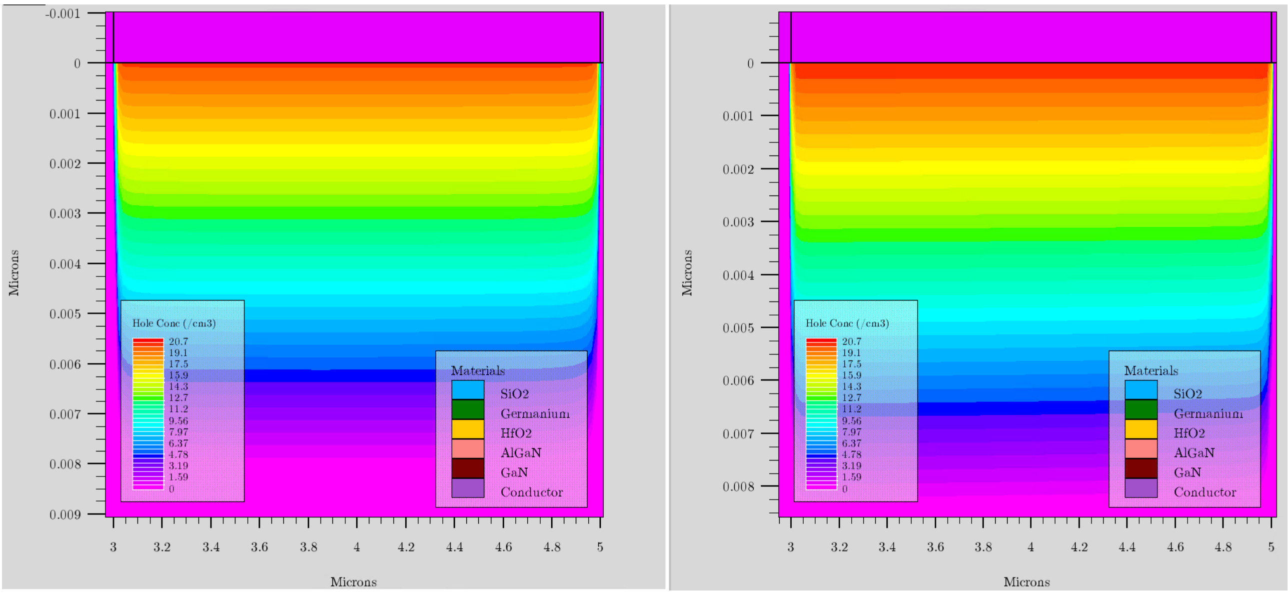
Drain current with antiparallel polarization (figure 9).



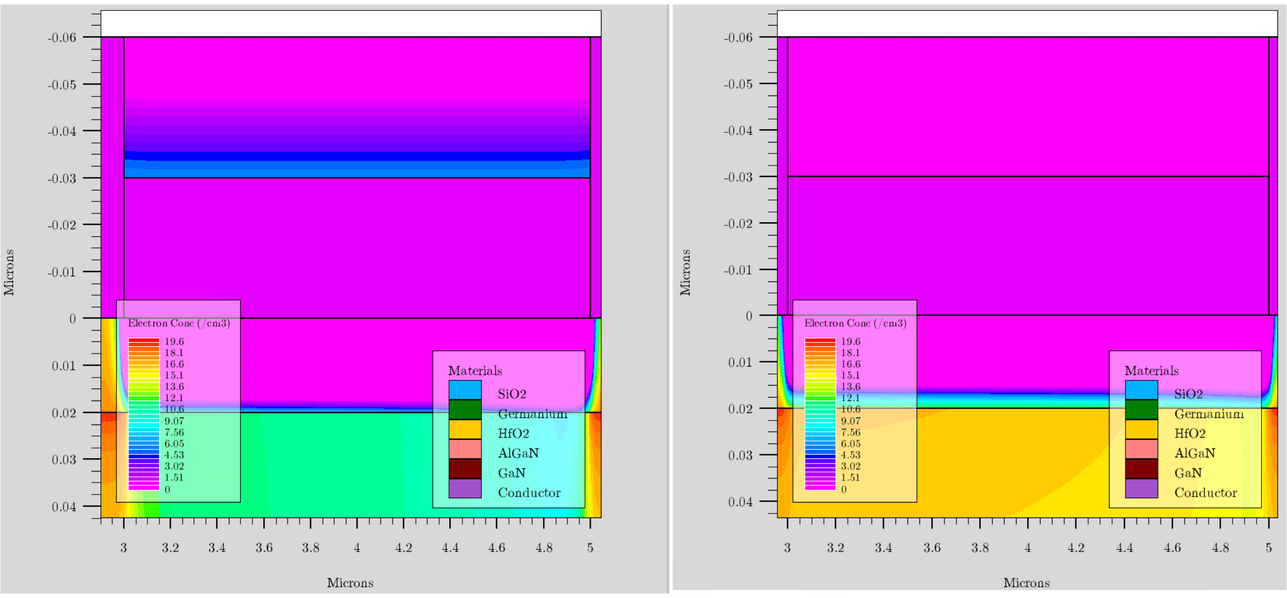
Drain current with antiparallel polarization (figure 9), logarithmic y-axis.



