

ECE 4333-301

Translation of RF GaN HEMT from Nextnano into

Silvaco Atlas

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Abstract

This paper discusses the creation of an RF GaN HEMT device in Silvaco Atlas from a reference 1D design in Nextnano and how to extract S-parameters from that device. The covered topics include translation of material parameters across software suites, sensible assumptions on structural design, determining similarity across translations, and appropriate simulation parameters.

Acknowledgments

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1. Introduction

1.1 Background

For many applications, the High Electron Mobility Transistor (HEMT) is the next evolution of the MOSFET. The planar silicon MOSFET has reached the limit of speed, causing subsequent generations to find clever structural designs to create more rapid transistors. HEMTs offer a solution by having a faster electron mobility (μ) by virtue of being composed of materials with an inherently higher μ . These devices are most relevant in the sphere of high-frequency and high-power applications- telecommunication systems and power systems- not simply because their μ is higher, but because this property is important in many other aspects of transistors. For example, if we take the well-known MOSFET drain current equations, we can see that if all else is equal we will linearly gain current purely by having an increased μ .

$$I_{Dsat} = \frac{1}{2} \frac{W}{L} C_{OX} \mu (V_{GS} - V_T)^2$$

However, as they are different in both material and structure, they cannot always be simply characterized by MOSFET equations and understandings.

Firstly, HEMTs' semiconductors are inherently n-type, thus p-type doping is especially challenging. Additionally, atop and below their main semiconductor layer (e.g. GaN or GaAs), they have an insulating material (AlN or delta-doped AlGaAs, respectively) that further guides the electrons along the channel semiconductor to increase carrier velocity. Figure 1 illustrates this structure.

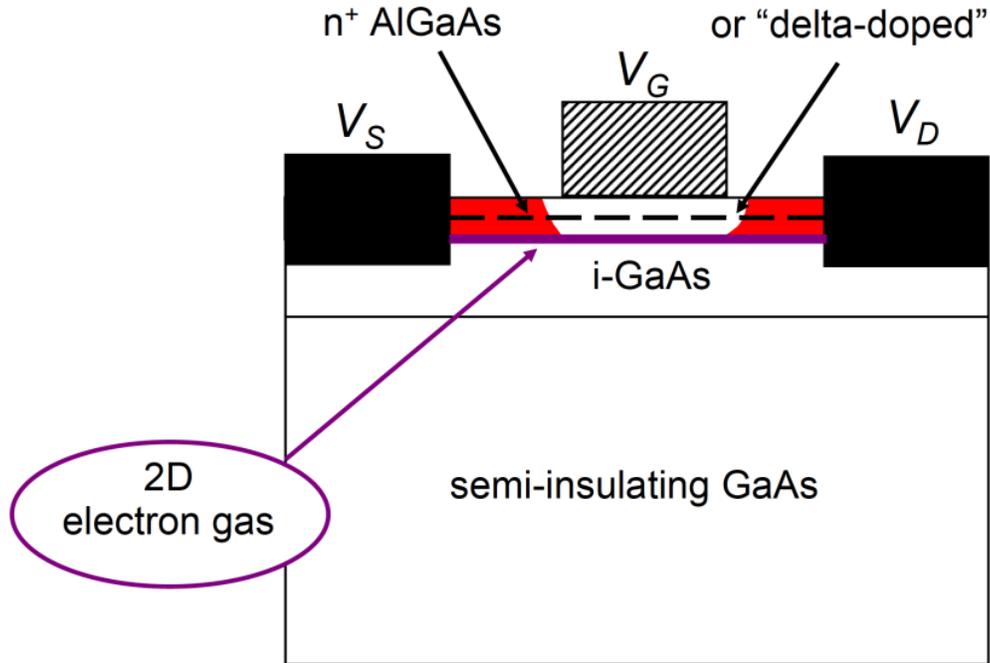


Figure 1: Diagram of an HEMT Device [1].

This structure allows a 2 Dimensional Electron Gas (2DEG) region to form. The product of which is much higher mobility, as within the 2DEG region, electrons can cross the structure with minimal interference. A graphical explanation of this effect is showcased in Figure 2 through the use of an energy band diagram. Energy band diagrams are crucial in understanding many aspects of transistor devices, as they allow us to see the distribution of electrons and holes (and their energies) along the structure. Figure 2 shows this diagram with the x-axis being the depth- as in, the structure from gate towards substrate.

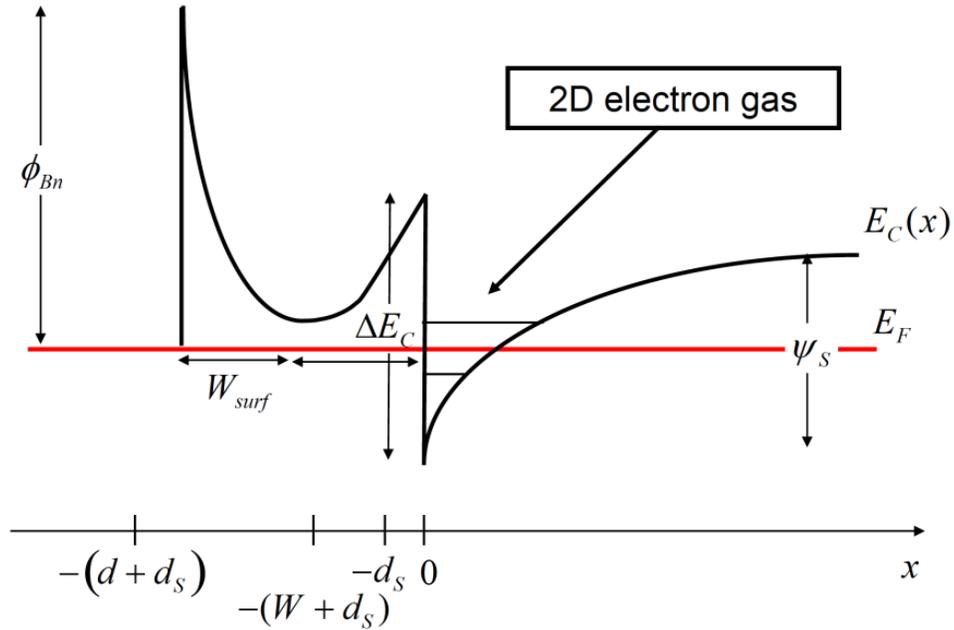


Figure 2: Generic Energy Band Diagram of an HEMT Device in Strong Inversion [1].

The 2DEG region is also often called a “quantum well,” as at this region a significant amount of quantum carriers are present- electrons in this case. The importance of these carriers in the scope of this paper does not go past the fact that they move across the structure more rapidly, so we will not be going into detail about them, however a mention felt appropriate.

1.2 Structure of Paper

The paper will begin with describing the translation of the simulated device from Nextnano to Silvaco Atlas in Section 2, including how to verify whether the device is appropriately translated. Section 3 will describe the simulation methods and some rough results given certain obstacles at the present stage, which will be explained in Section 4. Section 5 will conclude the paper with a summary of the work. In the Appendices, one can find notable pieces of code, project disclaimers, and project progress.

2. Translation of Device

2.1 Material Parameters

An important aspect of these devices, as stated in the introduction, is the materials. Even if we were using default material models in one software, we would need to at least verify that in a different software their parameters are equal. However, in our Nextnano simulation, the materials of GaN and AlN are heavily modified, so it is to be assumed that modifications are necessary in Silvaco Atlas as well.

Table A in Appendix A.1 shows the material defaults of GaN and AlN in Atlas, and Figure 9 in the same appendix shows the material modifications of the two materials in Nextnano. Of importance is to read the commented portions of the Nextnano to the far right of the page, as those roughly match the Syntax column of Table A to the Nextnano parameters. Some of the more important parameters are the direct band gap, the electron effective masses, and the hole effective masses.

To set material parameters in Atlas, one simply calls the "MATERIAL" statement, declares the material to be modified, and adjusts the material per the "Syntax" column.

For example, if we wanted GaN to have a bandgap of 3.51 eV, we write the following:

```
MATERIAL MATERIAL=GaN EG300=3.51
```

Some parameters and their syntax in Atlas are not obviously stated in the manual, for example the dielectric constants of these materials (which turns out to be "PERMITTIVITY") [2]. An easy way to check the total material parameters is to include the statement "MODEL PRINT" in the Atlas input file. This will at least give insight into the values of these parameters. To find the syntax, one needs to reach the last chapter of any Atlas manual- titled "Statements"- and shift through the "MATERIAL" statement's parameters until the desired parameter is found. Using these tools help with other materials which do not have in-depth tables- in our case, AlGaN.

Both in Nextnano and Atlas, the material parameters of AlGaN are calculated based on the parameters of GaN & AlN and the x composition of the material. The x composition is the ratio of aluminum to gallium- $\text{Al}_x\text{Ga}_{1-x}\text{N}$. The Atlas defaults are 0.30; based on Nextnano we desire the x composition to be 0.45. From there, we could let Atlas determine the rest of the material parameters for us. However, there is a slight discrepancy between what Nextnano calculates the AlGaN parameters to be and what Atlas calculates, even though they are supposed to be fully determined by the GaN and AlN parameters that have been set. Therefore, the best course of action is to find the material parameter file outputted by Nextnano and transfer those values to Atlas explicitly. For easier readability, the Nextnano++ version of the output file is provided in Appendix A.1 as Figure 10 (the input file is written in the Nextnano³ syntax, hence the differentiation).

