Simulations with TCAD

Tutorial

Overview

- 1.) Building a structure
  - Using a scheme command file
- 2.) Define simulation parameters
  - Using an Input command file

  - **Example: ‘Simple’ Diode**

1.) Geometry file

- A scheme file consists of
  - Parameter definitions
  - Geometry definitions
  - Doping profile definitions
  - Meshing definitions
  - Contact definitions and placements
  - Operation orders

1.A Parameter definition

- You could define:
  - Geometry sizes:
    - **(define Diode_thickness 320.0);**

(define Diode_width 500.0); (define Oxide_thickness 1.2); (define Al_thickness 1); (define Doping_thickness_BP 10); (define Doping_thickness_implant 1); (define Connection_hole_width 10)

  - Or doping concentrations
    - **(define concentration_bulk 1.5e12);**

(define concentration_implant 1e19); (define concentration_BP 1e19)

1.B Geometry

- (sdegeo:create-rectangle (position 0 0 0) (position Diode_width Diode_thickness 0) "Silicon" "bulk")

Material could be a default material or a self define material; material properties could be change in the Material.par file

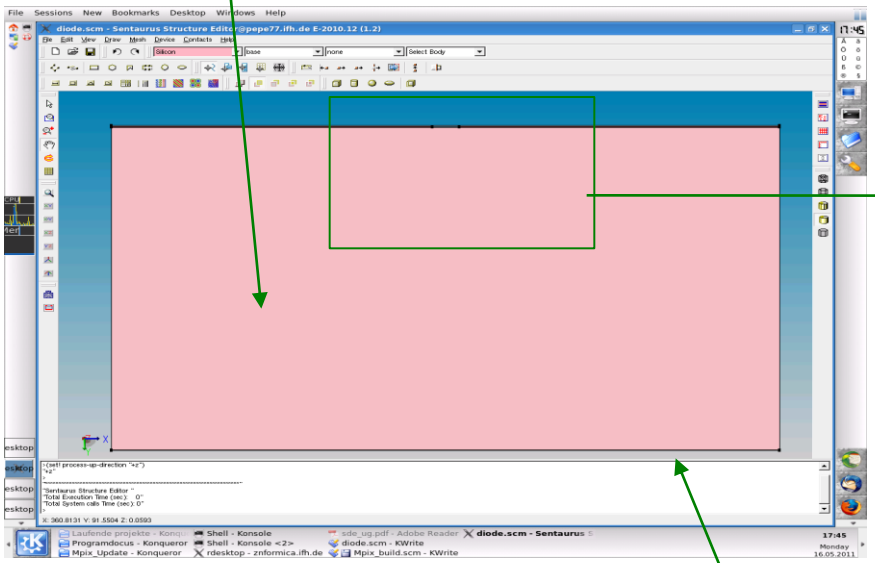
- (sdegeo:create-rectangle (position 0 (* -1 Oxide_thickness) 0) (position Diode_width (* -1 (+ Oxide_thickness Al_thickness)) 0) "Aluminum" "TopCon")

