

Computational Electronics

Introduction to Drift-Diffusion Modeling With PADRE

Prepared by
Dragica Vasileska
Associate Professor
Arizona State University

The need for semiconductor device modeling:

1. Increased costs for R&D and production facilities, which are becoming too large for any one company or country to accept.
2. Shorter process technology life cycles.
3. Emphasis on faster characterization of manufacturing processes, assisted by modeling and simulation.

Computer simulations, often called technology for computer assisted design (TCAD) offer many advantages such as:

1. Evaluating "what-if" scenarios rapidly
2. Providing problem diagnostics
3. Providing full-field, in-depth understanding
4. Providing insight into extremely complex problems/phenomena/product sets
5. Decreasing design cycle time (savings on hardware build lead-time, gain insight for next product/process)
6. Shortening time to market

Some TCAD prerequisites are:

1. Modeling and simulation require enormous technical depth and expertise not only in simulation techniques and tools but also in the fields of physics and chemistry.
2. Laboratory infrastructure and experimental expertise are essential for both model verification and input parameter evaluations in order to have truly effective and predictive simulations.
3. Software and tool vendors need to be closely tied to development activities in the research and development laboratories.

Historical Development of Device Simulations

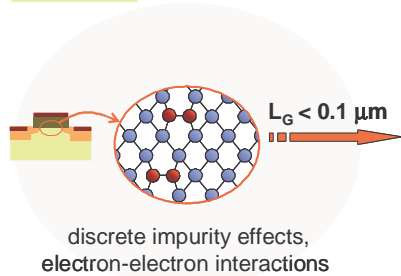
1964: Gummel introduced the decoupled scheme for the solution of the Poisson and the continuity equations for a BJT

1968: de Mari introduced the scaling of variables that is used even today and prevents effectively overflows and underflows

1969: Sharfetter and Gummel, in their seminal paper that describes the simulation of a 1D Silicon Read (IMPATT) diode, introduced the so-called Sharfetter-Gummel discretization of the continuity equation

Existing Device Simulators

2D MOS: MINIMOS, GEMINI, PISCES, CADDET, HFIELDS,
CURRY, PADRE
3D MOS: WATMOS, FIELDAY, MINIMOS3D, PADRE
1D BJT: SEDAN, BIPOLE, LUSTRE
2D BJT: BAMBI, CURRY, PADRE
MESFETs: CUPID

**Drift-Diffusion Model:**

- * Good for devices with $L_G > 0.5 \mu\text{m}$
- * Can't deal with hot carrier effects

Hydrodynamic Model:

- * Hot carrier effects, such as velocity overshoot, included into the model
- * Overestimates the velocity at high fields

Particle-Based Simulation:

- * Accurate up to classical limits
- * Allows proper treatment of the discrete impurity effects and $e-e$ and $e-i$ interactions
- * Time consuming

Padre is a computer program that numerically solves the semiconductor equations (Poisson, Continuity, and/or Energy Balance), thus allowing one to simulate the performance of electronic devices.

nanoHUB.org
online simulations and more

More about Padre

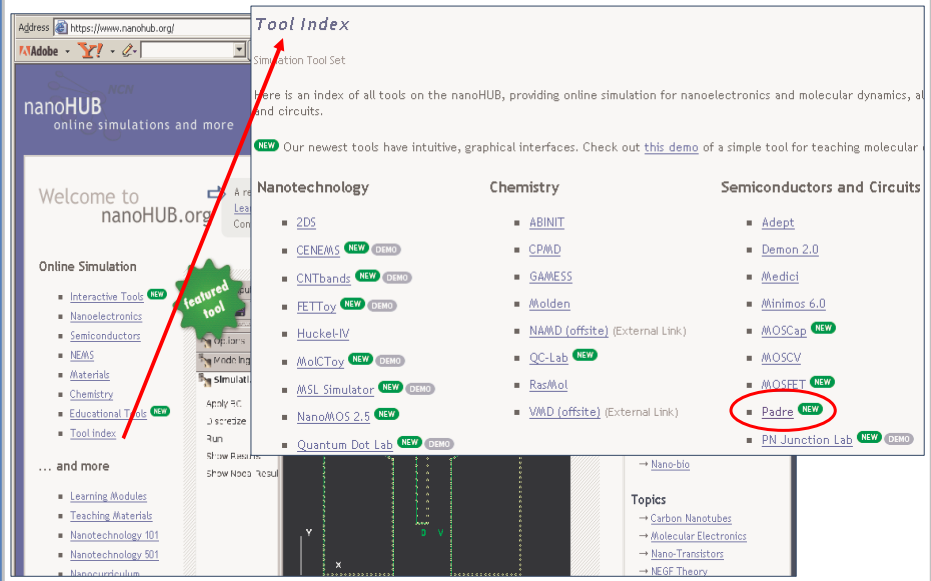
To find out more about Padre....

From www.nanohub.org, select the Padre tool, and then select Padre Tool Information. From there, you can download the complete Padre manual or access an online manual.

Network for Computational Nanotechnology 


nanoHUB.org
online simulations and more

Where Can I Find the Padre Tool?