The last material to mention is silicon carbide, which is the substrate of the device. This also required modification, even though in Nextnano SiC is left as-is. Most notably, the bandgaps differ between the two programs, Nextnano calling for 6.0 eV and Atlas calling for 2.9 eV.

One crucial parameter that does not get mentioned in the Atlas tables or the Nextnano input file is electron affinity, denoted as χ . This is the energy difference between the vacuum level and the conduction band. Manually setting χ of materials is not quite straight-forward. In Atlas, there are two ways to set a material's χ : through explicit instruction (with the "AFFINITY" parameter) or the "ALIGN" parameter. The ALIGN parameter is far more useful when we do not know χ directly, as the calculations are done

with respect to the material with the smallest bandgap and the conduction band discontinuities. That is, the sudden jumps the conduction band makes since each material in the device creates a heterojunction (a junction between two materials with different band gaps). To align a material that is immediately neighboring the reference material- GaN in our case- one must use this equation:

$$A = \frac{\Delta E_C}{E_{g2} - E_{g1}} = \frac{\Delta E_C}{\Delta E_{g21}} \quad (1) [2]$$

Where E_{g1} is the reference material, E_{g2} is the material to be aligned, and ΔE_C is the conduction band discontinuity between the two materials. For a material that is not immediately neighboring the reference material, the following formula is used:

$$A = \frac{\Delta E_{g32}}{\Delta E_{g31}} \frac{\Delta E_{C32}}{\Delta E_{g32}} \quad (2) [2]$$

As an example, if we have a GaN region with a bandgap of 3.51 eV as declared above, and we want to align a region of AlN followed by a region of AlGaIn with bandgaps of 6.25 eV and 4.66 eV respectively, we would use Equation 1 to solve for AlN's alignment and Equation 2 for AlGaIn. To find ΔE_C , in this case, we can use the energy band diagrams generated from our prior Nextnano sim, as seen in Figure 3. In this diagram, from left to right, the materials are: a metal, AlGaIn, AlN, and GaN. By inspection of the graph, we can deduce that the ΔE_C between GaN & AlN is about 1.92 eV and between AlN & AlGaIn is about 1.07 eV. Also note that the Schottky barrier height (the conduction band discontinuity between the metal and the AlGaIn region) is precisely 1 eV.

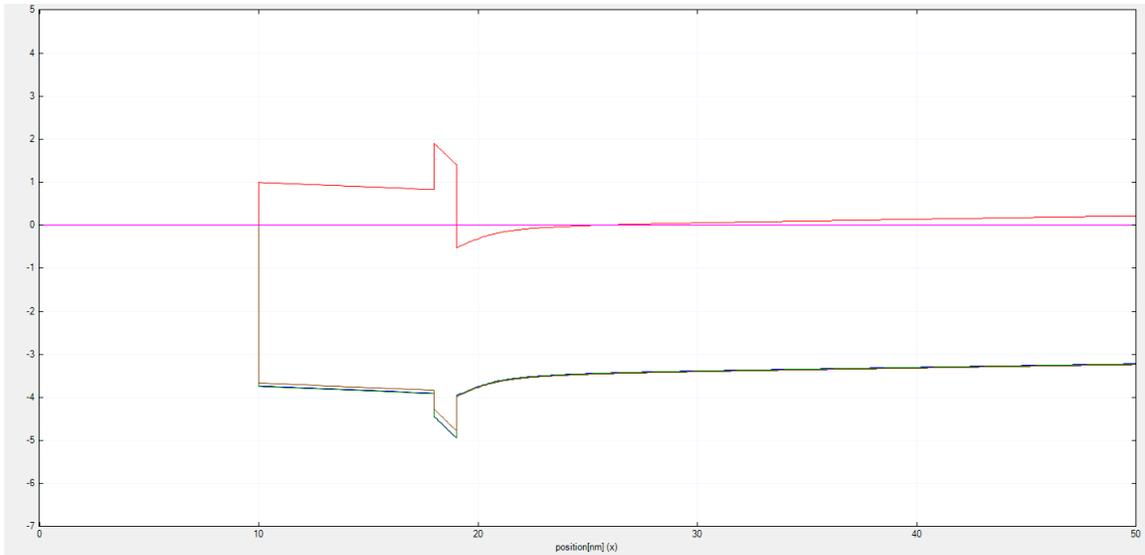


Figure 3: Energy Band Diagram of GaN HEMT Generated by Nextnano. Gate Bias is at 0 V

Plugging these values into the equations above, we get that to align AlN, the A value is 0.7, and to align AlGaN it is about 0.94. That means that 70% and 94%, respectively, of the band discontinuity will be on the conduction side. We can see that this looks about right as the valence band discontinuity (ΔE_v) accounts for a third of the discontinuity between the GaN and AlN regions and nearly none between the GaN and the AlGaN regions.

To set the metal work function (W_M), simply add 1 eV to the χ that will result onto the AlGaN region. If, for example, χ is 1.5 eV, W_M will be 2.5 eV. Thus, include this statement in the simulation file:

```
contact name=gate workfunction=2.5
```

The results of this process can be found in Appendix A.1, Figure 11. Note that some parameters are not adjusted (such as the lattice constants of GaN and AlN) since there are some parameters that are identical between programs. Also, the SiC parameters are lacking as Nextnano does not provide as in-depth parameters at output for that material.

2.2 Structure Specifications

The structure has two components in both Nextnano and Atlas and is thus one of the more straight-forward portions of the project. Both have a mesh and a definition of regions. The main difference is in the fact that our Nextnano simulation is monodimensional- from gate to substrate- whereas in Atlas we also need the drain and source contacts, so a bidimensional structure is necessary.

The mesh is simply the resolution of the structure to be calculated. Both are split into comparable units of spacing (Atlas) and nodes (Nextnano), where each refers to the distance between each meshline. Because our region of interest is in the GaN region, we set the mesh along that region to have a high resolution; everywhere else can have a relatively low resolution. For example, to set a mesh of 100 nm wide and 50 nm deep with a resolution of 100x50, one may write:

```
x.mesh loc=0.000 spac=0.001  
  
x.mesh loc=0.100 spac=0.001  
  
y.mesh loc=0.000 spac=0.001  
  
y.mesh loc=0.050 spac=0.001
```

It is important to note that whereas Nextnano's nodes are a fixed distance apart within a certain region, if two neighboring meshes have different spacing in Atlas then there will be a gradient towards the next mesh region. For example, if one writes the same example as above, but changes the y mesh spacing as so:

```
y.mesh loc=0.000 spac=0.001  
  
y.mesh loc=0.050 spac=0.005
```

Then the mesh of the structure will seem as it does in Figure 4:

