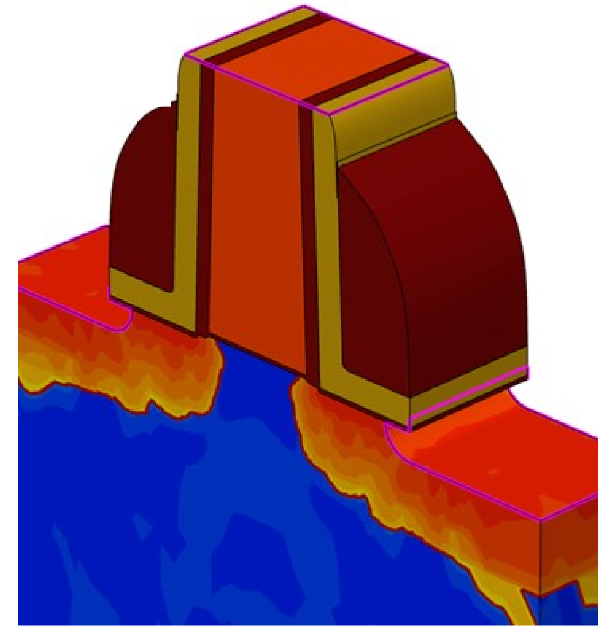
Technology Computer Aided Design (TCAD) Laboratory

Lecture 5, integrated diode



[Source: Synopsys]

Giovanni Betti Beneventi

E-mail: giovanni.betti2@unibo.it ; giobettibeneventi@gmail.com

Office: Engineering faculty, ARCES lab. (Ex. 3.2 room), viale del Risorgimento 2, Bologna

Phone: +39-051-209-3773

Advanced Research Center on Electronic Systems (ARCES)

University of Bologna, Italy

Outline

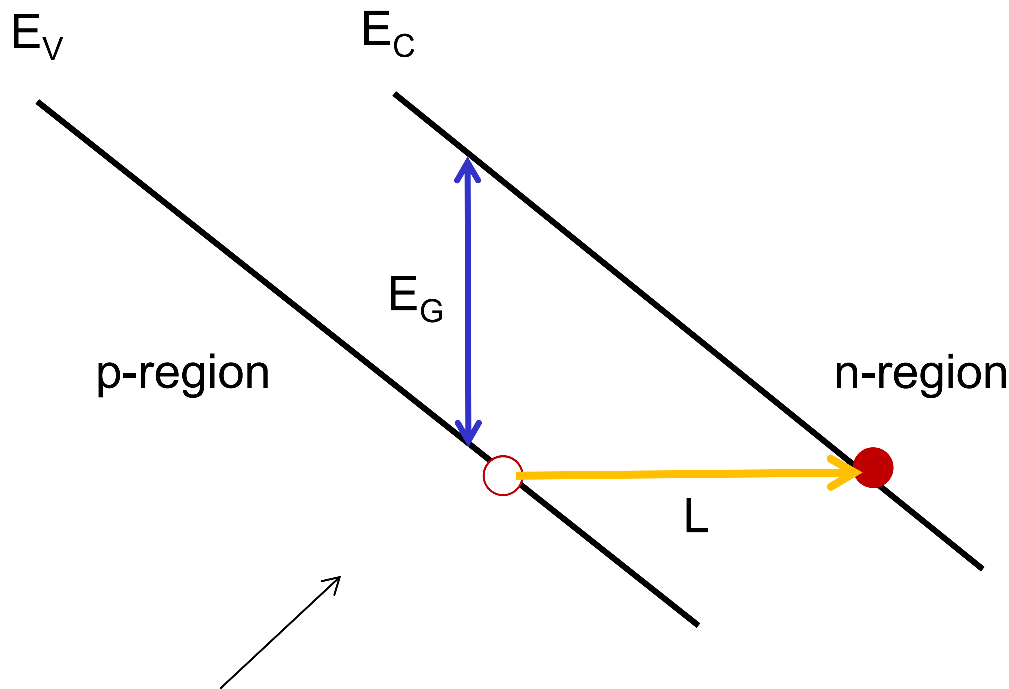
- Introduction
- Implementation of Input files
  - Sentaurus Structure Editor (SDE) command file
  - Sentaurus Device (SDevice)
    - command file
    - parameter file
- Run the simulation
- Post-processing of results

Introduction

- In this lesson we will implement a more realistic version of the pn-junction diode.
- The goal is to build a prototype device which could be similar to actual integrated diodes.
- The more realistic diode has features such as finite doping abruptness which makes it more suitable to simulate the reverse bias region including effects such as the band-to-band tunneling (i.e. Zener effect) or avalanche generation (i.e. Impact Ionization).
- The reason why these phenomena must be simulated with finite doping abruptness is that they depend exponentially on the applied field, and steep fields at the abrupt junctions could lead to convergence issues.

Qualitative understanding of band-to-band tunneling (1)

- Band-to-band tunneling is a carrier generation phenomenon.

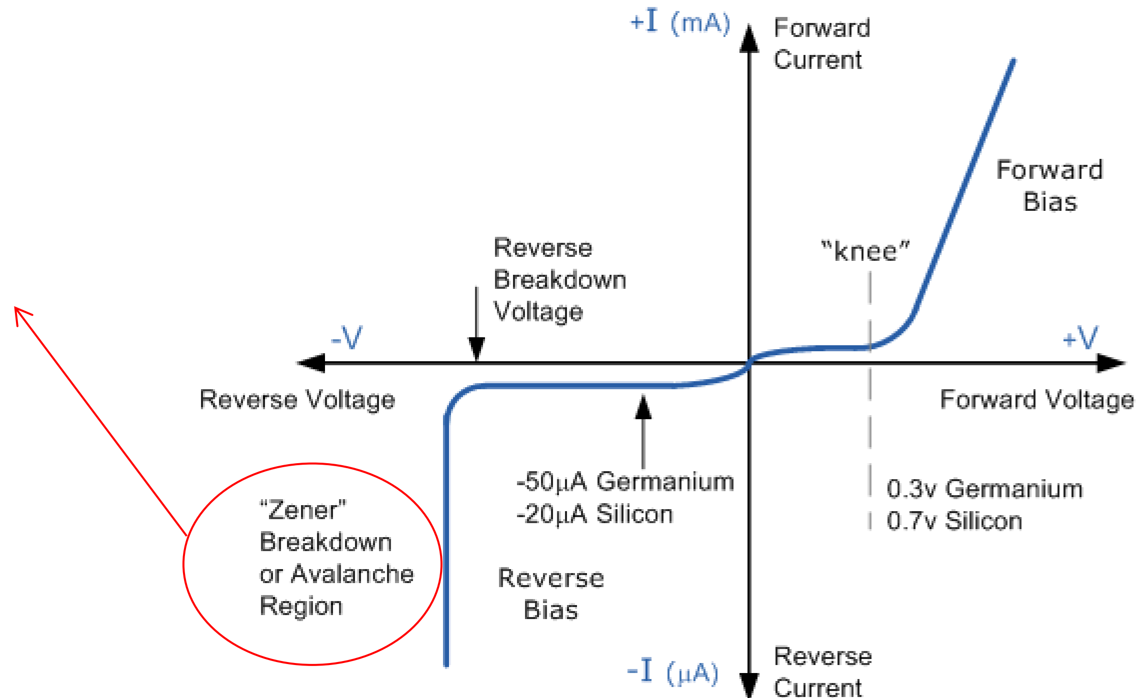


According to quantum mechanics, if L is short enough and if E_G is small enough there is a not-negligible probability of an electron to tunnel from the valence band of the *p*-region to the conduction band of the *n*-region. In this way, an electron is injected in the conduction band and a hole is freed at the valence band, and can contribute to current conduction. This carrier-generation process is shown to increase exponentially with the increase of the module of the reverse electric field. This phenomenon is also called "Zener breakdown".