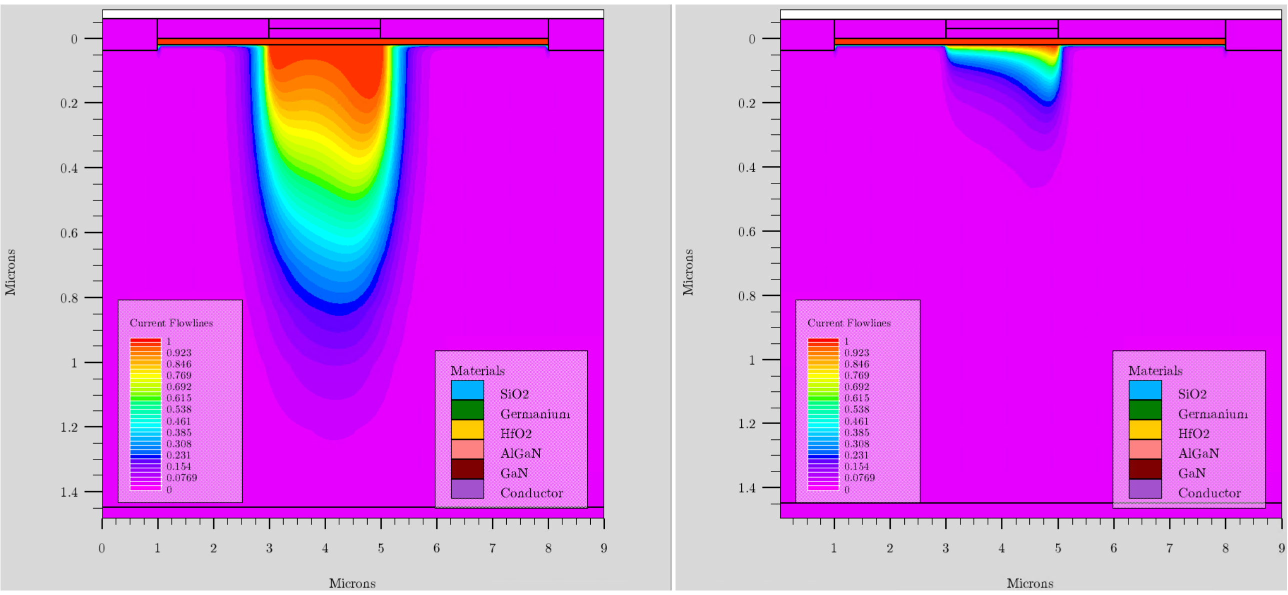
Electron concentration at $0V_{Gate}$, with parallel (left) and antiparallel (right) polarization (figure 8).



Hole concentration in the top of the AlGaN $0V_{Gate}$, with parallel (left) and antiparallel (right) polarization (figure 10).



Electron concentration at the gate region at $0V_{Gate}$, with parallel (left) and antiparallel (right) polarization (figure 11).



Current flowlines with a relative scale, with parallel (left) and antiparallel (right) polarization (figure 12).