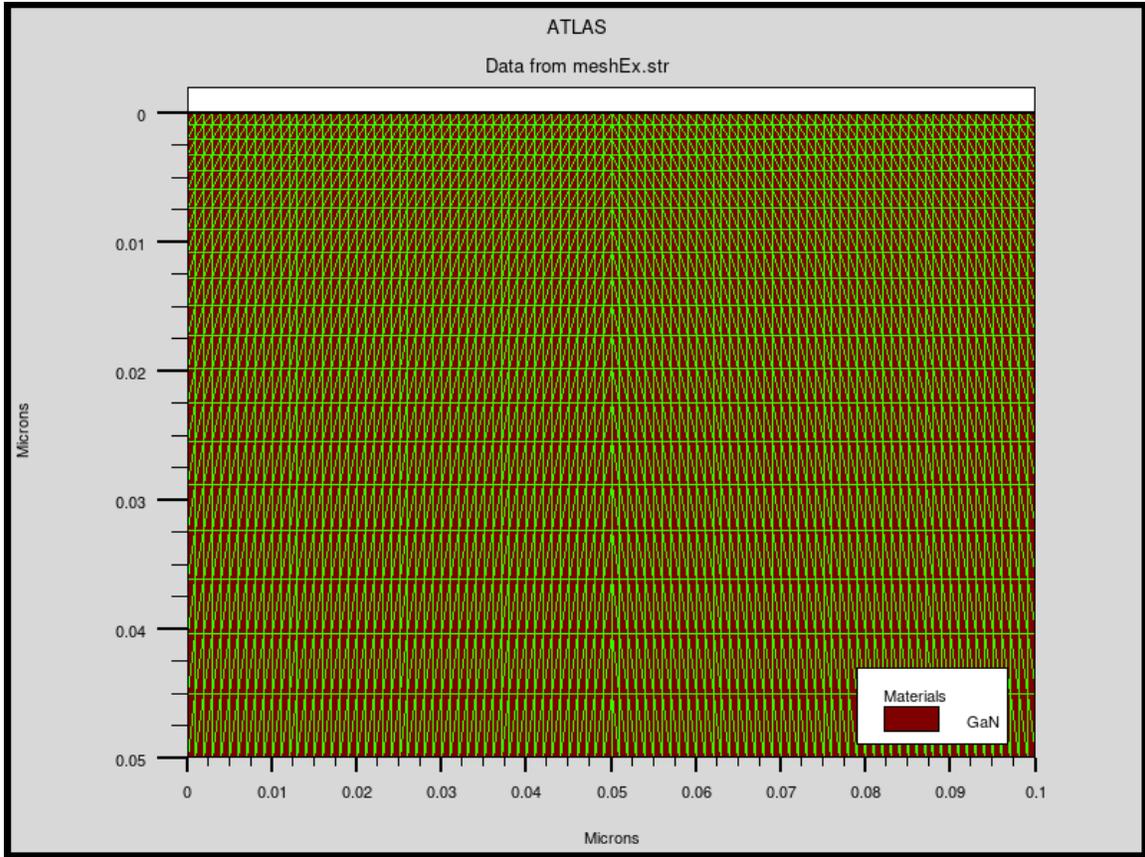


Figure 4: Variable Mesh of a Monolithic Structure

As per the region definitions, those essentially specify what material goes where. Usually, one matches the mesh boundaries with the various regions. Additionally on Atlas, one can set where electrodes and contacts are and their characteristics- though those fall under their own statements of "ELEC" and "CONTACT", the latter of which is seen in the previous section. For brevity, refer to Appendix A.2, Figures 12 and 13 for detailed definitions of both the meshes and regions for both programs. Figure 5 shows the final structure designed in Atlas. Note that the AlN layer above the GaN layer is not visible as it is just 1 nm deep, whereas the rest of the structure is 1 micron deep.

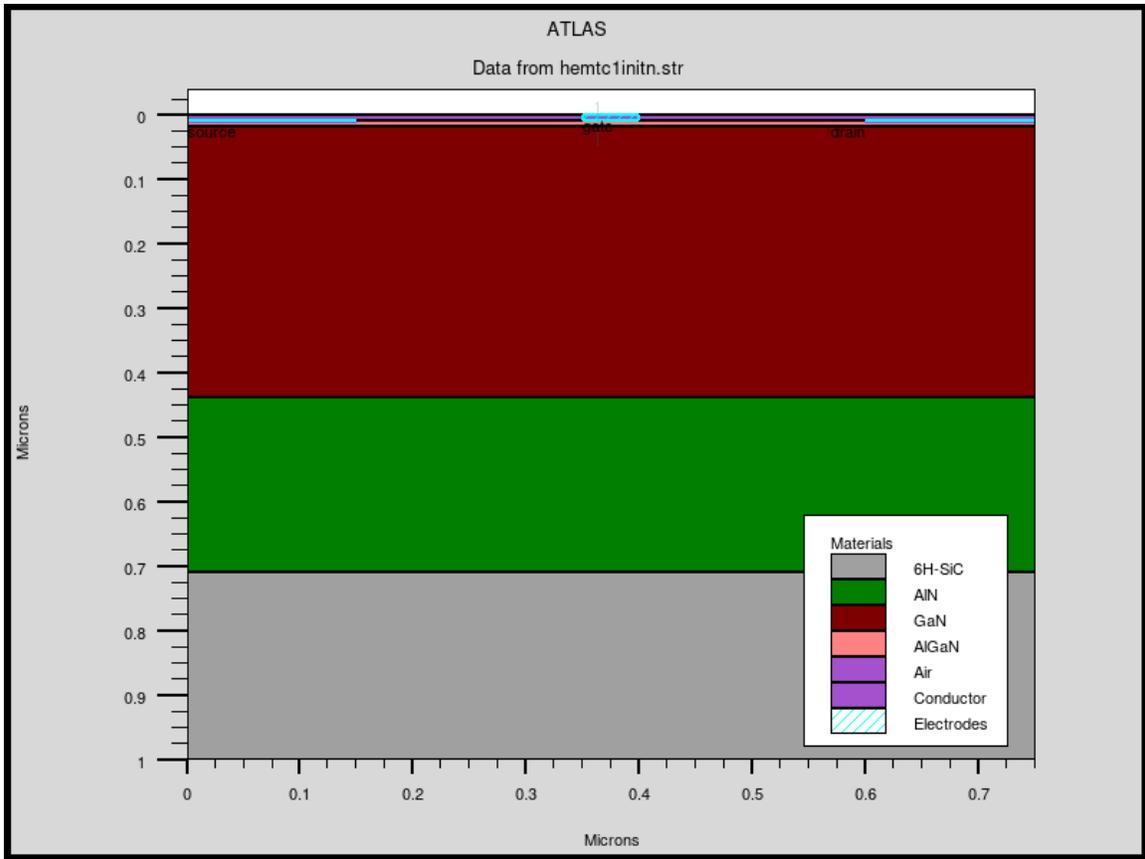


Figure 5: GaN HEMT Structure

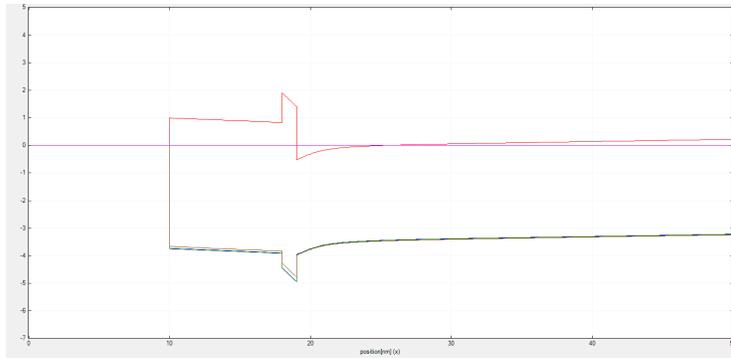
The placement and size of the electrodes is a topic which requires some amount of personal judgment, as the Nextnano simulator does not include them in its definitions, and the physical structures are not clearly defined. For the gate electrode, the conclusion is to overlay it onto the metal layer. As per the drain and source electrodes, there are a few choices. One could simply place them above the metal layer, however some HEMT schematics show the electrodes in the structure. For the latter option, one must make sure that the electrodes reach a depth well below the quantum well region. [3] Conventional MOSFET design has the general rule-of-thumb of having the junctions reach 30% of the

channel layer's depth [4]. As seen in Figure 5, the first option was chosen- as some unpublished literature on this specific transistor showed this to be the case [5].

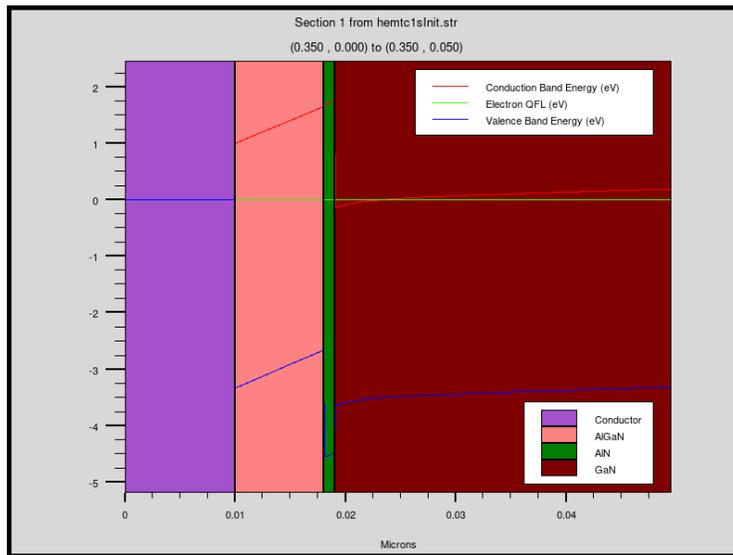
2.3 Verification Methodology

To verify the translation from Nextnano to Atlas, we can find many answers in if the energy band diagrams match. To generate an energy band diagram in Atlas, one simply needs to open the solved structure in Silvaco's plotting program Tonyplot, make a cutline through the region of interest, and select the desired band parameters. In the following figures, the cutline will be made through the center of the structure along the x axis and 50 nm deep.

As an example, Figure 6 shows the energy band diagrams generated by Nextnano and Atlas at 0 V gate bias. These band diagrams have a slight difference in how much the GaN region bends down, limiting the amount of 2DEG. Additionally, the AlN and AlGaIn regions do not have the appropriate shape.



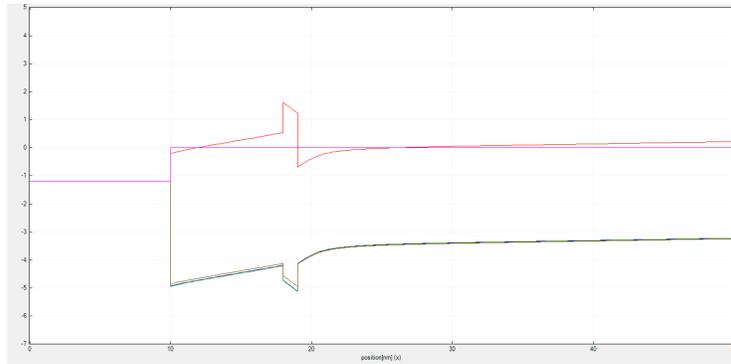
a.