Qualitative understanding of band-to-band tunneling (2)

- Once triggered, band-to-band tunneling produces a steep increase of the current in the current-voltage (IV) diode characteristics.
- This is due to the sudden increase of current due to the generation of a large number of free carriers.

Zener (band-to-band tunneling) or Avalanche (impact ionization) can be both triggered in the reverse bias region; which one is triggered at lower voltages depends on the physical characteristics of the diode (doping in particular)



Band-to-band tunneling & impact ionization

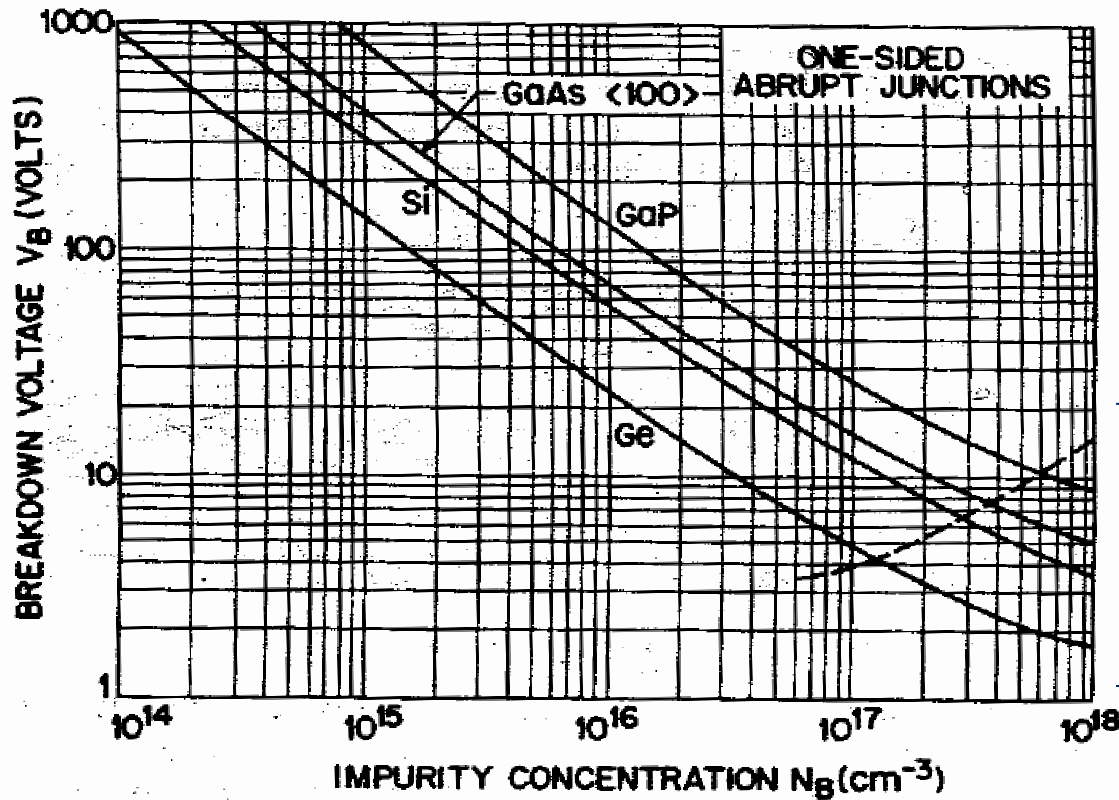
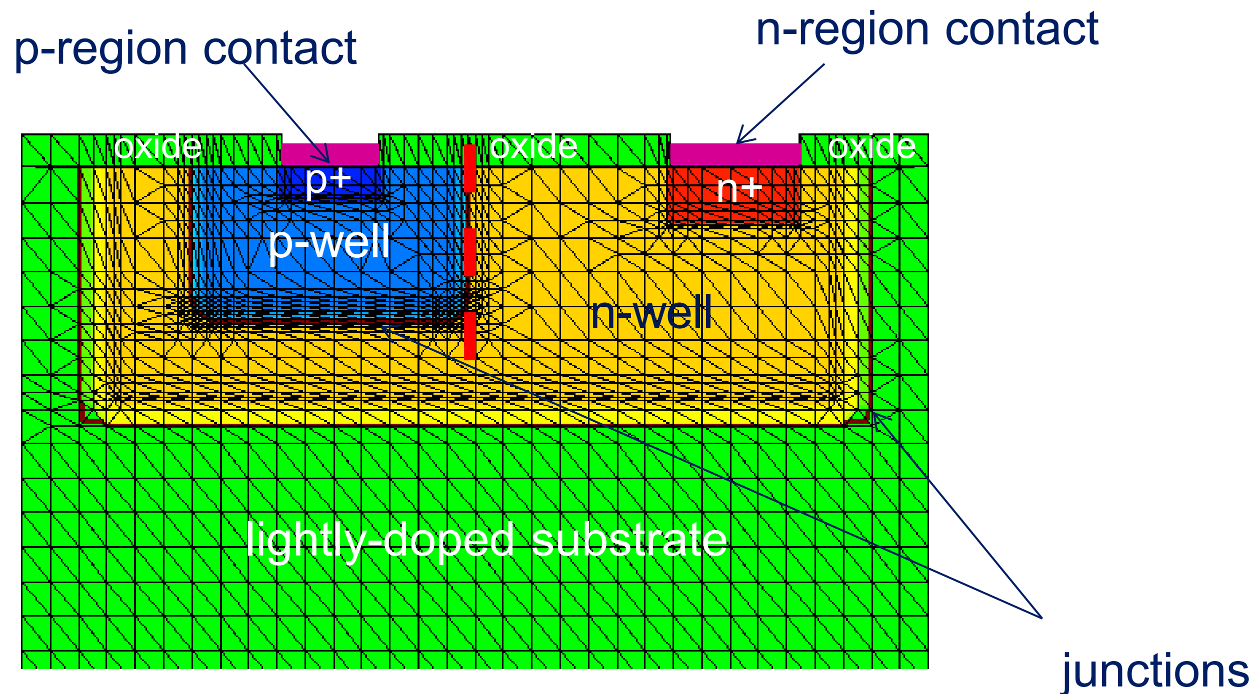


Fig. 26 Avalanche breakdown voltage versus impurity concentration for one-sided abrupt junctions in Ge, Si, ⟨100⟩-oriented GaAs, and GaP. The dashed line indicates the maximum doping beyond which the tunneling mechanism will dominate the voltage breakdown characteristics. (After Sze and Gibbons, Ref. 35.)