Input file

```
go atlas

# AlGaN/GaN HEMT, set layer thicknesses
set tPZT=0.06
set tALGAN=0.02
set tHfO2=0.03

# pz refers to the net polarization charge at each interface, setting sheet charge values
set pz=0.8e13
set pzPZT=8e13
set pzHfO2=-2.7e13
set meshratio=0.5
mesh space.mult=1.0

set vgstep=0.1

# Define mesh in horizontal direction
x.mesh loc=0.00                         spac=0.02
x.mesh loc=1.00                         spac=0.02
x.mesh loc=3.00                         spac=0.02
x.mesh loc=5.00                         spac=0.02
x.mesh loc=8.00                    spac=0.02
x.mesh loc=9.00                    spac=0.02

# Define mesh in vertical direction
y.mesh loc=-1*$tPZT                     spac=($tPZT-$tHfO2)/20
y.mesh loc=-0.5*($tPZT-$tHfO2)-$tHfO2   spac=($tPZT-$tHfO2)/20
y.mesh loc=-0.1*($tPZT-$tHfO2)-$tHfO2   spac=($tPZT-$tHfO2)/20

y.mesh loc=-1*$tHfO2          spac=$tHfO2/40
y.mesh loc=-0.9*$tHfO2        spac=$tHfO2/20
y.mesh loc=-0.5*$tHfO2        spac=$tHfO2/10
y.mesh loc=-0.1*$tHfO2        spac=$tHfO2/20

y.mesh loc=0                     spac=$tPZT/200
y.mesh loc=0.1*$tALGAN                spac=$tALGAN/40
y.mesh loc=0.5*$tALGAN                spac=$tALGAN/10
y.mesh loc=0.9*$tALGAN                spac=$tALGAN/40
y.mesh loc=$tALGAN                  spac=$tALGAN/60
y.mesh loc=1.1*$tALGAN                spac=$tALGAN/10
y.mesh loc=3.00                    spac=0.5

# Define several regions, e.g., insulator or semiconductor layers
region num=1 material=oxide
region num=2 material=germanium y.min=-1*$tPZT     y.max=-1*$tHfO2          x.min=3 x.max=5
region num=3 material=HfO2     y.min=-1*$tHfO2     y.max=0                  x.min=3 x.max=5
region num=4 material=algan      y.min=0           y.max=$tALGAN x.comp=0.2   x.min=1 x.max=8
region num=5 material=gan      y.min=$tALGAN       y.max=1.5+$tALGAN

# Define electrodes
electr name=gate              y.min=-1*$tPZT y.max=-1*$tPZT           x.min=3 x.max=5
electr name=source            y.min=-1*$tPZT y.max=0.02+$tALGAN         x.min=0 x.max=1
electr name=drain             y.min=-1*$tPZT y.max=0.02+$tALGAN         x.min=8 x.max=9
electr name=substrate bottom

# Put a certain amount of interface charge to mimic the effect of polarization differences
interface charge=$pzPZT s.s   y.min=-1*$tHfO2      y.max=-1*$tHfO2       x.min=3 x.max=5
interface charge=$pzHfO2 s.s   y.min=0      y.max=0       x.min=3 x.max=5
interface charge=$pz    s.s   y.min=$tALGAN  y.max=$tALGAN    x.min=1 x.max=8

# Switch on models (which have to be completed for mobility)
models print srh fermi

# Adjust material parameters
material material=gan      eg300=3.43   affinity=4.1  permittivity=9.5 mun=1800  mup=10 NC300=2.23e18 NV300=4.62e19  vsatn=1.9e7
material material=algan     eg300=3.832  affinity=3.84 permittivity=9.4 mun=20    mup=10 NC300=2.95e18 NV300=1.084e20 vsatn=1.1e7
material material=germanium eg300=3.4    affinity=3.5  permittivity=600 mun=25    mup=25 NC300=1.4e20  NV300=3.4e20
```

```
material material=HfO2      eg300=5.8    affinity=2.0  permittivity=25  mun=150   mup=150  NC300=2.8e19 NV300=1.04e19


# Impact ionization needed for breakdown
impact selb material=gan

# Adjust workfunction Schottky gate; source and drain regions are in principle ohmic
contact name=gate workfunction=4.96
contact name=source workfunction=4.2
contact name=drain workfunction=4.2

# Variables which should be plotted in case of TonyPlot
output con.band val.band band.param flowlines charge traps e.mob h.mob e.velocity ex.vel ey.velocity h.vel hx.vel hy.vel qss polar.charge

# Indicate what numerical methodology is used for the calculations: first adopt Gummel method, after 5 iterations the Newton method
method gummel newton gum.init=5 carriers=2 autonr

# Start calculations at thermal equilibrium
solve init

# Save the solution in a structure file for studying the device properties, e.g., plotting band diagrams or conduction current
save outfile=PZT_HEMT.str

############################################
# Calculation of I-V curves
############################################

# Solve equations for one charge carrier
method gummel newton gum.init=5 carriers=2 autonr

# Solve the equations for a fixed drain voltage
solve vdrain=0.25

# Make a log file for storing the I-V data
log outfile=Id_Vgs.log no.trap

solve vgate=-3 vstep=$vgstep vfinal=-3 name=gate
save outfile=Id_Vgs.str

solve vgate=-3+$vgstep vstep=$vgstep vfinal=0 name=gate
save outfile=Id_Vgs2.str

solve vgate=$vgstep vstep=$vgstep vfinal=15 name=gate
save outfile=Id_Vgs3.str

# Stop storing the I-V data for the Id-Vds curve
tonyplot Id_Vgs.log Id_Vgs.str Id_Vgs2.str Id_Vgs3.str
quit
```