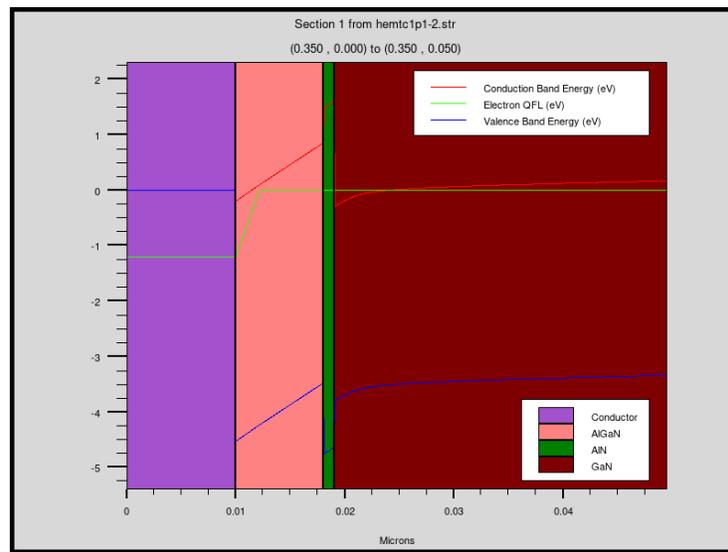
b.

Figure 6: Comparison of Nextnano (a.) and Atlas (b.) Devices at 0 V Gate Bias

Similarly, at 1.2 V gate bias per Figure 7, the energy band diagrams have some similarity in the GaN region, and the AlGaN region seems to behave better, however they differ significantly in the AlN layer.



a.



b.

Figure 7: Comparison of Nextnano (a.) and Atlas (b.) Devices at 1.2 V Gate Bias

Note that these Atlas results are of a recent, but not current, version of the code. The most up-to-date code, as seen in the Appendices, produces results that improve some aspects of the energy band diagrams in terms of objective accuracy. However, these energy band diagrams were more functionally accurate, hence their usage for this point.

3. Simulation

There are two simulation types done in this project: DC solutions for the energy band diagrams shown in the previous section, and AC analysis for the S-parameters this project aims to extract. The physics/simulation models used are the Schrodinger-Poisson models of Atlas (which match those of Nextnano). One of the parameters needed are the amount of eigenvalues, which essentially controls the precision of the simulation. Another is the type of carriers. In this case both electrons and holes are suitable for the model. [2] Hole and valence band calculations are not quite so important in the scope of this research, however they also do not pose any problems to be present. [3]

The simplest way to simulate and store DC simulations is to write the following statements:

```
solve vgate=1.2  
  
save outf=example.str
```

In this case, the gate will receive a bias voltage of 1.2 V and any other electrodes will remain at 0 V. If the next statement specifies a different electrode's bias, the gate bias will remain at 1.2 V for that measurement.

For AC analysis, a similar method can be used. However, to simulate at more than just one frequency a combination of log and set files are used. Log files catalog the simulations that occur since their declaration and set files specify the graphing of the results. As an example, the AC analysis has the following code written:

```

log outf=example.log master gains s.params inport=gate outport=drain width=50

solve ac freq=1e9 fstep=1e9 nstep=10

solve ac freq=2e10 fstep=1e10 nstep=5

tonyplot example.log -set example1.set

```

The S11, S22, S12, and S21 results of this simulation are as in Figure 8. Besides the inaccuracies of the structure, the output is still about what one could expect from these devices. [6] Though DC bias should have some effect on these characteristics, no real change in the output was realized by any sensible bias point. Hence, these simulations were run at 0 V bias at all ports.

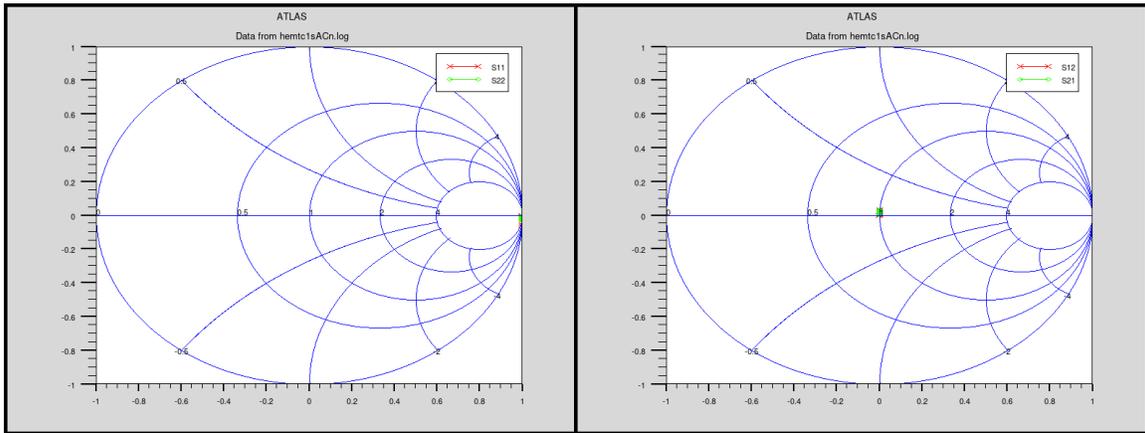


Figure 8: S-parameter Simulation Output

4. Present Issues

Suitable matching between the Atlas and Nextnano structures has not been realized. Explicit definitions assist in allowing for the band structures to have a decent relative behavior, however at the same bias the entire structures are considerably offset.

The most accurate structure, definition-wise, does not exhibit anywhere near the appropriate energy band diagram characteristics, and the most accurate structure energy band diagram-wise does not exhibit appropriate RF characteristics. The reason for all of these mismatches has not been found, and one could suppose it may be some minor detail in the depths of the Atlas simulator. This is the conclusion as all possibilities in adjusting material parameters and simulation methods and models have been exhausted. Some tactics attempted have been to use entirely default parameters, omit the AlN barrier layer, simply modify Atlas example files, and try radically different structural architectures, all to no avail.

5. Conclusion

The usage of various simulators is important to view certain devices from multiple angles, especially as different tools specialize in different aspects of the same subject. Importantly, they not only provide different data, but they can even present the same data in different ways, allowing for new and helpful relationships to be concluded. Therefore, deeper understanding of multiple software suites is paramount to simulating devices effectively.

Appendix A

A.1 Material Parameters

Table A: Electronic Band-Structure and Polarization Parameters for InN, GaN and AlN [2]

Parameter	Symbol	Syntax	Units	InN	GaN	AlN
Electron eff. mass (z)	m_{cz}	MZZ	m_0	0.11	0.20	0.33
Electron eff. mass (t)	m_{ct}	MTT	m_0	0.11	0.18	0.25
Hole eff. mass param.	A1	A1		-9.24	-7.24	-3.95
Hole eff. mass param.	A2	A2		-0.6	-0.51	-0.27
Hole eff. mass param.	A3	A3		8.68	6.73	3.68
Hole eff. mass param.	A4	A4		-4.34	-3.36	-1.84
Hole eff. mass param.	A5	A5		-4.32	-3.35	-1.92
Hole eff. mass param.	A6	A6		-6.08	-4.72	-2.91
Valence band reference	Ev0		eV	-1.59	-2.64	-3.44
Direct band gap (300K)	Eg(300)		eV	1.89	3.42	6.28
Spin-orbit split energy	D1	DELTA1	eV	0.041	0.019	-0.164