For relatively high doping concentrations, Zener tunneling occurs at lower voltages than Avalanche

The structure

- We want to create a structure like this one:



SWB

OPEN SWB FROM THE LINUX COMMAND LINE

`swb &`

STARTING (AND SAVING) A NEW SWB PROJECT

`Project` → `New` → `New Project`

`Project`→ `Save as` → `Project` → `pn_reale`

ADD TOOLS

left click on `No tools` → right click → `Add` → Name, scroll for `SDE` → select `Batch` → `Ok`

left click on `SDE` → right click → `Add` → Name → scroll for `Sdevice` → `Ok`

ADD PARAMETERS (WITH THEIR DEFAULT VALUES):

Click in the box just below `SDE` tool image and press `Add` →`Parameter` → `pwell_doping_concentration` → `default value` → `5e18`

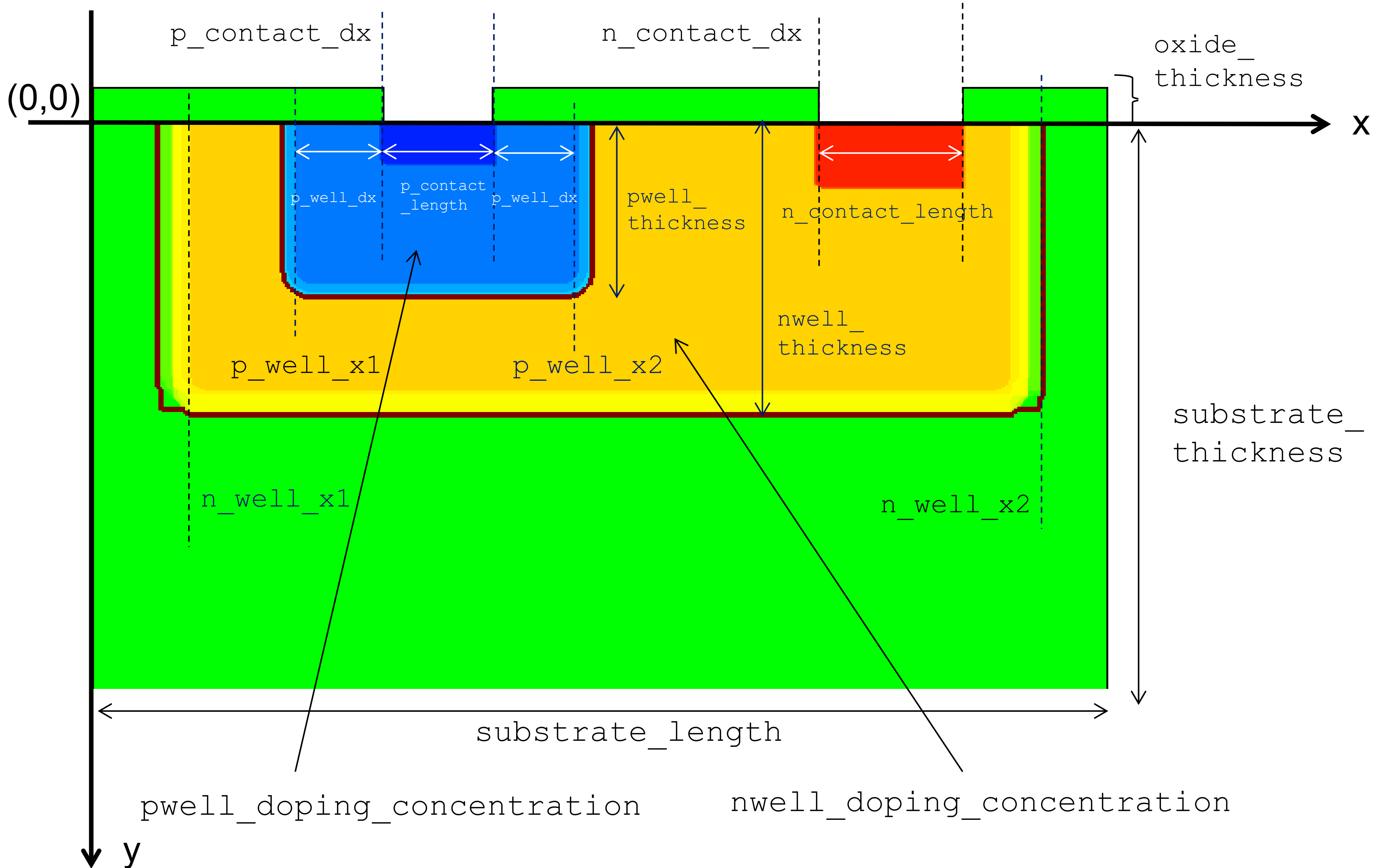
Right click on `pwell_doping_concentration` → `Add` → `Parameter` →`nwell_doping_concentration` → `default value` → `5e17`

Right click in the box just below `Sdevice` tool image and press `Add` →`Parameter` → `VR` → `default value` → `-6`

Right click on `VR` → `Add` → `Parameter` → `VD` → `default value` → `1`

`Experiment` → `Add New Experiment` → `pwell_doping_concentration` → `5e19` → `nwell_doping_concentration` → `5e18`

Geometrical definitions / integrated diode



SDE command file (1)

Select SDE image tool → Right Click → `Edit input` → `Commands`

then write in the text file the following commands:

```
; clear structure
(sde:clear)
; New-replace-old option (default)
(sdegeo:set-default-boolean "ABA")
; define minimum displacement
(define eps 0.001)
; SEMICONDUCTOR MATERIAL
(define semiconductor_material "Silicon")
; SUBSTRATE PARAMETERS
(define substrate_length 1.400)
(define substrate_thickness 0.800)
; PWELL PARAMETERS
(define pwell_thickness 0.200)
; x coordinate of pwell
(define p_contact_dx 0.400)
(define p_contact_length 0.150)
```

SDE command file (2)

```
; NWELL PARAMETERS
(define nwell_thickness 0.350)
; x coordinate of nwell
(define n_contact_dx 1.000)
(define n_contact_length 0.200)
; extra space at contacts
(define pwell_dx 0.100)
(define pwell_x1 (- p_contact_dx pwell_dx))
(define pwell_x2 (+ pwell_dx (+ p_contact_length p_contact_dx)))
(define nwell_x1 0.150)
(define nwell_x2 (- substrate_length 0.150))

; DOPING PARAMETERS
(define substrate_doping_concentration 1e12)
(define nwell_doping_concentration @nwell_doping_concentration@)
(define pwell_doping_concentration @pwell_doping_concentration@)
```

SDE command file (3)

```
(define nwell_value_at_depth substrate_doping_concentration)
(define nwell_depth 0.050)
(define pwell_value_at_depth substrate_doping_concentration)
(define pwell_depth 0.100)
; OXIDE
(define oxide_material "Oxide")
(define oxide_thickness 0.050)
; MESH PARAMETERS
(define substrate_xmax 0.056)
(define substrate_ymax 0.056)
(define substrate_xmin 0.028)
(define substrate_ymin 0.028)
(define wells_xmax 0.21)
(define wells_ymax 0.21)
(define wells_xmin 0.0056)
(define wells_ymin 0.0056)
```

parameter for Gaussian smoothing of doping (see next)

SDE command file (4)

```
; *** GEOMETRY
; convention: x=length y=thickness
; create semiconductor substrate
(sdegeo:create-rectangle (position 0 0 0) (position substrate_length
substrate_thickness 0) semiconductor_material "substrate-r")
; create oxidations
(sdegeo:create-rectangle (position 0 0 0) (position p_contact_dx (-
oxide_thickness) 0) oxide_material "oxide1-r")
(sdegeo:create-rectangle (position (+ p_contact_length p_contact_dx) 0 0)
(position n_contact_dx (- oxide_thickness) 0) oxide_material "oxide2-r")
(sdegeo:create-rectangle (position (+ n_contact_length n_contact_dx) 0 0)
(position substrate_length (- oxide_thickness) 0) oxide_material "oxide3-
r")
; *** CONTACTS ***
; a) SET VERTEXES
; 1st vertex on p_contact
(sdegeo:insert-vertex (position p_contact_dx 0 0))
; 2nd vertex on p_contact
(sdegeo:insert-vertex (position (+ p_contact_length p_contact_dx) 0 0))
```