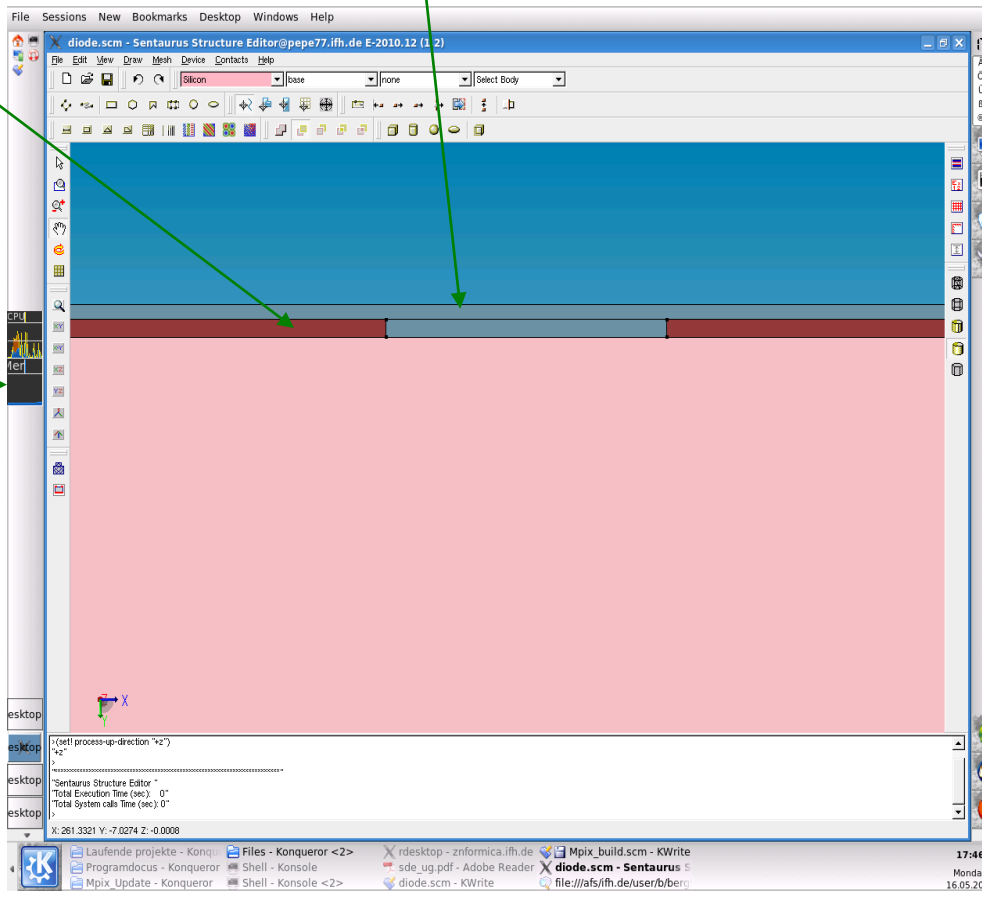
```
Epsilon
{ *  Ratio of the permittivities of material and vacuum

  * epsilon() = epsilon
epsilon   = 11.9     # default 11.7[1] }
```

Top metal

SiO_2

Bulk-Si





BP metal

1.C Doping profile I – Reference Window

- (sdedr:define-refeval-window "BP_DopingRefWin" "Line" (position 0 Diode_thickness 0) (position Diode_width Diode_thickness 0))

- (sdedr:define-refeval-window "Top_DopingRefWin" "Line" (position 0 0 0) (position Diode_width 0 0))

1.C Doping profile
II – Profile definition

- (sdedr:define-constant-profile "BulkDopingProfile" "BoronActiveConcentration" concentration_bulk)