The screenshot shows the nanoHUB.org website with the following structure:

- Address bar:** <https://www.nanohub.org>
- Page Title:** Tool Index
- Text:** Simulation Tool Set. There is an index of all tools on the nanoHUB, providing online simulation for nanoelectronics and molecular dynamics, and circuits.
- Introductory text:** Our newest tools have intuitive, graphical interfaces. Check out [this demo](#) of a simple tool for teaching molecular...
- Categories:**
 - Nanotechnology:** 2DS, CENEMS (NEW DEMO), CNTbands (NEW DEMO), FETToy (NEW DEMO), HuckeHIV, MolCToy (NEW DEMO), MSL Simulator (NEW DEMO), NanoMOS 2.5 (NEW), Quantum Dot Lab (NEW DEMO)
 - Chemistry:** ABINIT, CPAMD, GAMESS, Molden, NAMD (offsite) (External Link), QC-Lab (NEW), RasMol, VMD (offsite) (External Link)
 - Semiconductors and Circuits:** Adept, Demon 2.0, Medici, Minimos 6.0, MOSCap (NEW), MOSCV, MOSFET (NEW), Padre (NEW), PN Junction Lab (NEW DEMO)
- Left Sidebar:** Welcome to nanoHUB.org, Online Simulation (Interactive Tools, Nanoelectronics, Semiconductors, NEWS, Materials, Chemistry, Educational Tools, Tool Index), and more (Learning Modules, Teaching Materials, Nanotechnology 101, Nanotechnology 501, Nanotechnology).
- Right Sidebar:** Topics (Carbon Nanotubes, Molecular Electronics, Nano-Transistors, NEGF Theory)

Network for Computational Nanotechnology 

Some Hints on the PADRE Syntax

A PADRE command file is a list of commands for PADRE to execute.

This list is stored as an ASCII text file using any text editor.

The input file contains a sequence of statements.

Each statement consists of a keyword that identifies the statement and a set of parameters.

The general format is:

`<STATEMENT> <PARAMETER>=<VALUE>`

The statement keyword must come first, but after this the order of parameters within a statement is not important.

Any line beginning with # is ignored. These lines are used as comments. Note that the "#" can be put on any PADRE input line; all information to the left of the character is processed, and that to the right is ignored.

PADRE can read up to 256 characters on one line. However, it is best to spread long input statements over several lines to make the input file more readable.

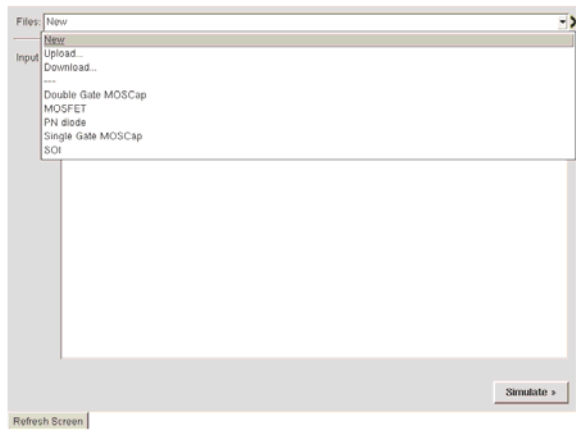
The character + at the beginning of a line indicates continuation.

Some Hints on the PADRE Syntax, Cont'd

Group		Statements
1. Structure Specification	—	MESH REGION ELECTRODE DOPING
2. Material Models Specification	—	MATERIAL MODELS CONTACT INTERFACE
3. Numerical Method Selection	—	METHOD
4. Solution Specification	—	LOG SOLVE LOAD SAVE

Your First PADRE Simulation: A PN Junction Example

When you start a Padre session, a window appears with a pull-down menu on the top right that allows you to upload/download individual source files or use some sample files for typical device structures such as a Double Gate MOS Capacitor, MOSFET,



After we select the PN diode example, a **list of statements** appears in the window as shown below. There is a **strict logic on how these statements have to be ordered**, and this is illustrated in the slides that follow on the example of simulation of pn-diode)

```

Files: PN diode
Input file:
title      pn diode (setup)
options    PO

mesh      rect nx=200 ny=3 width=1 outf=mesh
x.m       n=1  l=0 r=1
x.m       n=100 l=0.5 r=0.8
x.m       n=200 l=1.0 r=1.05
y.m       n=1  l=0 r=1
y.m       n=3  l=1 r=1

$ Regions specifications
region    rnm=1 ix l=1 ix.h=100 iy l=1 iy.h=3 silicon
region    rnm=1 ix l=100 ix.h=200 iy l=1 iy.h=3 silicon
elec      rnm=1 ix l=1 ix.h=1 iy l=1 iy.h=3
elec      rnm=2 ix l=200 ix.h=200 iy l=1 iy.h=3

$ Doping specification
dop       reg=1 p type conc=1e17 x l=0 x.r=0.5 y top=0 y.bot=1 uniform
dop       reg=1 n type conc=1e17 x l=0.5 x.r=1.0 y top=0 y.bot=1 uniform
plot.ld   log dop abs a.x=0 b.x=1.0 b.y=0.5 a.y=0.5 points ascii
*         outf=dop

$ Materials specifications
material  name=silicon tau=0.1e-06 tau=0.1e-06 trap.typ=0 etrap=0

$ Specify models
models   srh conmob fldmob impact temperature=300
system   electrons holes newton
  