SDE command file (5)

```
; 1st vertex on n_contact
(sdegeo:insert-vertex (position n_contact_dx 0 0))
; 2nd vertex on n_contact
(sdegeo:insert-vertex (position (+ n_contact_dx n_contact_length) 0 0))
; b) SET EDGE (DEFINITION AND ACTIVATION)
; p_contact
(sdegeo:define-contact-set "p_contact" 4 (color:rgb 1 0 0) "##")
(sdegeo:set-current-contact-set "p_contact")
(sdegeo:define-2d-contact (find-edge-id (position (+ eps p_contact_dx) 0 0))
"p_contact")
; n_contact
(sdegeo:define-contact-set "n_contact" 4 (color:rgb 1 0 0) "##")
(sdegeo:set-current-contact-set "n_contact")
(sdegeo:define-2d-contact (find-edge-id (position (+ eps n_contact_dx) 0 0))
"n_contact")
```

SDE command file (6)

```
; *** DOPING ****

; SUBSTRATE (p-type): CONSTANT PROFILE, ON A REGION

(sdedr:define-constant-profile "substrate-doping-profile"
"BoronActiveConcentration" substrate_doping_concentration)

(sdedr:define-constant-profile-region "substrate-doping-placement"
"substrate-doping-profile" "substrate-r")

(sdedr:define-constant-profile-placement "substrate-doping-placement"
"substrate-doping-profile" "substrate-doping-window" 0.000)

; NWELL (n-type): CONSTANT PROFILE, DEFINE RECTANGLE

(sdedr:define-refinement-window "nwell-doping-window" "Rectangle" (position
nwell_x1 0 0) (position nwell_x2 nwell_thickness 0))

(sdedr:define-constant-profile "nwell-doping-profile"
"PhosphorusActiveConcentration" nwell_doping_concentration)

(sdedr:define-constant-profile-placement "nwell-doping-placement" "nwell-
doping-profile" "nwell-doping-window" 0.000)

; NWELL (n-type): GAUSSIAN SMOOTHING

; horizontal line

(sdedr:define-refinement-window "nwell-doping-window-gauss-hor" "Line"
(position nwell_x1 nwell_thickness 0) (position nwell_x2 nwell_thickness
0))
```

SDE command file (7)

```
(sdedr:define-gaussian-profile "nwell-doping-profile-gauss-hor"
"PhosphorusActiveConcentration" "PeakPos" 0 "PeakVal"
nwell_doping_concentration "ValueAtDepth" nwell_value_at_depth "Depth"
nwell_depth "Gauss" "Factor" 1)

(sdedr:define-analytical-profile-placement "nwell-doping-placement-gauss-
hor" "nwell-doping-profile-gauss-hor" "nwell-doping-window-gauss-hor"
"Positive" "NoReplace" "Eval")

; side line 1 (sx)

(sdedr:define-refinement-window "nwell-doping-window-gauss-side1" "Line"
(position nwell_x1 0 0) (position nwell_x1 nwell_thickness 0))

(sdedr:define-gaussian-profile "nwell-doping-profile-gauss-side1"
"PhosphorusActiveConcentration" "PeakPos" 0 "PeakVal"
nwell_doping_concentration "ValueAtDepth" nwell_value_at_depth "Depth"
nwell_depth "Gauss" "Factor" 0)

(sdedr:define-analytical-profile-placement "nwell-doping-placement-gauss-
side1" "nwell-doping-profile-gauss-side1" "nwell-doping-window-gauss-side1"
"Positive" "NoReplace" "Eval")

; side line 2 (dx)

(sdedr:define-refinement-window "nwell-doping-window-gauss-side2" "Line"
(position nwell_x2 0 0) (position nwell_x2 nwell_thickness 0))
```

SDE command file (8)

```
(sdedr:define-gaussian-profile "nwell-doping-profile-gauss-side2"
"PhosphorusActiveConcentration" "PeakPos" 0 "PeakVal"
nwell_doping_concentration "ValueAtDepth" nwell_value_at_depth "Depth"
nwell_depth "Gauss" "Factor" 0)

(sdedr:define-analytical-profile-placement "nwell-doping-placement-gauss-
side2" "nwell-doping-profile-gauss-side2" "nwell-doping-window-gauss-side2"
"Negative" "NoReplace" "Eval")

; NWELL OHMIC CONTACT

(sdedr:define-refinement-window "nwell-doping-window-ohmic" "Rectangle"
(position n_contact_dx 0 0) (position (+ n_contact_dx n_contact_length) (*
0.25 nwell_thickness) 0))

(sdedr:define-constant-profile "nwell-doping-profile-ohmic"
"PhosphorusActiveConcentration" 1e20)

(sdedr:define-constant-profile-placement "nwell-doping-placement-ohmic"
"nwell-doping-profile-ohmic" "nwell-doping-window-ohmic" 0.000)

; PWELL (p-type): CONSTANT PROFILE

(sdedr:define-refinement-window "pwell-doping-window" "Rectangle" (position
pwell_x1 0 0) (position pwell_x2 pwell_thickness 0))

(sdedr:define-constant-profile "pwell-doping-profile"
"BoronActiveConcentration" pwell_doping_concentration)

(sdedr:define-constant-profile-placement "pwell-doping-placement" "pwell-
doping-profile" "pwell-doping-window" 0.000)
```

SDE command file (9)

```
; PWELL (p-type): GAUSSIAN SMOOTHING

; horizontal line

(sdedr:define-refinement-window "pwell-doping-window-gauss-hor" "Line"
(position pwell_x1 pwell_thickness 0) (position pwell_x2 pwell_thickness
0))

(sdedr:define-gaussian-profile "pwell-doping-profile-gauss-hor"
"BoronActiveConcentration" "PeakPos" 0 "PeakVal" pwell_doping_concentration
"ValueAtDepth" pwell_value_at_depth "Depth" pwell_depth "Gauss" "Factor" 1)

(sdedr:define-analytical-profile-placement "pwell-doping-placement-gauss-
hor" "pwell-doping-profile-gauss-hor" "pwell-doping-window-gauss-hor"
"Positive" "NoReplace" "Eval")

; side line 1 (sx)

(sdedr:define-refinement-window "pwell-doping-window-gauss-side1" "Line"
(position pwell_x1 0 0) (position pwell_x1 pwell_thickness 0))

(sdedr:define-gaussian-profile "pwell-doping-profile-gauss-side1"
"BoronActiveConcentration" "PeakPos" 0 "PeakVal" pwell_doping_concentration
"ValueAtDepth" pwell_value_at_depth "Depth" pwell_depth "Gauss" "Factor" 0)

(sdedr:define-analytical-profile-placement "pwell-doping-placement-gauss-
side1" "pwell-doping-profile-gauss-side1" "pwell-doping-window-gauss-side1"
"Positive" "NoReplace" "Eval")
```