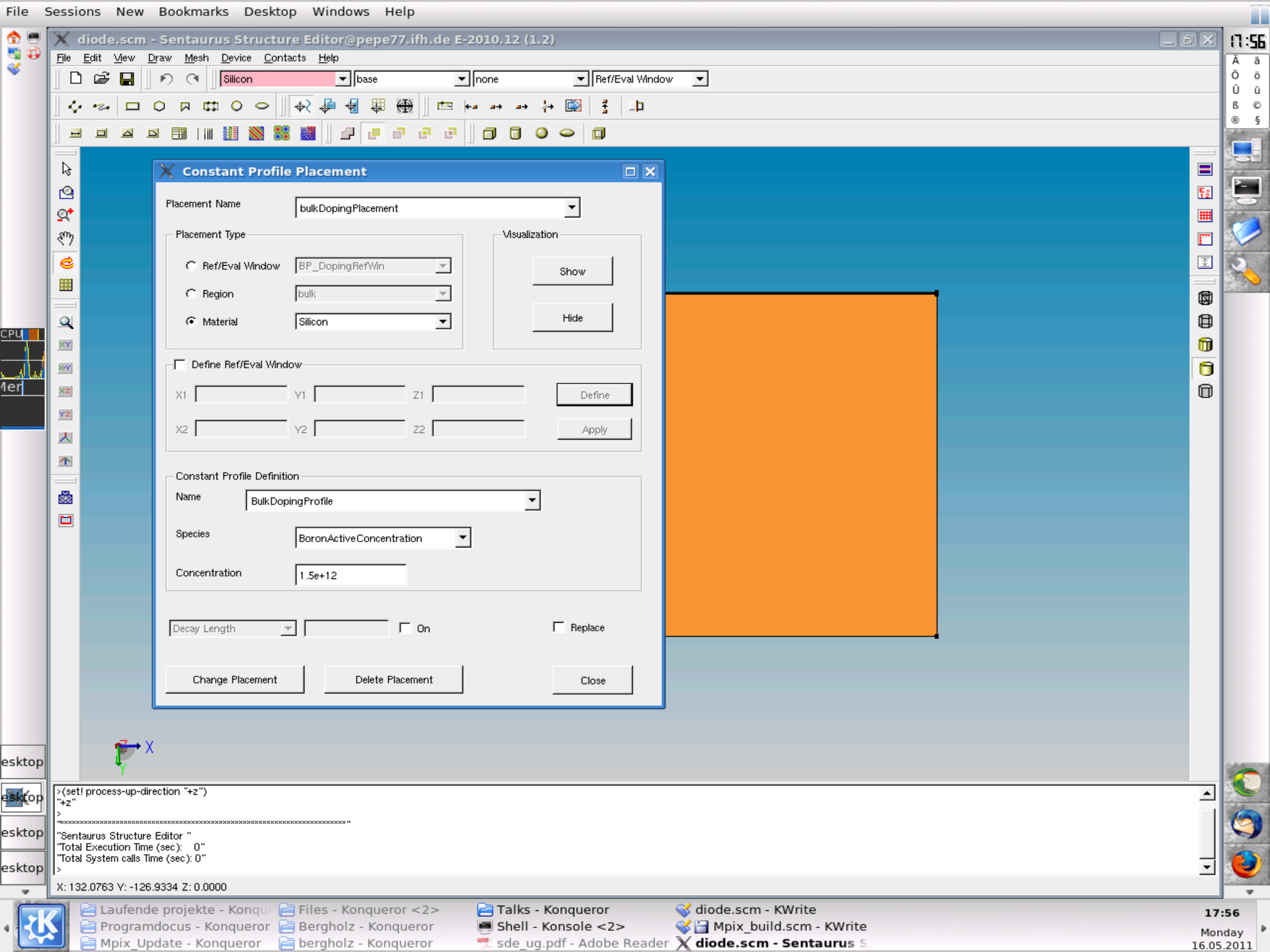
- (sdedr:define-gaussian-profile "BPDopingProfile" "BoronActiveConcentration" "PeakPos" 0 "PeakVal" concentration_BP "ValueAtDepth" concentration_bulk "Depth" Doping_thickness_BP "Gauss" "Factor" 0.5)

- (sdedr:define-gaussian-profile "TopDopingProfile" "PhosphorusActiveConcentration" "PeakPos" 0 "PeakVal" concentration_implant "ValueAtDepth" concentration_bulk "Depth" Doping_thickness_implant"Gauss" "Factor" 0.5)

1.C Doping profile
III – Create the profile

- (sdedr:define-constant-profile-material "bulkDopingPlacement" "BulkDopingProfile" "Silicon")
- (sdedr:define-analytical-profile-placement "BPDopingPlacement" "BPDopingProfile" "BP_DopingRefWin" "Both" "NoReplace" "Eval")

- (sdedr:define-analytical-profile-placement "TopDopingPlacement" "TopDopingProfile" "Top_DopingRefWin" "Both" "NoReplace" "Eval")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Silicon
base
none
Ref/Eval Window
Constant Profile Placement
Placement Name
bulkDopingPlacement
Placement Type
Ref/Eval Window
BP_DopingRefWin
Region
bulk
Material
Silicon
Visualization
Show
Hide
Define Ref/Eval Window
X1
Y1
Z1
Define
X2
Y2
Z2
Apply
Constant Profile Definition
Name
BulkDopingProfile
Species
BoronActiveConcentration
Concentration
1.5e+12
Decay Length
On
Replace
Change Placement
Delete Placement
Close
>(set! process-up-direction "+z")
"+z"
"Sentaurus Structure Editor "
"Total Execution Time (sec): 0"
"Total System calls Time (sec): 0"
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1.D Meshing
I – Reference window

- (sdedr:define-refeval-window “surfaceRefinementPlacement" "Rectangle" (position 0 0 0) (position Diode_width (* thickness_implant 1.5) 0))