```

```

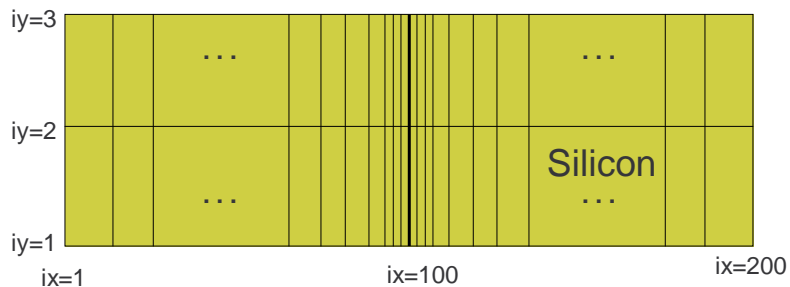
title      pn diode (setup)
options    PO
mesh      rect nx=200 ny=3 width=1 outf=mesh
x.m       n=1  l=0 r=1
x.m       n=100 l=0.5 r=0.8
x.m       n=200 l=1.0 r=1.05
y.m       n=1  l=0 r=1
y.m       n=3  l=1 r=1
  
```

- The **title** statement acts as a comment or reminder line. It is generally useful to include a meaningful title to identify the content of the file.
- The **mesh** statement states that the mesh is tensor product mesh (*rect*) and there are 200 mesh points along the x-axis (left to right) and 3 mesh points along the depth (top to bottom). The name **mesh** will be the output filename (*outf*) which contains the mesh attributes. The mesh length along x-axis and y-axis is 1 μm , as specified in the example.

```
title      pn diode (setup)
options    PO
mesh       rect nx=200 ny=3 width=1 outf=mesh
x.m        n=1   l=0  r=1
x.m        n=100 l=0.5 r=0.8
x.m        n=200 l=1.0 r=1.05
y.m        n=1   l=0  r=1
y.m        n=3   l=1  r=1
```

- The three `x.m` statements specify how we distribute the nodes. The first attribute defines the mesh point `n`, the second one the `location`, and the third one the mesh expansion `ratio`, i.e. the ratio of two neighboring mesh spacing.
- Similarly, the two `y.m` statements specify the mesh spacing in the `y`-direction.

Refer to the Padre manual for a complete discussion of the mesh statement and the other statements to be discussed in this tutorial.

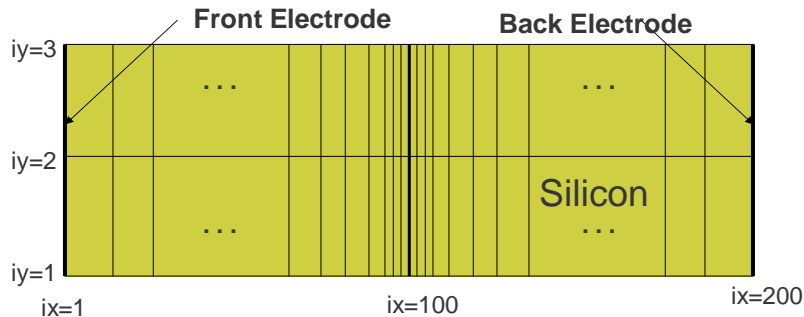


Mesh gets finer
towards the middle
section of the device.

\$ Regions specifications

```
region num=1 ix.l=1 ix.h=100 iy.l=1 iy.h=3 silicon
region num=1 ix.l=100 ix.h=200 iy.l=1 iy.h=3 silicon
elec num=1 ix.l=1 ix.h=1 iy.l=1 iy.h=3
elec num=2 ix.l=200 ix.h=200 iy.l=1 iy.h=3
```

- In this block we define regions. The first **region** statement states that from node `ix.low=1` to `ix.high=100` and `iy.low=1` to `iy.high=3` **silicon** is the material. This region is defined as `region num=1`. Similarly, the second **region** statement states that from node `ix.low=100` to `ix.high=200` and `iy.low=1` to `iy.high=3` **silicon** is the material system. This region is also defined as `region num=1`.
- The **electrode** statement defines the box that the program will treat as an electrode. In this case the box is defined with `ix.low=1`, `ix.high=1`, `iy.low=1` and `iy.high=3`. This is the first electrode, or the front electrode. The second (back) electrode is defined with the statement `ix.low=200`, `ix.high=200`, `iy.low=1` and `iy.high=3`.