Crystal-field split energy	D2	DELTA2	eV	0.0013	0.01413	0.01913
Lattice constant	a ₀	ALATTICE	Å	3.548	3.189	3.112
Elastic constant	C33	C33	GPa	200	392	382
Elastic constant	C13	C13	GPa	94	100	127
Hydrostatic deformation potential	ac	AC	eV	-4.08	-4.08	-4.08
Shear deform. potential	D1	D1	eV	-0.89	-0.89	-0.89
Shear deform. potential	D2	D2	eV	4.27	4.27	4.27
Shear deform. potential	D3	D3	eV	5.18	5.18	5.18
Shear deform. potential	D4	D4	eV	-2.59	-2.59	-2.59
Spontaneous polarization	P _{sp}	PSP	C/m ²	-0.04	-0.03	-0.09
Piezoelectric const. (z)	e ₃₃	E33	C/m ²	0.81	0.67	1.5
Piezoelectric const. (x,y)	e ₃₁	E31	C/m ²	-0.41	-0.34	-0.53

```

335 | Here we are overwriting the database entries for GaN.
336 | -----
337 |
338 | binary-wz-default
339 | binary-type
340 | conduction-band-masses
341 |
342 | = GaN-wz-default
343 | = 0.202d0 0.202d0 0.206d0 0.206d0
344 | = 1.430d0 0.330d0 0.330d0 0.330d0
345 | = 2.170d0 0.280d0 0.280d0 0.280d0
346 | = 1.45d0 1.45d0 1.45d0 1.45d0
347 | = 1.14d0 1.14d0 1.14d0 0.150d0
348 |
349 | band-gaps
350 | = 3.516d0 7d0 7d0
351 | = 2.7557d0 6.150d0 6.450d0
352 |
353 | varshni-parameters
354 | = 0.395d-3 0.00d0 0.00d0
355 | = 830d0 0.00d0 0.00d0
356 |
357 | static-dielectric-constants
358 | = 9.268d0 9.268d0 10.10d0 10.10d0
359 | = 8d0 8d0 8d0 8d0
360 |
361 | lattice-constants
362 | = 390d0 145d0 106d0 106d0
363 |
364 | piezo-electric-constants
365 | = 427d0 0.35d0 0.35d0 0.35d0
366 | = 6d0 6d0 6d0 6d0
367 |
368 | pyro-polarization
369 | = -6.8d0 -6.8d0 -8.6d0 -8.6d0
370 |
371 | absolute-deformation-potentials-cbs
372 | = -3.7d0 4.5d0 8.2d0
373 |
374 | uniax-vb-deformation-potentials
375 | = -7.2d0 0.6d0 -5.5d0 6.6d0
376 |
377 | 6x6kp-parameters
378 | = -3.46d0 -3.46d0 -4.8d0
379 | = 0.01d0 0.06567d0 0.0557d0
380 |
381 | Bend_JBinary-wz-default
382 |
383 | -----
384 | Here we are overwriting the database entries for AlN.
385 | -----
386 |
387 | binary-wz-default
388 | binary-type
389 | conduction-band-masses
390 |
391 | = AlN-wz-default
392 | = 3 5
393 | = 0.30d0 0.30d0 0.32d0 0.32d0
394 | = 0.22d0 0.22d0 0.23d0 0.23d0
395 | = 10.24d0 10.24d0 3.53d0 3.53d0
396 | = 0.24d0 0.24d0 3.53d0 3.53d0
397 | = 3.81d0 3.81d0 0.25d0 0.25d0
398 |
399 | valence-band-masses
400 | = 6.95d0 10d0 10d0
401 | = 4.72454583d0 5.710d0 5.41d0
402 | = -1.526d0
403 |
404 | band-gaps
405 | = 6.95d0 10d0 10d0
406 | = 4.72454583d0 5.710d0 5.41d0
407 | = -1.526d0
408 |
409 | conduction-band-energies
410 | = 6.95d0 10d0 10d0
411 | = 4.72454583d0 5.710d0 5.41d0
412 | = -1.526d0
413 |
414 | valence-band-energies
415 | = 6.95d0 10d0 10d0
416 | = 4.72454583d0 5.710d0 5.41d0
417 | = -1.526d0
418 |
419 | -----
420 | Notes: We use GaN Varshni parameters also for AlN.
421 | Then the conduction band edges of nextnano3 and nextnano++ coincide and
422 | therefore it is easier to compare the results of nextnano3 and nextnano++ with each other.
423 | The problem currently is that
424 | - nextnano++ interpolates both the Varshni parameters and the band gaps.
425 | - nextnano3 interpolates only the Varshni parameters.
426 | - nextnano++ uses different Varshni parameters
427 | have been applied which makes more sense.
428 | -----
429 |
430 | varshni-parameters
431 | = 0.395d-3 0.00d0 0.00d0 0.00d0
432 | = 830d0 0.00d0 0.00d0 0.00d0
433 | = 1.795d-3 0.00d0 0.00d0 0.00d0
434 | = 1462d0 0.00d0 0.00d0 0.00d0
435 |
436 | varshni-parameters
437 | = 1.795d-3 0.00d0 0.00d0 0.00d0
438 | = 1462d0 0.00d0 0.00d0 0.00d0
439 |
440 | lattice-dielectric-constants
441 | = 9.268d0 9.268d0 10.10d0 10.10d0
442 | = 8d0 8d0 8d0 8d0
443 |
444 | lattice-constants
445 | = 390d0 145d0 106d0 106d0
446 |
447 | lattice-constants-temp-coeff
448 | = 427d0 0.35d0 0.35d0 0.35d0
449 | = 6d0 6d0 6d0 6d0
450 |
451 | piezo-electric-constants
452 | = -6.8d0 -6.8d0 -8.6d0 -8.6d0
453 |
454 | pyro-polarization
455 | = -3.7d0 4.5d0 8.2d0
456 |
457 | absolute-deformation-potentials-cbs
458 | = -3.9d0 -3.9d0 -28.5d0
459 |
460 | uniax-vb-deformation-potentials
461 | = -17.1d0 7.3d0 8.8d0
462 |
463 | 6x6kp-parameters
464 | = -3.82d0 -3.82d0 -4.8d0
465 | = -1.32d0 -1.47d0 -1.54d0
466 | = -6.165d0 0.06633d0 0.0663d0
467 |
468 | Bend_JBinary-wz-default
469 |
470 | -----
471 | Here we are overwriting the database entries for GaN.
472 | -----
473 |
474 | binary-wz-default
475 | binary-type
476 | conduction-band-masses
477 |
478 | = GaN-wz-default
479 | = 0.202d0 0.202d0 0.206d0 0.206d0
480 | = 1.430d0 0.330d0 0.330d0 0.330d0
481 | = 2.170d0 0.280d0 0.280d0 0.280d0
482 | = 1.45d0 1.45d0 1.45d0 1.45d0
483 | = 1.14d0 1.14d0 1.14d0 0.150d0
484 |
485 | band-gaps
486 | = 3.516d0 7d0 7d0
487 | = 2.7557d0 6.150d0 6.450d0
488 |
489 | varshni-parameters
490 | = 0.395d-3 0.00d0 0.00d0
491 | = 830d0 0.00d0 0.00d0
492 |
493 | static-dielectric-constants
494 | = 9.268d0 9.268d0 10.10d0 10.10d0
495 | = 8d0 8d0 8d0 8d0
496 |
497 | lattice-constants
498 | = 390d0 145d0 106d0 106d0
499 |
500 | piezo-electric-constants
501 | = 427d0 0.35d0 0.35d0 0.35d0
502 | = 6d0 6d0 6d0 6d0
503 |
504 | pyro-polarization
505 | = -6.8d0 -6.8d0 -8.6d0 -8.6d0
506 |
507 | absolute-deformation-potentials-cbs
508 | = -3.7d0 4.5d0 8.2d0
509 |
510 | uniax-vb-deformation-potentials
511 | = -7.2d0 0.6d0 -5.5d0 6.6d0
512 |
513 | 6x6kp-parameters
514 | = -3.46d0 -3.46d0 -4.8d0
515 | = 0.01d0 0.06567d0 0.0557d0
516 |
517 | Bend_JBinary-wz-default
518 |
519 | -----
520 | Here we are overwriting the database entries for AlN.
521 | -----
522 |
523 | binary-wz-default
524 | binary-type
525 | conduction-band-masses
526 |
527 | = AlN-wz-default
528 | = 3 5
529 | = 0.30d0 0.30d0 0.32d0 0.32d0
530 | = 0.22d0 0.22d0 0.23d0 0.23d0
531 | = 10.24d0 10.24d0 3.53d0 3.53d0
532 | = 0.24d0 0.24d0 3.53d0 3.53d0
533 | = 3.81d0 3.81d0 0.25d0 0.25d0
534 |
535 | valence-band-masses
536 | = 6.95d0 10d0 10d0
537 | = 4.72454583d0 5.710d0 5.41d0
538 | = -1.526d0
539 |
540 | band-gaps
541 | = 6.95d0 10d0 10d0
542 | = 4.72454583d0 5.710d0 5.41d0
543 | = -1.526d0
544 |
545 | conduction-band-energies
546 | = 6.95d0 10d0 10d0
547 | = 4.72454583d0 5.710d0 5.41d0
548 | = -1.526d0
549 |
550 | valence-band-energies
551 | = 6.95d0 10d0 10d0
552 | = 4.72454583d0 5.710d0 5.41d0
553 | = -1.526d0
554 |
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563 | have been applied which makes more sense.
564 | -----
565 |
566 | varshni-parameters
567 | = 0.395d-3 0.00d0 0.00d0 0.00d0
568 | = 830d0 0.00d0 0.00d0 0.00d0
569 | = 1.795d-3 0.00d0 0.00d0 0.00d0
570 | = 1462d0 0.00d0 0.00d0 0.00d0
571 |
572 | varshni-parameters
573 | = 1.795d-3 0.00d0 0.00d0 0.00d0