SDE command file (10)

```
; side line 2 (dx)

(sdedr:define-refinement-window "pwell-doping-window-gauss-side2" "Line"
(position pwell_x2 0 0) (position pwell_x2 pwell_thickness 0))

(sdedr:define-gaussian-profile "pwell-doping-profile-gauss-side2"
"BoronActiveConcentration" "PeakPos" 0 "PeakVal" pwell_doping_concentration
"ValueAtDepth" pwell_value_at_depth "Depth" pwell_depth "Gauss" "Factor" 0)

(sdedr:define-analytical-profile-placement "pwell-doping-placement-gauss-
side2" "pwell-doping-profile-gauss-side2" "pwell-doping-window-gauss-side2"
"Negative" "NoReplace" "Eval")

; PWELL OHMIC CONTACT

(sdedr:define-refinement-window "pwell-doping-window-ohmic" "Rectangle"
(position p_contact_dx 0 0) (position (+ p_contact_dx p_contact_length)
(* 0.25 pwell_thickness) 0))

(sdedr:define-constant-profile "pwell-doping-profile-ohmic"
"BoronActiveConcentration" 1e20)

(sdedr:define-constant-profile-placement "pwell-doping-placement-ohmic"
"pwell-doping-profile-ohmic" "pwell-doping-window-ohmic" 0.000)
```

SDE command file (11)

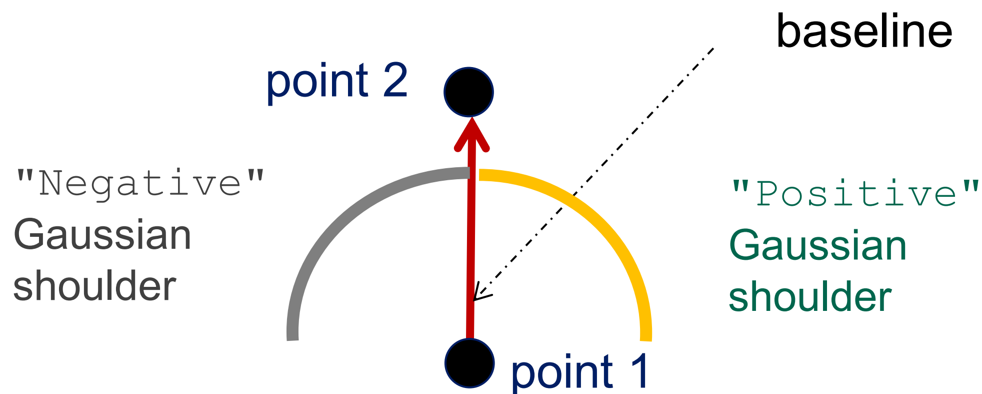
```
; *** MESH ***
; * SUBSTRATE (underneath refinement)
(sdedr:define-refeval-window "substrate-ref" "Rectangle" (position 0 0 0)
(position substrate_length substrate_thickness 0))
(sdedr:define-refinement-size "substrate-ref-size" substrate_xmax
substrate_ymax substrate_xmin substrate_ymin)
(sdedr:define-refinement-placement "substrate-ref-pl" "substrate-ref-size"
"substrate-ref")
; * WELLS
(sdedr:define-refeval-window "wells-ref" "Rectangle" (position nwell_x1 0
0) (position nwell_x2 nwell_thickness 0))
(sdedr:define-refinement-size "wells-ref-size" wells_xmax wells_ymax
wells_xmin wells_ymin)
(sdedr:define-refinement-placement "wells-ref-pl" "wells-ref-size" "wells-
ref")
; * p-n JUNCTION REFINEMENT
(sdedr:define-refinement-function "wells-ref-size" "DopingConcentration"
"MaxTransDiff" 0.1)
; * BUILDING MESH
(sde:build-mesh "snmesh" "-a -c boxmethod" "n@node@")
```

SDE command file (12)

- `Save` → `Quit`

➢ DONE SDE PART.

N.B how to handle `"Positive"` and `"Negative"` in the Gaussian doping profile:



Sdevice command file (1)

Select Sdevice image tool → Right Click → `Edit input` → `Commands`

then write in the text file the following commands:

```
File
{
   **** INPUT FILES
   * geometry, contacts doping and mesh
   Grid ="@tdr@"
   * physical parameters
   Parameter = "@parameter@"
   **** OUTPUT FILES
   * distributed variables
   Plot = "n@node@_des.tdr"
   * electrical characteristics at the electrodes
   Current= "n@node@_des.plt"
}
```

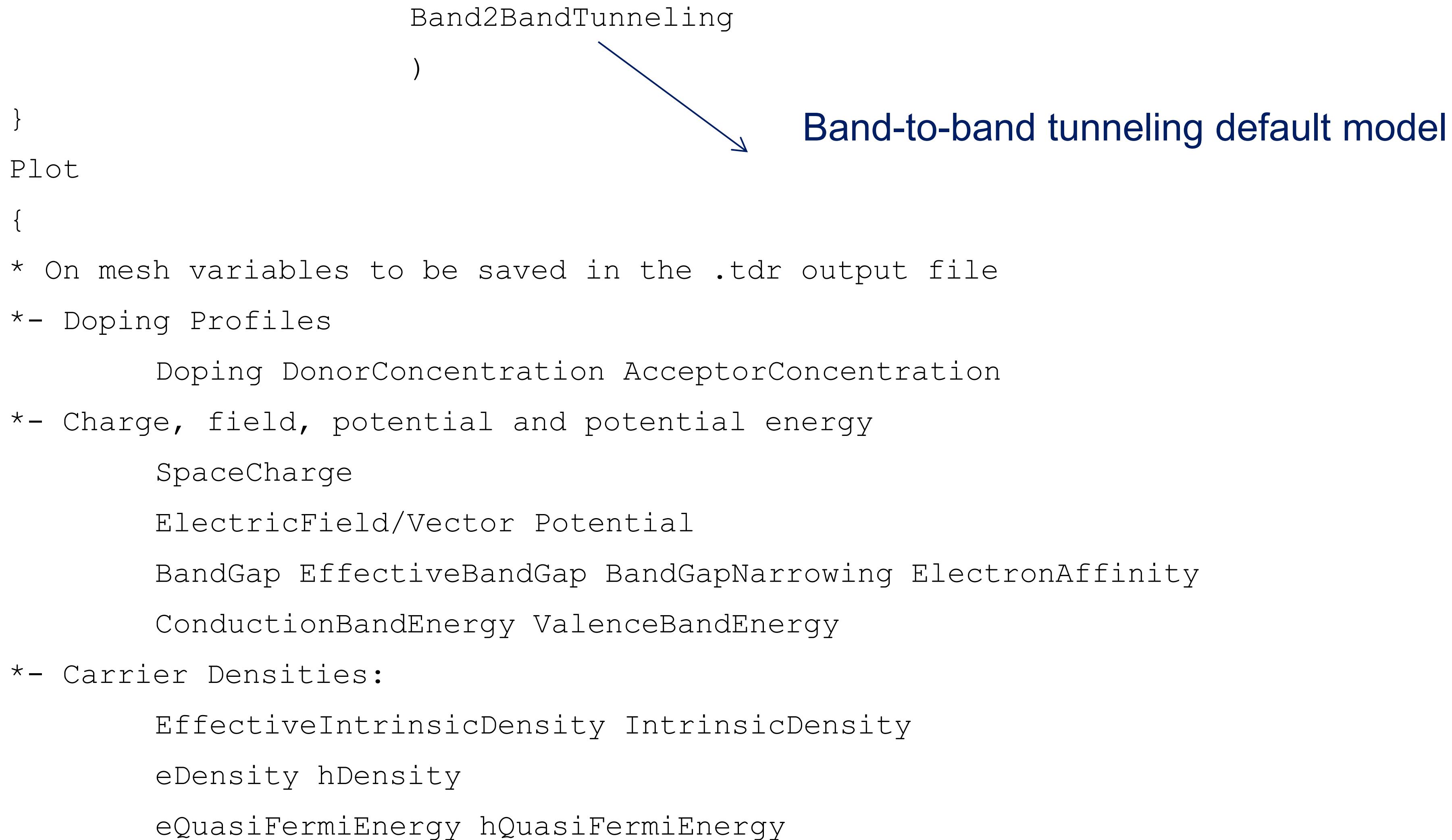
Sdevice command file (2)

```
Electrode
{
   * defines which contacts have to be treated as electrodes; initial bias
   * and boundary conditions
   * obviously, electrode names must match the contact names of the dvs.cmd file
   { name="p_contact" voltage=0.0 }
   { name="n_contact" voltage=0.0 }
}

Physics
{
        Mobility (
                  DopingDependence
                  )
        Recombination (
                      SRH (DopingDependence)
                      SRH (TemperatureDependence)
```