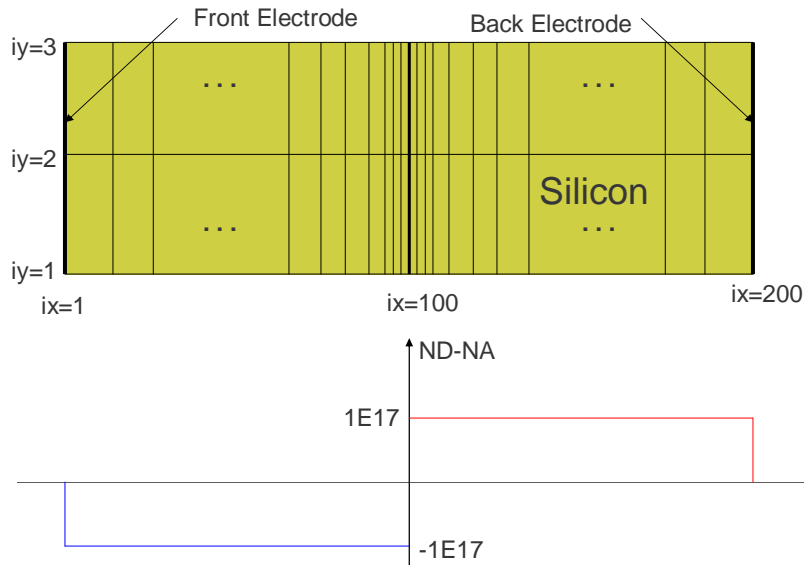


Mesh that gets finer
towards the middle
section of the device.

```
$ Doping specification
dop reg=1 p.type conc=1e+17 x.l=0 x.r=0.5
+      y.top=0 y.bot=1 uniform
dop reg=1 n.type conc=1e+17 x.l=0.5 x.r=1.0 y.top=0
+      y.bot=1 uniform
plot.1d log dop abs a.x=0 b.x=1.0 b.y=0.5 a.y=0.5
+      points ascii outf=dop
```

- The first statement says that in the region `x.left=0`, `x.right=0.5`, `y.top=0` and `y.bot=1` (in μm) we add a **uniform** concentration of acceptors (`p.type`) of $1e17 \text{ cm}^{-3}$.
- The second statement says that in the region `x.left=0.5`, `x.right=1.0`, `y.top=0` and `y.bot=1` (in μm) we add a **uniform** concentration of donors (`n.type`) of $1e17 \text{ cm}^{-3}$.
- The last statement is a `plot` statement along the x-axis and the middle of the y-axis. The output file (`outf`) where doping is stored is called `dop`.

Step 3: Doping Specification



Step 4. Materials Specification

```
& Materials specifications  
material name=silicon taun0=1e-06 taup0=1e-06  
+      trap.typ=0 etrap=0
```

- Within the **material** statement we can specify a variety of material properties such as minority carrier lifetime for electrons (**taun0**=1 us), minority carrier lifetime for holes (**taup0**=1 us), the type of traps (**trap.typ**=0 means no traps), and the energy level of the traps (in this case the energy level is **etrap**=0 eV).

```
$ Specify models
models srh conmob fldmob impact temperature=300
system electrons holes newton
```

- Under the **models** statement we specify that we include **srh** (Shockley-Read-Hall generation-recombination), **conmob** (concentration dependent mobility model), **fldmob** (field-dependent mobility model needed under high bias conditions) and **impact** (impact ionization process), and the **temperature** is 300 K.
- Under the **system** statement we specify that we have both **electrons** and **holes** and that the **newton** method will be used for the solution of the equations.

```
$ Solve for initial conditions
solve init
plot.1d pot a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=pot
plot.1d band.val a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=vband
plot.1d band.con a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=cband
plot.1d qfn a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=qfn
plot.1d qfp a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=qfp
plot.1d ele a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=ele
plot.1d hole a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=hole
plot.1d net.charge a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=ro
plot.1d e.field a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=efield
plot.1d recomb a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=recomb
```

- **solve init** statement specifies that we need to solve for the initial conditions, i.e. without bias applied to the electrodes.

```

$ Solve for initial conditions
solve init
plot.1d pot a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=pot
plot.1d band.val a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=vband
plot.1d band.con a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=cband
plot.1d qfn a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=qfn
plot.1d qfp a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=qfp
plot.1d ele a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=ele
plot.1d hole a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=hole
plot.1d net.charge a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=ro
plot.1d e.field a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=efield
plot.1d recomb a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=recomb

```

- The 10 plot statements save the data for 1D plots along the middle of the device in corresponding files. The variables that get plotted are **pot** (for potential), **vband** (valence band), **cband** (conduction band), **qfn** (quasi-Fermi level for electrons), **qfp** (quasi-Fermi level for holes), **ele** (electron density), **hole** (hole density), **ro** (total charge density), **efield** (the electric field) and **recomb** (net recombination rate).

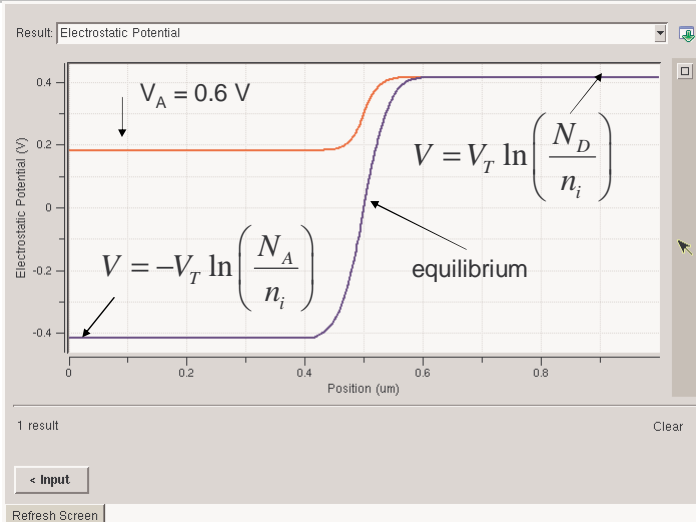
```

$ Solve for applied bias
log outf=iv
solve prev
solve proj vstep=0.03 nsteps=20 elect=1
plot.1d pot a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=potiv
plot.1d band.val a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=vbiv
plot.1d band.con a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=cbiv
plot.1d qfn a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=qfniv
plot.1d qfp a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=qfpiv
plot.1d ele a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=eleiv
plot.1d hole a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=holeiv
plot.1d net.charge a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii
+   outf=roiv
plot.1d e.field a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii
+   outf=efieldiv
plot.1d recomb a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=reiv
plot.1d j.electr a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii
+   outf=jelectr
plot.1d j.hole a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=jhole
plot.1d j.total a.x=0 b.x=1.0 a.y=0.5 b.y=0.5 ascii outf=jtot
end

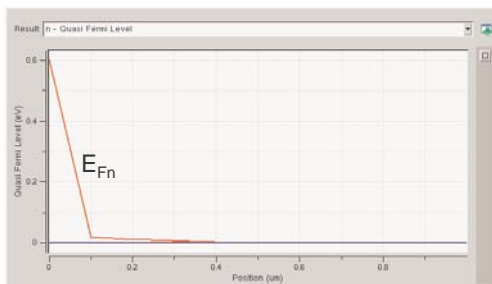
```