574 | = 1462d0 0.00d0 0.00d0 0.00d0
575 |
576 | lattice-dielectric-constants
577 | = 9.268d0 9.268d0 10.10d0 10.10d0
578 | = 8d0 8d0 8d0 8d0
579 |
580 | lattice-constants
581 | = 390d0 145d0 106d0 106d0
582 |
583 | lattice-constants-temp-coeff
584 | = 427d0 0.35d0 0.35d0 0.35d0
585 | = 6d0 6d0 6d0 6d0
586 |
587 | piezo-electric-constants
588 | = -6.8d0 -6.8d0 -8.6d0 -8.6d0
589 |
590 | pyro-polarization
591 | = -3.7d0 4.5d0 8.2d0
592 |
593 | absolute-deformation-potentials-cbs
594 | = -3.9d0 -3.9d0 -28.5d0
595 |
596 | uniax-vb-deformation-potentials
597 | = -17.1d0 7.3d0 8.8d0
598 |
599 | 6x6kp-parameters
600 | = -3.82d0 -3.82d0 -4.8d0
601 | = -1.32d0 -1.47d0 -1.54d0
602 | = -6.165d0 0.06633d0 0.0663d0
603 |
604 | Bend_JBinary-wz-default
605 |
606 | -----
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608 | -----
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610 | binary-wz-default
611 | binary-type
612 | conduction-band-masses
613 |
614 | = GaN-wz-default
615 | = 0.202d0 0.202d0 0.206d0 0.206d0
616 | = 1.430d0 0.330d0 0.330d0 0.330d0
617 | = 2.170d0 0.280d0 0.280d0 0.280d0
618 | = 1.45d0 1.45d0 1.45d0 1.45d0
619 | = 1.14d0 1.14d0 1.14d0 0.150d0
620 |
621 | band-gaps
622 | = 3.516d0 7d0 7d0
623 | = 2.7557d0 6.150d0 6.450d0
624 |
625 | varshni-parameters
626 | = 0.395d-3 0.00d0 0.00d0
627 | = 830d0 0.00d0 0.00d0
628 |
629 | static-dielectric-constants
630 | = 9.268d0 9.268d0 10.10d0 10.10d0
631 | = 8d0 8d0 8d0 8d0
632 |
633 | lattice-constants
634 | = 390d0 145d0 106d0 106d0
635 |
636 | piezo-electric-constants
637 | = 427d0 0.35d0 0.35d0 0.35d0
638 | = 6d0 6d0 6d0 6d0
639 |
640 | pyro-polarization
641 | = -6.8d0 -6.8d0 -8.6d0 -8.6d0
642 |
643 | absolute-deformation-potentials-cbs
644 | = -3.7d0 4.5d0 8.2d0
645 |
646 | uniax-vb-deformation-potentials
647 | = -7.2d0 0.6d0 -5.5d0 6.6d0
648 |
649 | 6x6kp-parameters
650 | = -3.46d0 -3.46d0 -4.8d0
651 | = 0.01d0 0.06567d0 0.0557d0
652 |
653 | Bend_JBinary-wz-default
654 |
655 | -----
656 | Here we are overwriting the database entries for AlN.
657 | -----
658 |
659 | binary-wz-default
660 | binary-type
661 | conduction-band-masses
662 |
663 | = AlN-wz-default
664 | = 3 5
665 | = 0.30d0 0.30d0 0.32d0 0.32d0
666 | = 0.22d0 0.22d0 0.23d0 0.23d0
667 | = 10.24d0 10.24d0 3.53d0 3.53d0
668 | = 0.24d0 0.24d0 3.53d0 3.53d0
669 | = 3.81d0 3.81d0 0.25d0 0.25d0
670 |
671 | valence-band-masses
672 | = 6.95d0 10d0 10d0
673 | = 4.72454583d0 5.710d0 5.41d0
674 | = -1.526d0
675 |
676 | band-gaps
677 | = 6.95d0 10d0 10d0
678 | = 4.72454583d0 5.710d0 5.41d0
679 | = -1.526d0
680 |
681 | conduction-band-energies
682 | = 6.95d0 10d0 10d0
683 | = 4.72454583d0 5.710d0 5.41d0
684 | = -1.526d0
685 |
686 | valence-band-energies
687 | = 6.95d0 10d0 10d0
688 | = 4.72454583d0 5.710d0 5.41d0
689 | = -1.526d0
690 |
691 | -----
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700 | -----
701 |
702 | varshni-parameters
703 | = 0.395d-3 0.00d0 0.00d0 0.00d0
704 | = 830d0 0.00d0 0.00d0 0.00d0
705 | = 1.795d-3 0.00d0 0.00d0 0.00d0
706 | = 1462d0 0.00d0 0.00d0 0.00d0
707 |
708 | varshni-parameters
709 | = 1.795d-3 0.00d0 0.00d0 0.00d0
710 | = 1462d0 0.00d0 0.00d0 0.00d0
711 |
712 | lattice-dielectric-constants
713 | = 9.268d0 9.268d0 10.10d0 10.10d0
714 | = 8d0 8d0 8d0 8d0
715 |
716 | lattice-constants
717 | = 390d0 145d0 106d0 106d0
718 |
719 | lattice-constants-temp-coeff
720 | = 427d0 0.35d0 0.35d0 0.35d0
721 | = 6d0 6d0 6d0 6d0
722 |
723 | piezo-electric-constants
724 | = -6.8d0 -6.8d0 -8.6d0 -8.6d0
725 |
726 | pyro-polarization
727 | = -3.7d0 4.5d0 8.2d0
728 |
729 | absolute-deformation-potentials-cbs
730 | = -3.9d0 -3.9d0 -28.5d0
731 |
732 | uniax-vb-deformation-potentials
733 | = -17.1d0 7.3d0 8.8d0
734 |
735 | 6x6kp-parameters
736 | = -3.82d0 -3.82d0 -4.8d0
737 | = -1.32d0 -1.47d0 -1.54d0
738 | = -6.165d0 0.06633d0 0.0663d0
739 |
740 | Bend_JBinary-wz-default
741 |
742 | -----
743 | Here we are overwriting the database entries for GaN.
744 | -----
745 |
746 | binary-wz-default
747 | binary-type
748 | conduction-band-masses
749 |
750 | = GaN-wz-default
751 | = 0.202d0 0.202d0 0.206d0 0.206d0
752 | = 1.430d0 0.330d0 0.330d0 0.330d0
753 | = 2.170d0 0.280d0 0.280d0 0.280d0
754 | = 1.45d0 1.45d0 1.45d0 1.45d0
755 | = 1.14d0 1.14d0 1.14d0 0.150d0
756 |
757 | band-gaps
758 | = 3.516d0 7d0 7d0
759 | = 2.7557d0 6.150d0 6.450d0
760 |
761 | varshni-parameters
762 | = 0.395d-3 0.00d0 0.00d0
763 | = 830d0 0.00d0 0.00d0
764 |
765 | static-dielectric-constants
766 | = 9.268d0 9.268d0 10.10d0 10.10d0
767 | = 8d0 8d0 8d0 8d0
768 |
769 | lattice-constants
770 | = 390d0 145d0 106d0 106d0
771 |
772 | piezo-electric-constants
773 | = 427d0 0.35d0 0.35d0 0.35d0
774 | = 6d0 6d0 6d0 6d0
775 |
776 | pyro-polarization
777 | = -6.8d0 -6.8d0 -8.6d0 -8.6d0
778 |
779 | absolute-deformation-potentials-cbs
780 | = -3.7d0 4.5d0 8.2d0
781 |
782 | uniax-vb-deformation-potentials
783 | = -7.2d0 0.6d0 -5.5d0 6.6d0
784 |
785 | 6x6kp-parameters
786 | = -3.46d0 -3.46d0 -4.8d0
787 | = 0.01d0 0.06567d0 0.0557d0
788 |
789 | Bend_JBinary-wz-default
790 |
791 | -----
792 | Here we are overwriting the database entries for AlN.
793 | -----
794 |
795 | binary-wz-default
796 | binary-type
797 | conduction-band-masses
798 |
799 | = AlN-wz-default
800 | = 3 5
801 | = 0.30d0 0.30d0 0.32d0 0.32d0
802 | = 0.22d0 0.22d0 0.23d0 0.23d0
803 | = 10.24d0 10.24d0 3.53d0 3.53d0
804 | = 0.24d0 0.24d0 3.53d0 3.53d0
805 | = 3.81d0 3.81d0 0.25d0 0.25d0
806 |
807 | valence-band-masses
808 | = 6.95d0 10d0 10d0
809 | = 4.72454583d0 5.710d0 5.41d0
810 | = -1.526d0
811 |
812 | band-gaps
813 | = 6.95d0 10d0 10d0
814 | = 4.72454583d0 5.710d0 5.41d0
815 | = -1.526d0
816 |
817 | conduction-band-energies
818 | = 6.95d0 10d0 10d0
819 | = 4.72454583d0 5.710d0 5.41d0
820 | = -1.526d0
821 |
822 | valence-band-energies
823 | = 6.95d0 10d0 10d0
824 | = 4.72454583d0 5.710d0 5.41d0
825 | = -1.526d0
826 |
827 | -----
828 | Notes: We use GaN Varshni parameters also for AlN.
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836 | -----
837 |
838 | varshni-parameters
839 | = 0.395d-3 0.00d0 0.00d0 0.00d0
840 | = 830d0 0.00d0 0.00d0 0.00d0
841 | = 1.795d-3 0.00d0 0.00d0 0.00d0
842 | = 1462d0 0.00d0 0.00d0 0.00d0
843 |
844 | varshni-parameters
845 | = 1.795d-3 0.00d0 0.00d0 0.00d0
846 | = 1462d0 0.00d0 0.00d0 0.00d0
847 |
848 | lattice-dielectric-constants
849 | = 9.268d0 9.268d0 10.10d0 10.10d0
850 | = 8d0 8d0 8d0 8d0
851 |
852 | lattice-constants
853 | = 390d0 145d0 106d0 106d0
854 |
855 | lattice-constants-temp-coeff
856 | = 427d0 0.35d0 0.35d0 0.35d0