advanced SRH models

Sdevice command file (3)




```
                        Band2BandTunneling
                        )
}
Plot
{
* On mesh variables to be saved in the .tdr output file
*- Doping Profiles
        Doping DonorConcentration AcceptorConcentration
*- Charge, field, potential and potential energy
        SpaceCharge
        ElectricField/Vector Potential
        BandGap EffectiveBandGap BandGapNarrowing ElectronAffinity
        ConductionBandEnergy ValenceBandEnergy
*- Carrier Densities:
        EffectiveIntrinsicDensity IntrinsicDensity
        eDensity hDensity
        eQuasiFermiEnergy hQuasiFermiEnergy
```

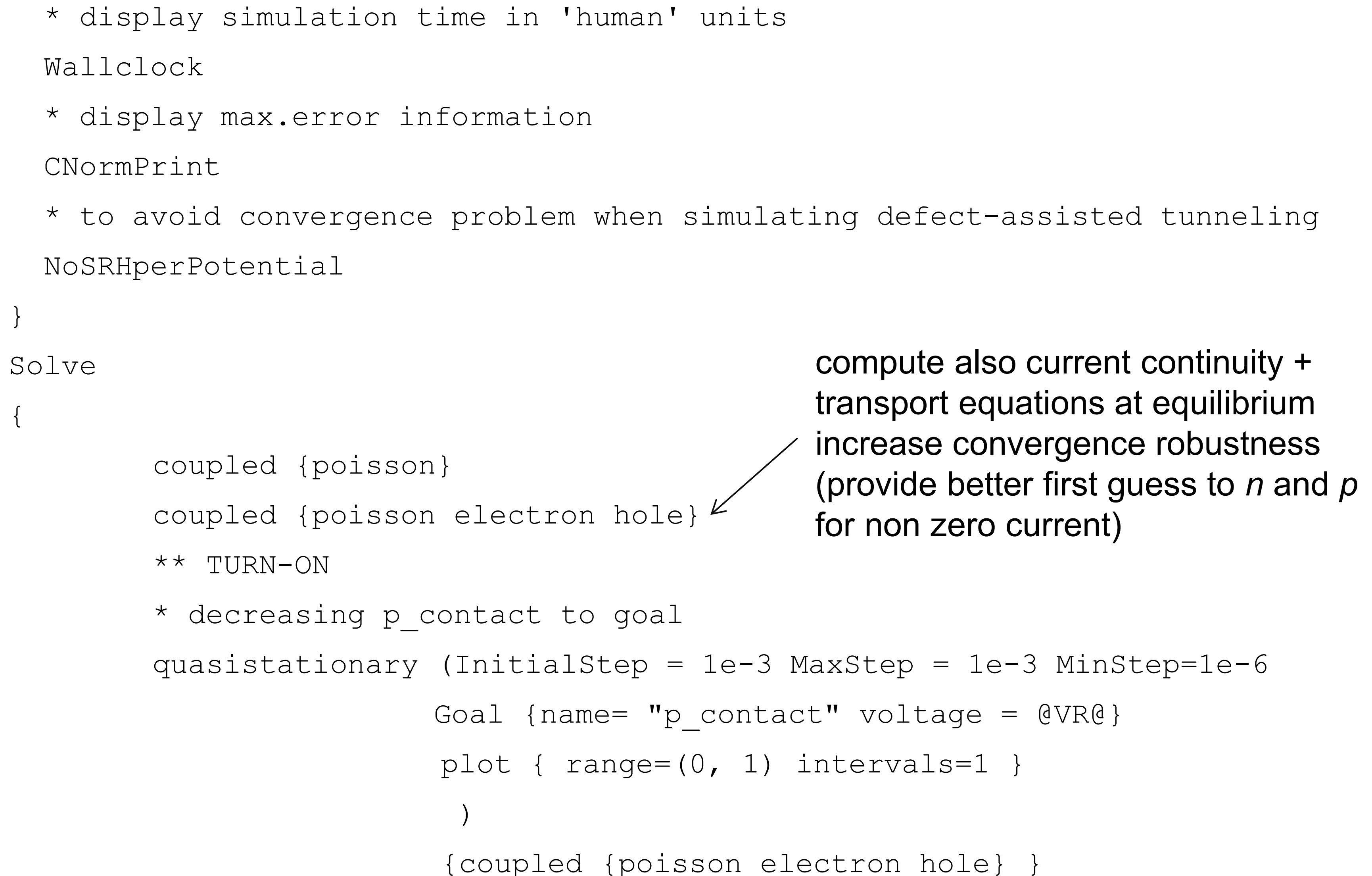
Sdevice command file (4)

```
*- Currents and current components:
        eGradQuasiFermi/Vector hGradQuasiFermi/Vector
        eMobility hMobility eVelocity hVelocity
        Current/Vector eCurrent/Vector hCurrent/Vector
        eDriftVelocity/Vector hDriftVelocity/Vector
*- SRH & interfacial traps
        SRHrecombination
        tSRHrecombination
*- Band2Band Tunneling
        eBand2BandGeneration hBand2BandGeneration Band2BandGeneration
        eAvalanche hAvalanche
}
Math
{
  * use previous two solutions (if any) to extrapolate next
  Extrapolate
```

Sdevice command file (5)

```
* use full derivatives in Newton method
Derivatives
* control on relative errors
RelErrControl
* relative error= 10^(-Digits)
Digits=7
* absolute error
Error(electron)=1e8
Error(hole)=1e8
* numerical parameter for space-charge regions
eDrForceRefDens=1e10
hDrForceRefDens=1e10
* maximum number of iteration at each step
Iterations=20
Method=ParDiSo
```

Sdevice command file (6)

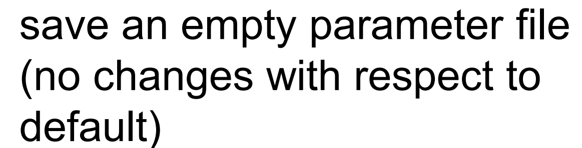


```
  * display simulation time in 'human' units
  Wallclock
  * display max.error information
  CNormPrint
  * to avoid convergence problem when simulating defect-assisted tunneling
  NoSRHperPotential
}
Solve
{
        coupled {poisson}
        coupled {poisson electron hole}
        ** TURN-ON
        * decreasing p_contact to goal
        quasistationary (InitialStep = 1e-3 MaxStep = 1e-3 MinStep=1e-6
                    Goal {name= "p_contact" voltage = @VR@}
                    plot { range=(0, 1) intervals=1 }
                    )
                    {coupled {poisson electron hole} }
```

Sdevice command file (7) & Sdevice parameter file & run

```
quasistationary (InitialStep = 1e-2 MaxStep = 1e-2 MinStep=1e-6
                 Goal {name= "p_contact" voltage = @VD@}
                  )
                 {coupled {poisson electron hole} }
                 }
```

save an empty parameter file (no changes with respect to default)



- `Save` → `Quit`
- Select Sdevice image tool → Right Click → `Edit input` → `Parameter` → `No` → `Save` → `Quit`

➢ DONE Sdevice command file PART.