- `log outf` states that a file called `iv` will be open for storing the IV-data.
- `solve prev` resolves for previous bias conditions.
- `solve proj` specifies that if necessary it will use the projection method to converge. Also specified here is that the voltage step (`vstep`) is 0.03V, the number of steps (`nsteps`) is 1, and the voltage is applied to the `electrode num=1` which is the anode.
- The meaning of the plot statements is the same as in Step 6. The specified variables are plotted at the final bias point which in our case is $0.03 \times 20 = 0.6$ V. Additional variables that are plotted are the net electron and hole current densities (`jelectr` and `jhole`) and the total current density along the device (`jtot`) which must be constant to ensure conservation of particles in the device.

In the next few slides we will show some sample simulation results for both EQUILIBRIUM and NONEQUILIBRIUM conditions that will provide us with a better understanding of the PN-diode operation.



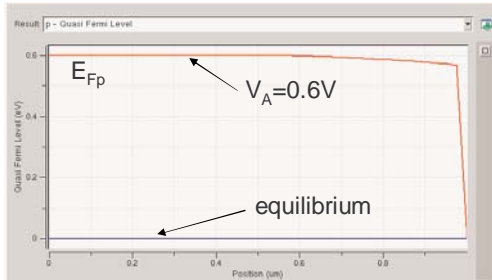
The electrostatic potential in equilibrium gives the position of the Fermi level with respect to the intrinsic level.

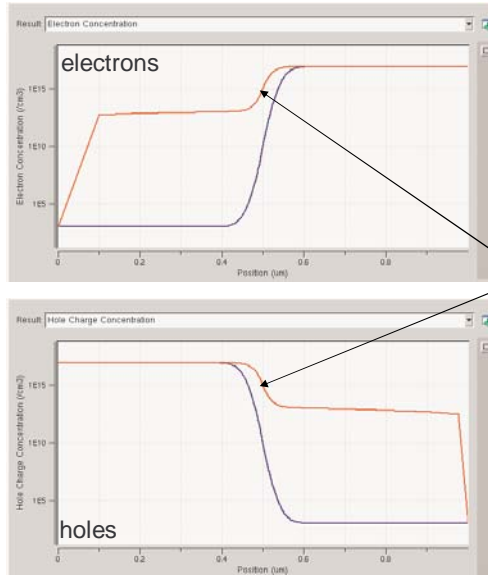


In equilibrium, the Fermi level is constant and represents a reference level.

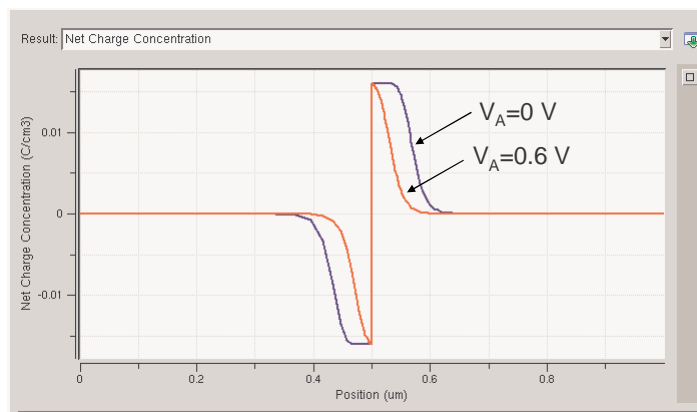
Under applied bias, throughout the most of the device, except the contacts (where the quasi-Fermi levels merge), we have

$$E_{Fp} - E_{Fn} \approx qV_A$$

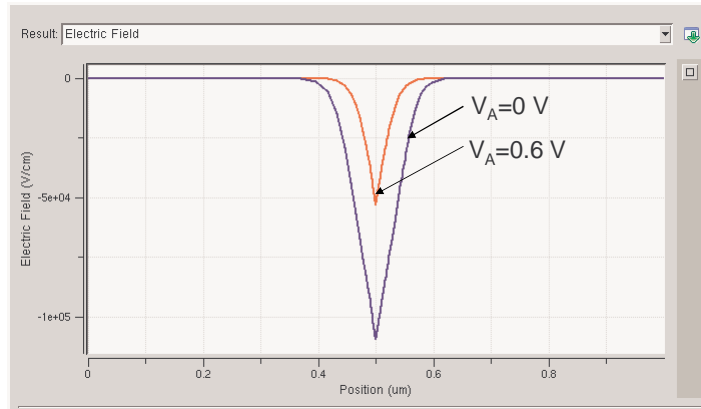




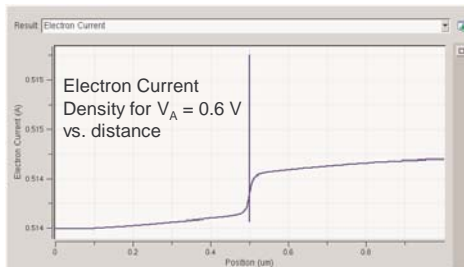
Increase of both electron and hole concentration under forward bias.