857 | = 6d0 6d0 6d0 6d0
858 |
859 | piezo-electric-constants
860 | = -6.8d0 -6.8d0 -8.6d0 -8.6d0
861 |
862 | pyro-polarization
863 | = -3.7d0 4.5d0 8.2d0
864 |
865 | absolute-deformation-potentials-cbs
866 | = -3.9d0 -3.9d0 -28.5d0
867 |
868 | uniax-vb-deformation-potentials
869 | = -17.1d0 7.3d0 8.8d0
870 |
871 | 6x6kp-parameters
872 | = -3.82d0 -3.82d0 -4.8d0
873 | = -1.32d0 -1.47d0 -1.54d0
874 | = -6.165d0 0.06633d0 0.0663d0
875 |
876 | Bend_JBinary-wz-default
877 |
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879 | Here we are overwriting the database entries for GaN.
880 | -----
881 |
882 | binary-wz-default
883 | binary-type
884 | conduction-band-masses
885 |
886 | = GaN-wz-default
887 | = 0.202d0 0.202d0 0.206d0 0.206d0
888 | = 1.430d0 0.330d0 0.330d0 0.330d0
889 | = 2.170d0 0.280d0 0.280d0 0.280d0
890 | = 1.45d0 1.45d0 1.45d0 1.45d0
891 | = 1.14d0 1.14d0 1.14d0 0.150d0
892 |
893 | band-gaps
894 | = 3.516d0 7d0 7d0
895 | = 2.7557d0 6.150d0 6.450d0
896 |
897 | varshni-parameters
898 | = 0.395d-3 0.00d0 0.00d0
899 | = 830d0 0.00d0 0.00d0
900 |
901 | static-dielectric-constants
902 | = 9.268d0 9.268d0 10.10d0 10.10d0
903 | = 8d0 8d0 8d0 8d0
904 |
905 | lattice-constants
906 | = 390d0 145d0 106d0 106d0
907 |
908 | piezo-electric-constants
909 | = 427d0 0.35d0 0.35d0 0.35d0
910 | = 6d0 6d0 6d0 6d0
911 |
912 | pyro-polarization
913 | = -6.8d0 -6.8d0 -8.6d0 -8.6d0
914 |
915 | absolute-deformation-potentials-cbs
916 | = -3.7d0 4.5d0 8.2d0
917 |
918 | uniax-vb-deformation-potentials
919 | = -7.2d0 0.6d0 -5.5d0 6.6d0
920 |
921 | 6x6kp-parameters
922 | = -3.46d0 -3.46d0 -4.8d0
923 | = 0.01d0 0.06567d0 0.0557d0
924 |
925 | Bend_JBinary-wz-default
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927 | -----
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929 | -----
930 |
931 | binary-wz-default
932 | binary-type
933 | conduction-band-masses
934 |
935 | = AlN-wz-default
936 | = 3 5
937 | = 0.30d0 0.30d0 0.32d0 0.32d0
938 | = 0.22d0 0.22d0 0.23d0 0.23d0
939 | = 10.24d0 10.24d0 3.53d0 3.53d0
940 | = 0.24d0 0.24d0 3.53d0 3.53d0
941 | = 3.81d0 3.81d0 0.25d0 0.25d0
942 |
943 | valence-band-masses
944 | = 6.95d0 10d0 10d0
945 | = 4.72454583d0 5.710d0 5.41d0
946 | = -1.526d0
947 |
948 | band-gaps
949 | = 6.95d0 10d0 10d0
950 | = 4.72454583d0 5.710d0 5.41d0
951 | = -1.526d0
952 |
953 | conduction-band-energies
954 | = 6.95d0 10d0 10d0
955 | = 4.72454583d0 5.710d0 5.41d0
956 | = -1.526d0
957 |
958 | valence-band-energies
959 | = 6.95d0 10d0 10d0
960 | = 4.72454583d0 5.710d0 5.41d0
961 | = -1.526d0
962 |
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973 |
974 | varshni-parameters
975 | = 0.395d-3 0.00d0 0.00d0 0.00d0
976 | = 830d0 0.00d0 0.00d0 0.00d0
977 | = 1.795d-3 0.00d0 0.00d0 0.00d0
978 | = 1462d0 0.00d0 0.00d0 0.00d0
979 |
980 | varshni-parameters
981 | = 1.795d-3 0.00d0 0.00d0 0.00d0
982 | = 1462d0 0.00d0 0.00d0 0.00d0
983 |
984 | lattice-dielectric-constants
985 | = 9.268d0 9.268d0 10.10d0 10.10d0
986 | = 8d0 8d0 8d0 8d0
987 |
988 | lattice-constants
989 | = 390d0 145d0 106d0 106d0
990 |
991 | lattice-constants-temp-coeff
992 | = 427d0 0.35d0 0.35d0 0.35d0
993 | = 6d0 6d0 6d0 6d0
994 |
995 | piezo-electric-constants
996 | = -6.8d0 -6.8d0 -8.6d0 -8.6d0
997 |
998 | pyro-polarization
999 | = -3.7d0 4.5d0 8.2d0
1000 |
1001 | absolute-deformation-potentials-cbs
1002 | = -3.9d0 -3.9d0 -28.5d0
1003 |
1004 | uniax-vb-deformation-potentials
1005 | = -17.1d0 7.3d0 8.8d0
1006 |
1007 | 6x6kp-parameters
1008 | = -3.82d0 -3.82d0 -4.8d0
1009 | = -1.32d0 -1.47d0 -1.54d0
1010 | = -6.165d0 0.06633d0 0.0663d0
1011 |
1012 | Bend_JBinary-wz-default
1013 |
1014 | -----
1015 | Here we are overwriting the database entries for GaN.
1016 | -----
1017 |
1018 | binary-wz-default
1019 | binary-type
1020 | conduction-band-masses
1021 |
1022 | = GaN-wz-default
1023 | = 0.202d0 0.202d0 0.206d0 0.206d0
1024 | = 1.430d0 0.330d0 0.330d0 0.330d0
1025 | = 2.170d0 0.280d0 0.280d0 0.280d0
1026 | = 1.45d0 1.45d0 1.45d0 1.45d0
1027 | = 1.14d0 1.14d0 1.14d0 0.150d0
1028 |
1029 | band-gaps
1030 | = 3.516d0 7d0 7d0
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1033 | varshni-parameters
1034 | = 0.395d-3 0.00d0 0.00d0
1035 | = 830d0 0.00d0 0.00d0
1036 |
1037 | static-dielectric-constants
1038 | = 9.268d0 9.268d0 10.10d0 10.10d0
1039 | = 8d0 8d0 8d0 8d0
1040 |
1041 | lattice-constants
1042 | = 390d0 145d0 106d0 106d0
1043 |
1044 | piezo-electric-constants
1045 | = 427d0 0.35d0 0.35d0 0.35d0
1046 | = 6d0 6d0 6d0 6d0
1047 |
1048 | pyro-polarization
1049 | = -6.8d0 -6.8d0 -8.6d0 -8.6d0
1050 |
1051 | absolute-deformation-potentials-cbs
1052 | = -3.7d0 4.5d0 8.2d0
1053 |
1054 | uniax-vb-deformation-potentials
1055 | = -7.2d0 0.6d0 -5.5d0 6.6d0
1056 |
1057 | 6x6kp-parameters
1058 | = -3.46d0 -3.46d0 -4
```

```

1 binary_wz{
2   name = "Al(x)Ga(1-x)N,x=0.450,1-x=0.550"
3   valence = "(unknown)"
4   lattice_consts{
5     a = 3.15435
6     a_expansion = 0.00000
7     c = 5.09365
8     c_expansion = 0.00000
9   }
10  dielectric_consts{
11    static_a = 9.00550
12    static_c = 9.41150
13    optical_a = 5.01550
14    optical_c = 5.01550
15  }
16  elastic_consts{
17    c11 = 392.700
18    c12 = 141.400
19    c13 = 106.900
20    c33 = 386.750
21    c44 = 109.950
22  }
23  piezoelectric_consts{
24    e31 = -0.417500
25    e33 = 1.50400
26    e15 = -0.381000
27  }
28  pyroelectric_consts{
29    p1 = -0.540025E-01
30  }
31  conduction_bands{
32    Gamma{
33      mass_l = 0.257300
34      mass_t = 0.246100
35      bandgap = 4.66183
36      bandgap_alpha = 0.00000
37      bandgap_beta = 0.00000
38      defpot_absolute_l = -13.9550
39      defpot_absolute_t = -5.49500
40    }
41  }
42  valence_bands{
43    bandoffset = -1.08600
44    defpotentials = [ -9.73000 , 6.03000 , 8.47000 , -4.01000 , -3.73000 , -4.55500 ]
45    delta = [ -0.705500E-01 , 0.596700E-02 , 0.596700E-02 ]
46    HH{
47      mass_l = 2.19350
48      mass_t = 5.56900
49    }
50    LH{
51      mass_l = 2.19350
52      mass_t = 0.190500
53    }
54    SO{
55      mass_l = 0.195000
56      mass_t = 2.31950
57    }
58  }
59  kp_6_bands{
60    A1 = -5.70250
61    A2 = -0.354500
62    A3 = 5.28500
63    A4 = -2.49700
64    A5 = -2.53150
65    A6 = -3.43300
66  }
67  kp_8_bands{
68    S1 = 0.838550
69    S2 = 0.984950
70    E_P1 = 14.2250
71    E_P2 = 14.2250
72    B1 = 0.515350E-01
73    B2 = 0.515350E-01
74    B3 = 0.515350E-01
75    A1 = -2.46455
76    A2 = -0.354500
77    A3 = 2.04705
78    A4 = -0.878300
79    A5 = -0.912800
80    A6 = 1.05065
81  }
82 }
83