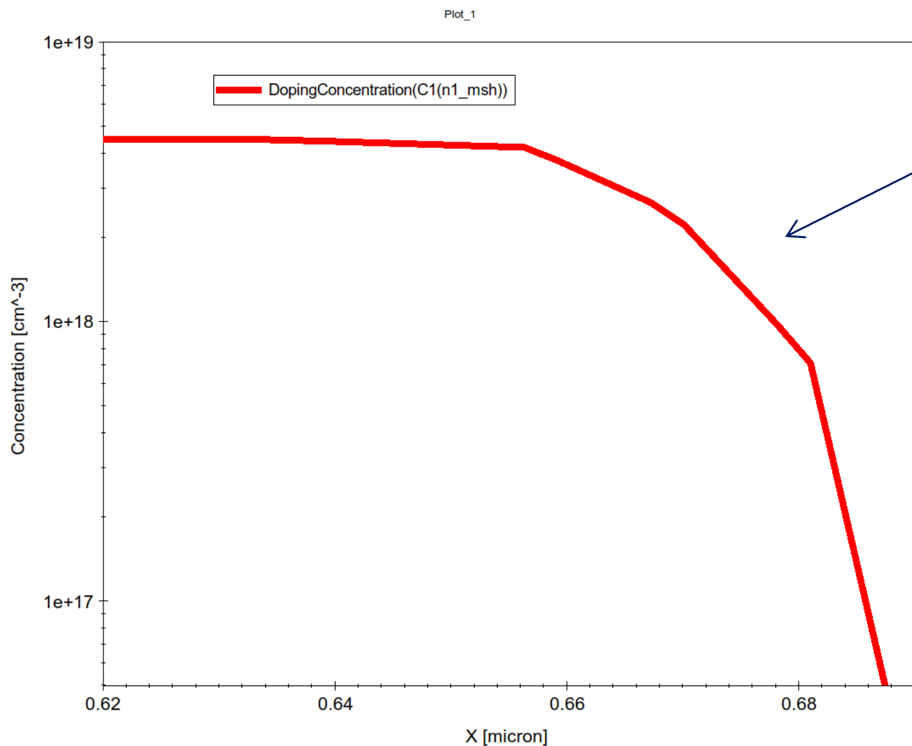
<u>Pre-processing and Run:</u>

Select nodes `n1` and `n8` (sde real nodes) → `CTRL-R` → `local:priority` → `Run`

Select nodes `n2` and `n11` (sdevice real nodes) → `CTRL-R` → `local:priority` → `Run`

Post-processing: doping profile

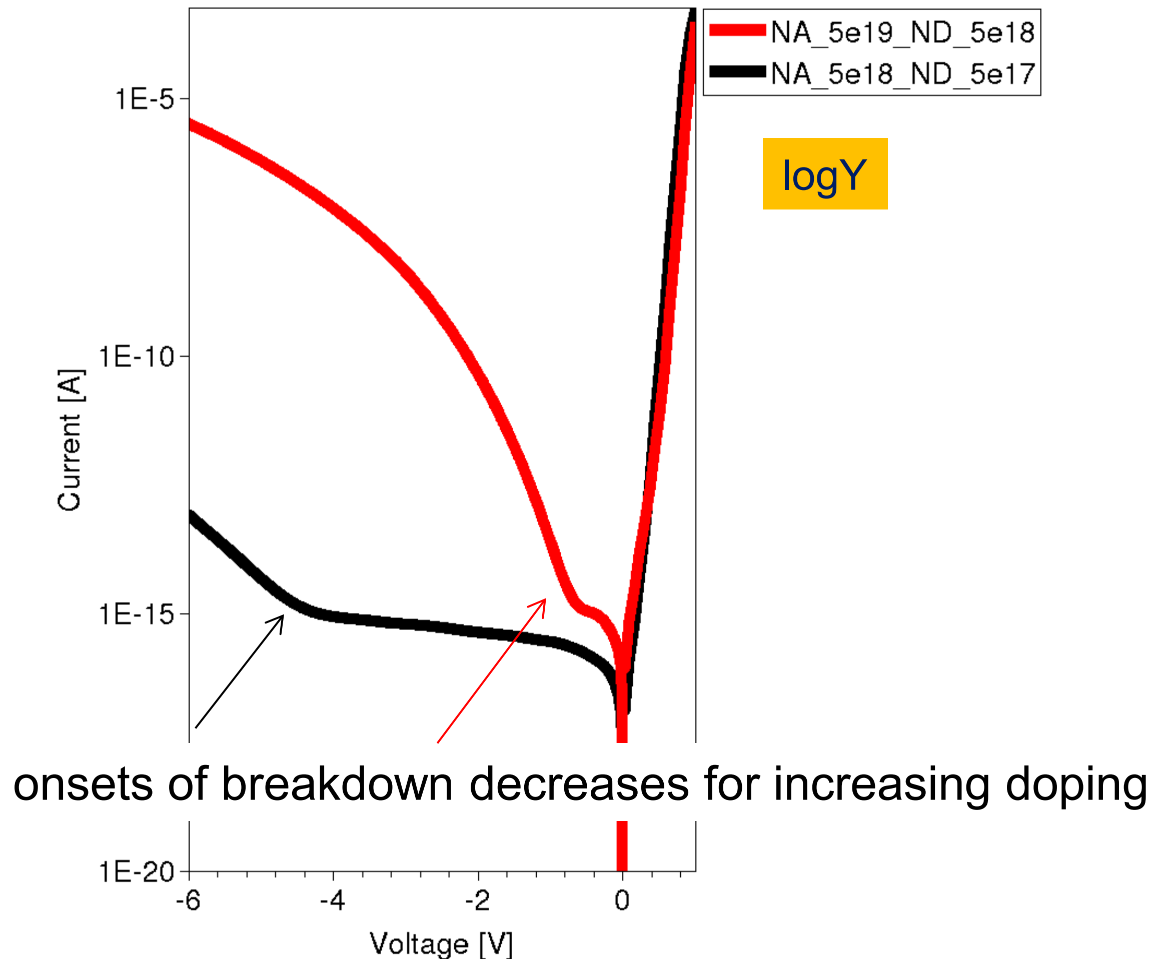
- Right click on `n1` → `Visualize` → `Svisual (Select File…)`
- Select `n1_msh.tdr` → `Ok`
- `Precision Cuts` → `Y` → `0.010`
- `Window` → `Plot_n1_msh` → Double click on X-axis → `Axis Properties` → `Min: 0.62 Max: 0.69`
- Double click on Y-axis → `Axis Properties` → `Min: 5e16 Max: 1e19` → Select `LogScale`



gaussian profile
("pwell-side2")