- (sdedr:define-refeval-window "overshutRefinementPlacement" "Rectangle" (position 0 0 0) (position Diode_width (* (+ Al_thickness Oxide_thickness) -1) 0))
- (sdedr:define-refeval-window "bulkRefinementPlacement" "Rectangle" (position 0 (* thickness_implant 1.5) 0) (position Diode_width (- Diode_thickness (* thickness_BPimplant 1.5)) 0))
- (sdedr:define-refeval-window "BPRefinementPlacement" "Rectangle" (position 0 (- Diode_thickness (* thickness_BPimplant 1.5)) 0) (position Diode_width (+ Diode_thickness Al_thickness) 0))

1.D Meshing
II – Refinement

- (sdedr:define-refinement-size "surfaceRefinementSize" (/ Diode_width 200) (/ Doping_thickness_implant 20) (/ Diode_width 2000) (/ Doping_thickness_implant 200))

- (sdedr:define-refinement-size "overshutRefinementSize" (/ Diode_width 20) (/ Oxide_thickness 2) (/ Diode_width 200) (/ Oxide_thickness 10))
- (sdedr:define-refinement-size "BulkRefinementSize" (/ Diode_width 10) (/ Diode_thicknes 20) (/ Diode_width 200) (/ Diode_thicknesr 100))
- (sdedr:define-refinement-size "BPRefinementSize" (/ Diode_width 50) (/ Doping_thickness_BP 10) (/ Diode_width 250) (/ Doping_thickness_BP 100))

1.D Meshing
III – Refinement function

- (sdedr:define-refinement-function "surfaceRefinementSize" "DopingConcentration" "MaxGradient" 1)

- (sdedr:define-refinement-function "overshutRefinementSize" "DopingConcentration" "MaxGradient" 1
- (sdedr:define-refinement-function "BulkRefinementSize" "DopingConcentration" "MaxGradient" 1)
- (sdedr:define-refinement-function "BPRefinementSize" "DopingConcentration" "MaxGradient" 1)