```

Figure 10: Nextnano AlGa_N Material Definition

```

# MATERIAL PARAMS
# GaN mod - order based on Atlas manual
MATERIAL MATERIAL=GaN MZZ=0.206 MTT=0.202 A1=-7.21 A2=-0.44 A3=6.68 A4=-3.46 A5=-3.40 A6=-4.90 \
EG300=3.51 DELTA1=0.010 DELTA2=0.00567 C33=398 C13=106 AC=-6.8 \
D1=-3.7 D2=4.5 D3=8.2 D4=-4.1 E33=1.27 E31=-0.034
#MATERIAL MATERIAL=GaN PERMITTIVITY=9.28

# AlN mod - order based on Atlas manual
MATERIAL MATERIAL=AlN MZZ=0.32 MTT=0.30 A1=-3.86 A2=-0.25 A3=3.58 A4=-1.32 A5=-1.47 A6=-1.64 \
EG300=6.25 DELTA1=-0.169 DELTA2=0.00633 C33=373 C13=108 AC=-3.9 \
D1=-17.1 D2=7.9 D3=8.8 D4=-3.9 E33=1.79 E31=-0.50
MATERIAL MATERIAL=AlN ALIGN=0.7024777372
#MATERIAL MATERIAL=AlN PERMITTIVITY=8.67

#SiC mod - Order based on nn++ material params. list
MATERIAL MATERIAL=SiC-6H ALATTICE=4.3596 PERMITTIVITY=9.72 C11=290 C12=235 MC=0.68 \
EG300=6.0
MATERIAL MATERIAL=SiC-6H ALIGN=0.5426787149

# AlGaIn mod - order matches GaN and AlN + explicitly stating certain parameters
MATERIAL MATERIAL=AlGaIn MZZ=0.2573 MTT=0.2461 A1=-5.7025 A2=-0.3545 A3=5.285 A4=-2.497 \
A5=-2.5315 A6=-3.433 DELTA1=-0.07055 DELTA2=-0.005967 C33=386.75 \
C13=106.9 EG300=4.66 AC=-5.495 D1=-9.73 D2=6.03 D3=8.47 D4=-4.01 \
E33=1.504 E31=-0.4175 ALATTICE=3.15435
MATERIAL MATERIAL=AlGaIn ALIGN=0.9350469565
#MATERIAL MATERIAL=AlGaIn PERMITTIVITY=9.0055

```

Figure 11: Material Modifications in Silvaco Atlas

A.2 Structural Specifications

```

215 $regions
216
217 !-----!
218 ! These are the regions of the AlGaIn/GaN region (without surface or GaN cap layer).
219 !-----!
220 region-number = 1 base-geometry = line region-priority = 1
221 x-coordinates = 0d0 10d0
222
223 region-number = 2 base-geometry = line region-priority = 1
224 x-coordinates = 10d0 18d0
225
226 region-number = 3 base-geometry = line region-priority = 1
227 x-coordinates = 18d0 19d0
228
229 region-number = 4 base-geometry = line region-priority = 1
230 x-coordinates = 19d0 439d0
231
232
233 !-----!
234 ! These are the regions left of the AlGaIn/GaN region, i.e. the GaN cap and the surface.
235 !-----!
236 region-number = 5 base-geometry = line region-priority = 1
237 x-coordinates = 439d0 709d0 ! air
238
239 region-number = 6 base-geometry = line region-priority = 1
240 x-coordinates = 709d0 1000d0
241
242 $end_regions
243 !-----!
244
245 !-----!
246 ! For every boundary between regions, there has to exist a grid line. And
247 ! between these grid lines there are a certain number of nodes which
248 ! determine the resolution of the simulated region. In order to specify
249 ! inhomogeneous grids you can use a grid factor different from one. This
250 ! means that the distance between each node is increased by this factor
251 ! from i to i+1.
252 !-----!
253 $grid-specification
254 grid-type = 1 0 0
255 x-grid-lines = 0d0 10d0 18d0 19d0 439d0 709d0 1000d0
256 x-nodes = 5 25 15 1050 50 20 ! originally: [blank] 5 25 15 1050 50 20
257 x-grid-factors = 1d0 1d0 1d0 1d0 1d0 1d0
258 $end_grid-specification
259 !-----!

```

Figure 12: Nextnano Region and Grid Specifications

```
mesh
x.mesh loc=-50   spac=.5
#x.mesh loc=0.15 spac=0.05
#x.mesh loc=0.60 spac=0.05
x.mesh loc=50   spac=.5

y.mesh loc=0.000 spac=0.002
y.mesh loc=0.010 spac=0.002
y.mesh loc=0.018 spac=0.003
y.mesh loc=0.019 spac=0.0001
y.mesh loc=0.439 spac=0.010
y.mesh loc=0.709 spac=0.010
y.mesh loc=1.000 spac=0.010

# STRUCTURE SPEC
region num=1 material=SiC-6H y.min=0.709 y.max=1.000
region num=2 material=AlN    y.min=0.439 y.max=0.709
region num=3 material=GaN    y.min=0.019 y.max=0.439 \
qwll well.nx=10500 well.ny=5
region num=4 material=AlN    y.min=0.018 y.max=0.019
region num=5 material=AlGaN  y.min=0.010 y.max=0.018 x.comp=0.45
region num=6 material=Air    y.min=0.000 y.max=0.010

elec num=1 name=source x.min=-50 x.max=-27.5 y.min=0.000 y.max=0.010
elec num=2 name=gate   x.min=-22.5 x.max=22.5 y.min=0.000 y.max=0.010
elec num=3 name=drain  x.min=27.5 x.max=50 y.min=0.000 y.max=0.010

contact name=gate workfun=4.23
```

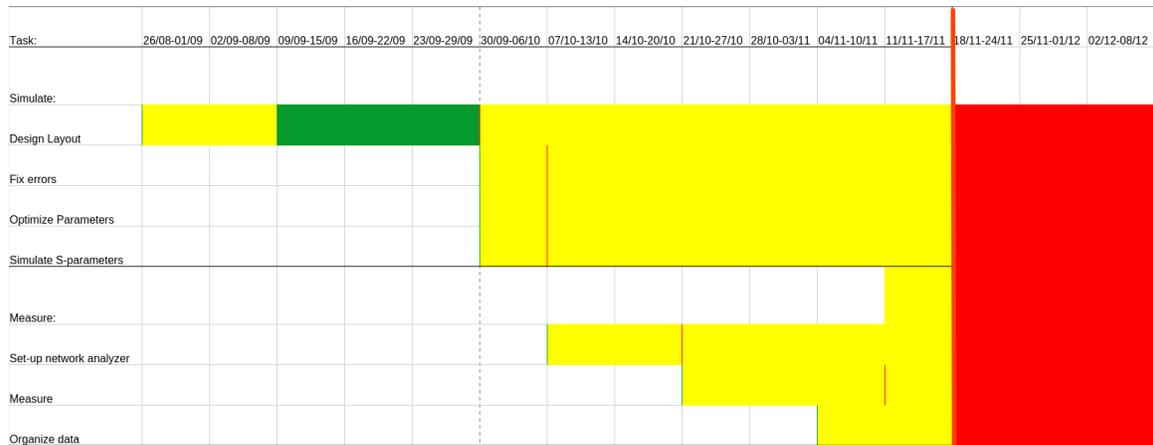
Figure 13: Atlas Region and Mesh Specifications

Appendix B

B.1 Safety, Environmental, and Social Impacts Disclaimer

Due to the nature of this project, especially up to this point, there are no reportable safety, environmental, or social considerations. All of the work until now is done virtually, and any future lab work will be with low-voltage lab equipment on a wafer that is already fabricated.

B.2 Gantt Chart



B.3 Budget Chart

Week	Hours	Cost
26/08-01/09	2	30
02/09-08/09	6	90
09/09-15/09	6	90
16/09-22/09	6	90
23/09-29/09	12	180
30/09-06/10	2	30
07/10-13/10	14	210
14/10-20/10	18	270
21/10-27/10	8	120
28/10-03/11	8	120
04/11-10/11	8	120
11/11-17/11	8	120
18/11-24/11	4	60
Totals:	102	1530

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3. Kim, TW Ph.D. Personal Interviews, September-November 2024.
4. Stephen A. Campbell, Fabrication Engineering at the Micro- and Nanoscale, Oxford University Press, New York, NY, pp. 132, 2013.
5. S. Chakraborty, W. Amir et al. "Addressing Reliability Issues in AlGaIn/GaN HEMTs: State-of-the-Art Developments and Future Prospects". University of Ulsan, *not yet published*.
6. L. Dunleavy, "Model-Based GaN PA Design Basics: GaN Transistor S-Parameters, Linear Stability Analysis and Resistive Stabilization," Qorvo Inc., 28 August 2019.