Post-processing: IV curve

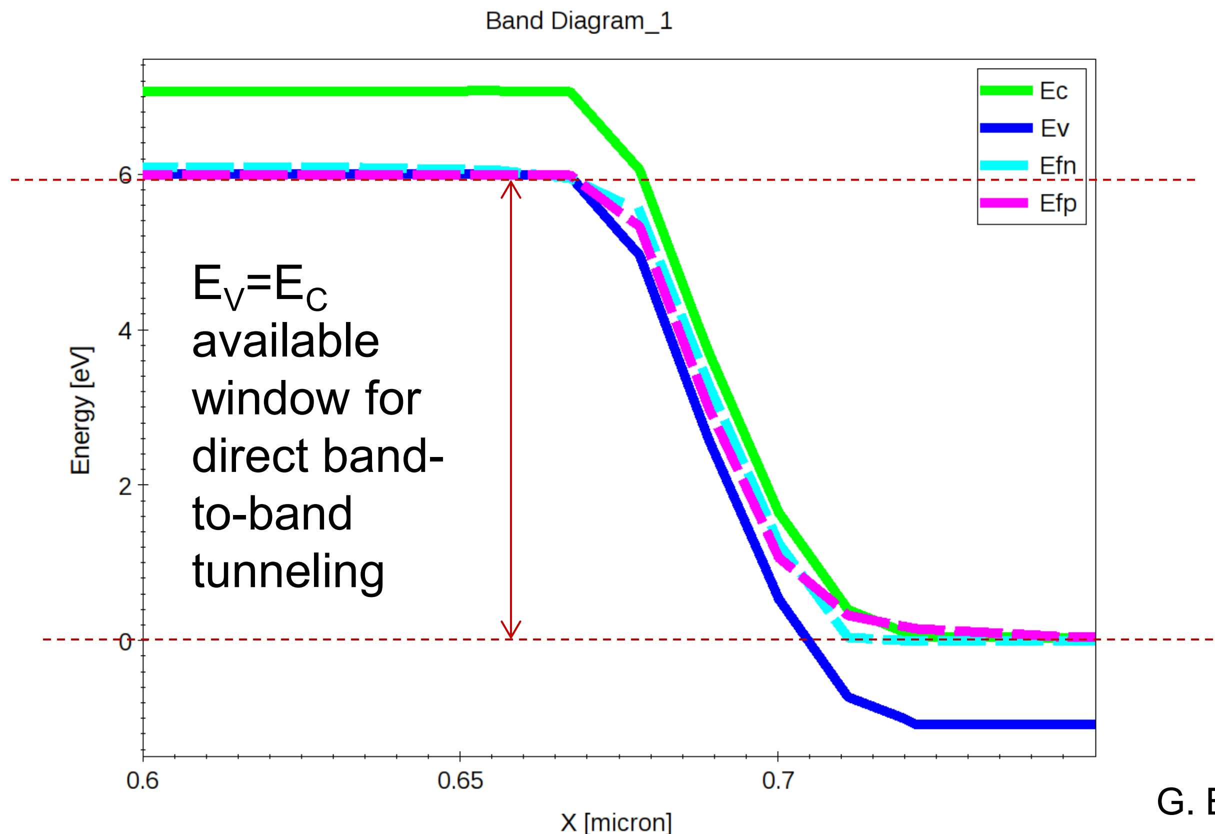
- Right click on `n2` and `n11` → `Visualize` → `Inspect (All Files)`
- Select `n2` and `n11` on the `Datasets` part → `p_contact` → `OuterVoltage` → `To X-Axis` → `TotalCurrent` → `To Left-Y-Axis`
- Select `logY` on the upper toolbar



onsets of breakdown decreases for increasing doping

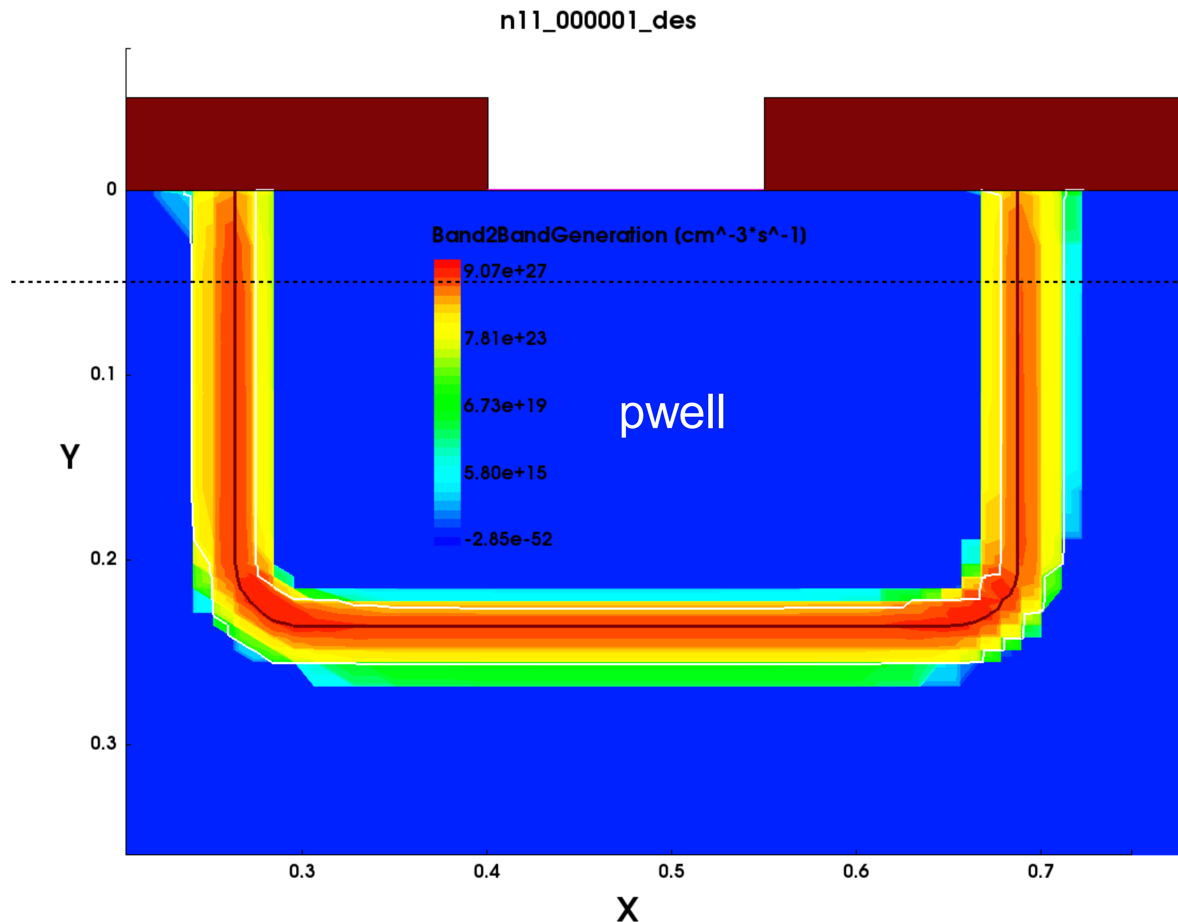
Post-processing: reverse bias bands

- Right click on `n11` → `Visualize` → `Svisual (Select File…)`
- Select `n11_000001_des` → `Ok`
- `Precision Cuts` → `Y` → `0.05` → `Plot Band Diagram`
- Double click on the x-axis of the band diagram → `Axis Properties` → `Min.` → `0.60` → `Max.` → `0.75`
- `Window` → `Plot n11_000001_des`



Post-processing: band-to-band generation rates

- `Window` → `Plot n11_000001_des` → `Window` → `Plot1`
- `Scalars` → `Band2BandGeneration` → zoom at the junction



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