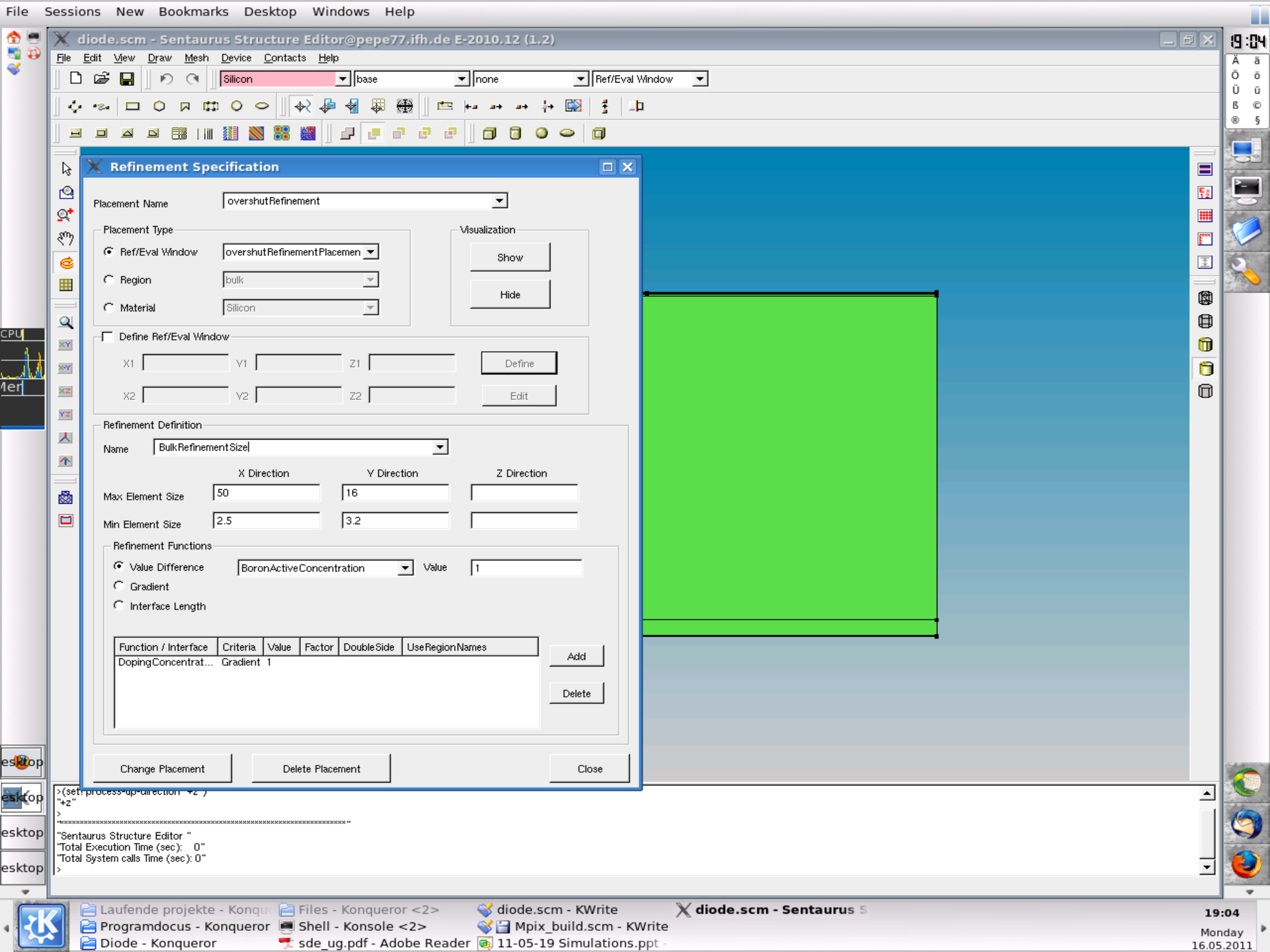
1.D Meshing
IV – Build the Refinement

```
(sdedr:define-refinement-placement "surfaceRefinement"
    "surfaceRefinementSize"
    "surfaceRefinementPlacement"
```

```
(sdedr:define-refinement-placement "overshutRefinement" "overshutRefinementSize"
    "overshutRefinementPlacement")

 sdedr:define-refinement-placement "bulkRefinement" "BulkRefinementSize"
    "bulkRefinementPlacement")

(sdedr:define-refinement-placement "BPRefinement" "BPRefinementSize"
    "BPRefinementPlacement")
```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Silicon
base
none
Ref/Eval Window
Refinement Specification
Placement Name
overshutRefinement
Placement Type
Ref/Eval Window
overshutRefinementPlacemen
Region
bulk
Material
Silicon
Visualization
Show
Hide
Define Ref/Eval Window
X1
Y1
Z1
X2
Y2
Z2
Define
Edit
Refinement Definition
Name
BulkRefinementSize
X Direction
Y Direction
Z Direction
Max Element Size
50
16
Min Element Size
2.5
3.2
Refinement Functions
Value Difference
BoronActiveConcentration
Value
1
Gradient
Interface Length
Function / Interface
Criteria
Value
Factor
DoubleSide
UseRegionNames
DopingConcentrat...
Gradient
1
Add
Delete
Change Placement
Delete Placement
Close
"+z"
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"Total System calls Time (sec): 0"
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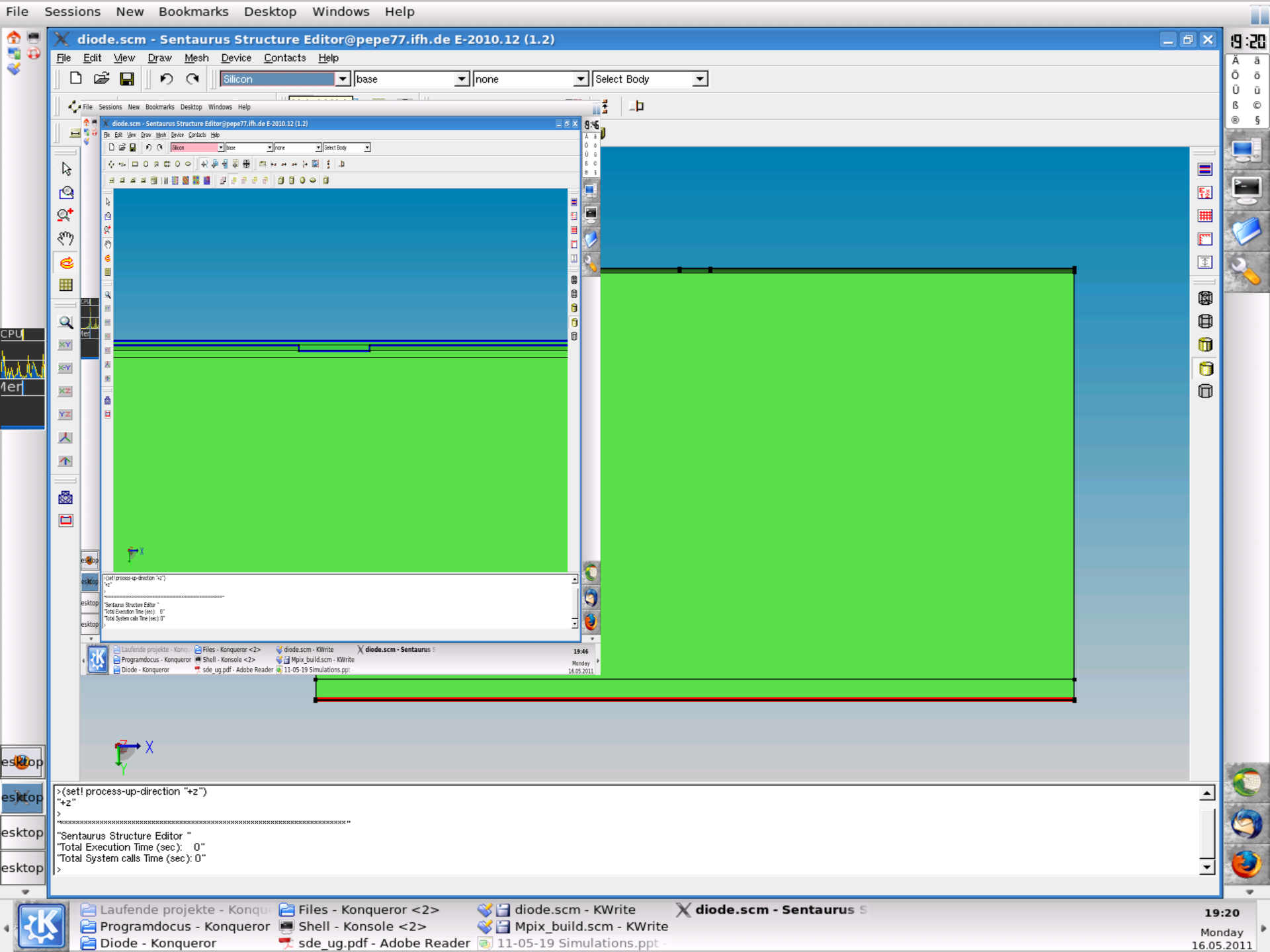
1.E Contact definition