The boundaries of the depletion region are marked by the presence of a finite charge in that segment of the device. In the example above, we clearly see that the width of the depletion region shrinks under forward bias conditions, As it is predicted theoretically with the depletion charge approximation.



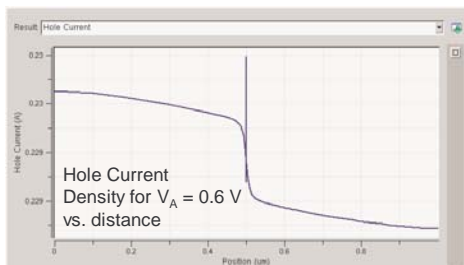
A finite net charge at some point in the device implies a finite electric field. Therefore, a finite electric field also means presence of a depletion region. Again we see that under forward bias the width of the depletion region decreases.



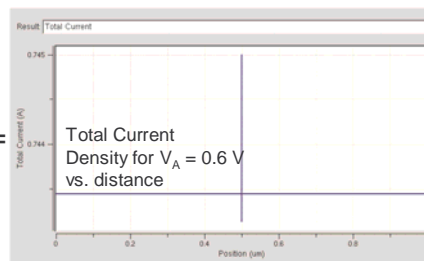
Electron current density + Hole current density = Total current density

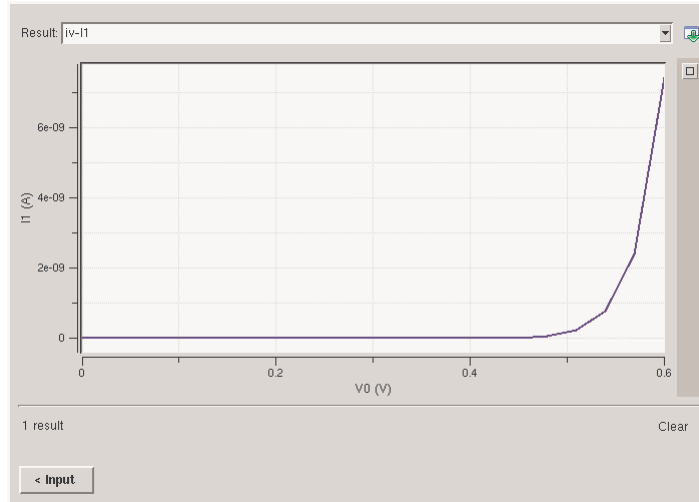
A constant total current density is a signature that we have conservation of particles in the system. (i.e. negligible recombination)

+



=





From the Padre tool input select window, select a few example input files. Work through each one line by line with the Padre manual to understand how to set up various kinds of Padre simulations.

Your Second PADRE Simulation:

MOS Capacitor

```
$ Mesh Specification
mesh      rect nx=3 ny=60
y.m       n=1  l=0 r=1
y.m       n=10 l=0.001 r=0.8
y.m       n=60 l=0.1 r=1.05
x.m       n=1  l=0 r=1
x.m       n=3  l=1 r=1

$ Regions specification
region   num=1 ix.l=1 ix.h=3 iy.l=1 iy.h=10
+ name=siO2 INS
region   num=2 ix.l=1 ix.h=3 iy.l=10 iy.h=60
+ name=silicon SEMI
$ Electrodes specification
elec     num=1 ix.l=1 ix.h=3 iy.l=1 iy.h=1
elec     num=2 ix.l=1 ix.h=3 iy.l=60 iy.h=60
$ Doping specification
dop reg=2 p.type conc=1e18 uniform
```

```
$ Contact specification
contact all neutral
contact num=1 aluminum
$ one can add as options: n.polysilicon, p.polysilicon,
$ tungsten
$ Specify models
models srh conmob fldmob
system electrons holes newton
$ Solve for initial conditions
solve init
plot.ld pot a.y=0 b.y=0.1 a.x=0.5 b.x=0.5 ascii
+ outf=pot.plot
plot.ld ele a.y=0 b.y=0.1 a.x=0.5 b.x=0.5 ascii
+ outf=ele.plot
plot.ld net.charge a.y=0 b.y=0.1 a.x=0.5 b.x=0.5 ascii
+ outf=ro.plot
plot.ld e.field a.y=0 b.y=0.1 a.x=0.5 b.x=0.5 ascii
+ outf=efield.plot
```

```
$ Solve for applied bias
solve prev
solve proj vstep=0.2 nsteps=10 elect=1
plot.ld pot a.y=0 b.y=0.1 a.x=0.5 b.x=0.5 ascii
+ outf=potne.plot
plot.ld ele a.y=0 b.y=0.1 a.x=0.5 b.x=0.5 ascii
+ outf=elene.plot
plot.ld net.charge a.y=0 b.y=0.1 a.x=0.5 b.x=0.5 ascii
+ outf=rone.plot
plot.ld e.field a.y=0 b.y=0.1 a.x=0.5 b.x=0.5 ascii
+ outf=efieldne.plot
end
```

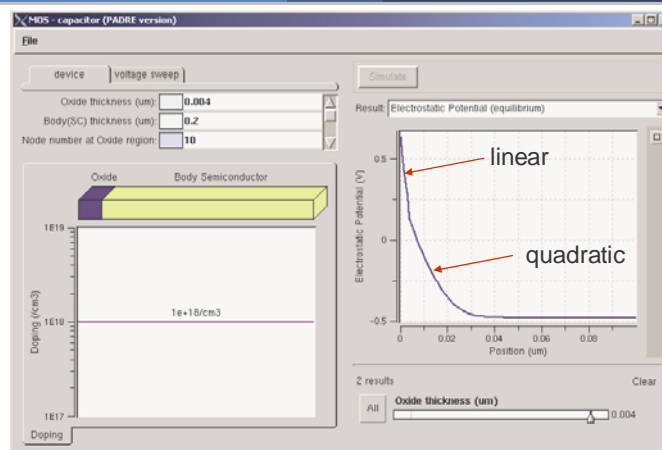
Consider a simple MOS capacitor. The gate is made of aluminum, the thickness of the SiO_2 layer is $t_{\text{ox}}=4$ nm and the doping of the p-type substrate is $N_A=10^{18} \text{ cm}^{-3}$. For this device structure plot:

At equilibrium

- the electrostatic potential,
- the total charge density,
- the electric field profile.

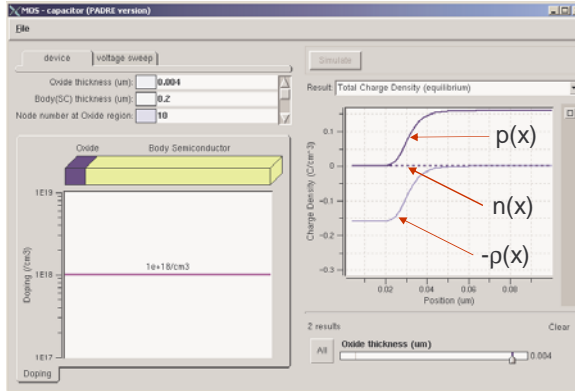
Under applied gate bias of 2V

- the inversion electron density vs. position



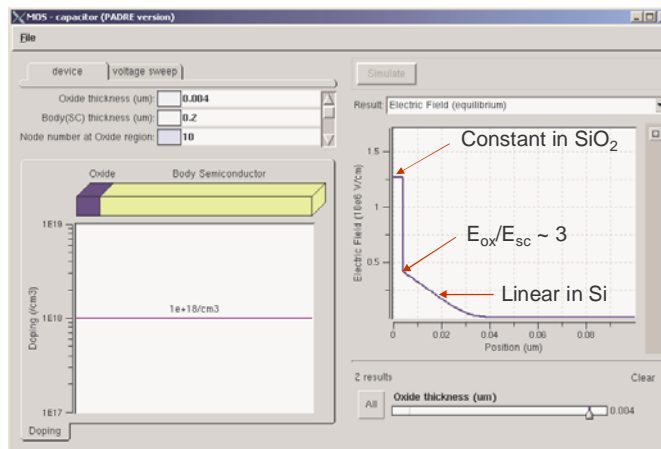
Question: Comment on the variation of the electrostatic potential in the semiconductor and in the oxide.

Answer: Since there are no charges in the oxide, the variation of the electrostatic potential in the oxide region is linear. In the semiconductor, due to the presence of the depletion region, we have quadratic variation of the potential vs. depth.



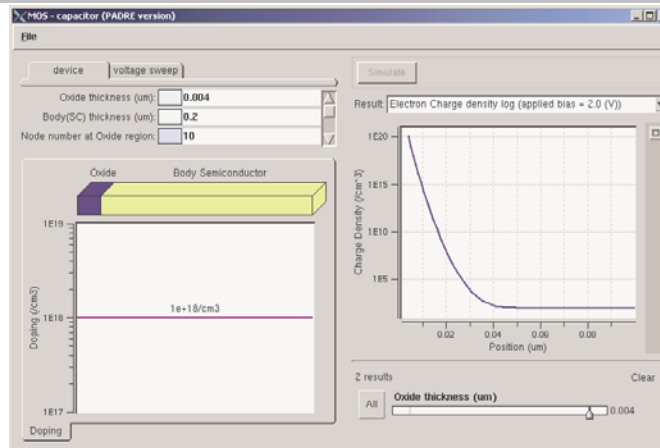
Question: Comment on the charge density components and their variation with distance.

Answer: The total charge density in this particular case equals the $N_A(x) + n(x) - p(x)$. The electron density is negligible, which means that the inversion layer has not formed yet. Therefore the net charge density is $N_A(x) - p(x)$ and depicts the extension of the depletion region in the semiconductor.



Question: Comment on the electric field variation with distance.

Answer: The electric field is constant in the oxide, varies linearly in the semiconductor since the doping is constant and the ratio of the electric fields in the oxide and in the semiconductor at the sc/oxide interface equals the ratio of sc/oxide dielectric constants.

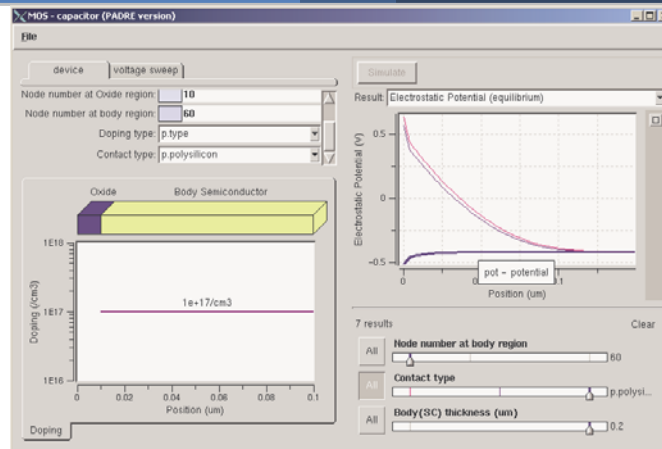


Question: Comment on the electron density variation for $V=2V$.

Answer: For $V_G=2V$, the inversion layer has formed. Since the potential is peaked at the sc/oxide interface, the electron density peaks at the interface and then decays exponentially into the bulk semiconductor region. This is what the classical picture predicts.

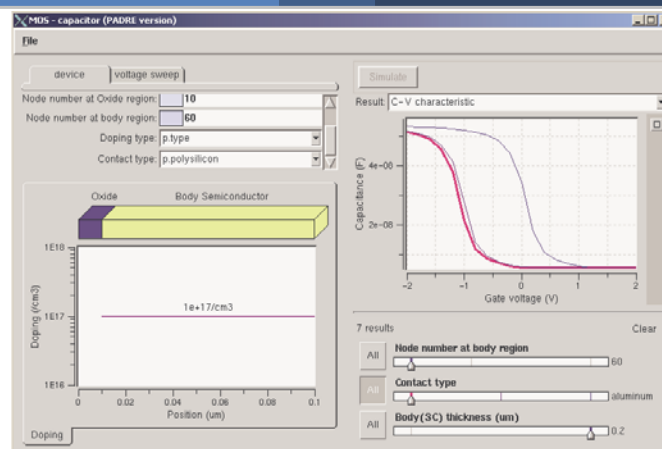
Consider a MOS capacitor structure found in conventional MOSFET devices. The thickness of the oxide region equals 4 nm and the substrate is p-type with doping N_A .

- Assume that $N_A=10^{17} \text{ cm}^{-3}$. Plot the conduction band profile under equilibrium conditions assuming aluminum gate, n+-polysilicon and p+-polysilicon gate.
- Vary the gate voltage from -2 to 2 V and calculate the high-frequency CV curves using $f=1\text{MHz}$. How does the change in the type of the gate electrode (aluminum vs. n+-polysilicon vs. p+-polysilicon) reflects on the HF CV-curves.
- Assume aluminum gate and plot the HF CV-curves for $f=1\text{MHz}$. How does the change in substrate doping reflects itself on the HF CV-curves. Support your reasoning with a physical model. Assume that $N_A=10^{16}$, 10^{17} and 10^{18} cm^{-3} .



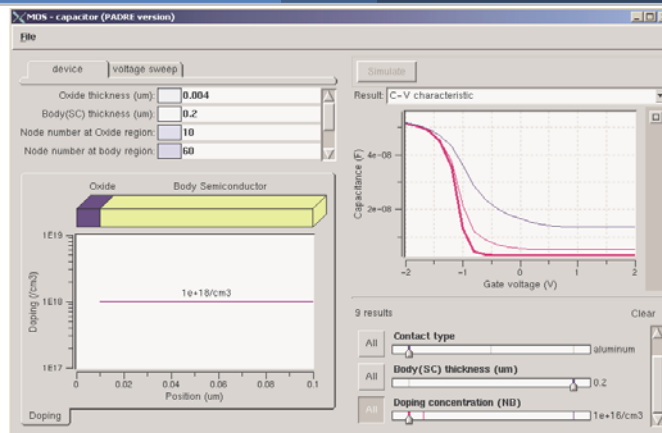
Question: Comment on the variation of the electrostatic potential in the semiconductor and in the oxide versus the choice of the gate electrode at equilibrium.

Answer: The aluminum and the n+-polysilicon gate make the MOS capacitor to be in the depletion/inversion mode. The very large value of the workfunction of the p+-polysilicon gate completely switches the picture and reverts it to accumulation mode.



Question: Comment on the modification of the HF CV-curves with the variation of the type of the gate electrode.

Answer: The change in the type of the gate electrode affects the metal-semiconductor workfunction difference and leads to rigid shift of the HF CV-curves. There is no distortion of the curves that can be produced, for example, by interface traps.



Question: Comment on the variation of the HF capacitance under depletion condition due to the variation of the substrate concentration.

Answer: The total gate capacitance under depletion conditions is a serial combination of the oxide and of the depletion layer capacitance. Since the thickness of the depletion layer varies as $N_A^{-1/2}$, with increasing N_A the depletion capacitance increases.