- (sdegeo:define-contact-set "BPContact" (color:rgb 1 0 0) "##")

- (sdegeo:define-2d-contact (list (car (find-edge-id (position (/ Diode_width 2) Diode_thickness 0))) (car (find-edge-id (position 0 (+ Diode_thickness (/ Al_thickness 2)) 0))) (car (find-edge-id (position Diode_width (+ Diode_thickness (/ Al_thickness 2)) 0))) (car (find-edge-id (position (/ Diode_width 2) (+ Diode_thickness Al_thickness) 0)))) "BPContact")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diode.scm - Sentaurus Structure Editor@pepe77.ifh.de E-2010.12 (1.2)
File Edit View Draw Mesh Device Contacts Help
Silicon
base
none
Select Body
>(set! process-up-direction "+z")
"+z"
>
"Sentaurus Structure Editor "
"Total Execution Time (sec): 0"
"Total System calls Time (sec): 0"
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Programdocus - Konqueror
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diode.scm - KWrite
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11-05-19 Simulations.ppt
diode.scm - Sentaurus
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Monday
16.05.2011

Starting with mesh building

- Additional Options
  - (sde:save-model "/afs/ifh.de/group/cms/bergholz/daten/TCAD/Diode/diodeModel")
  - (sde:build-mesh "snmesh" "-a -c boxmethod" "/afs/ifh.de/group/cms/bergholz/daten/TCAD/Diode/diodeMesh")
- **sde -e -l SchemeFile.scm**

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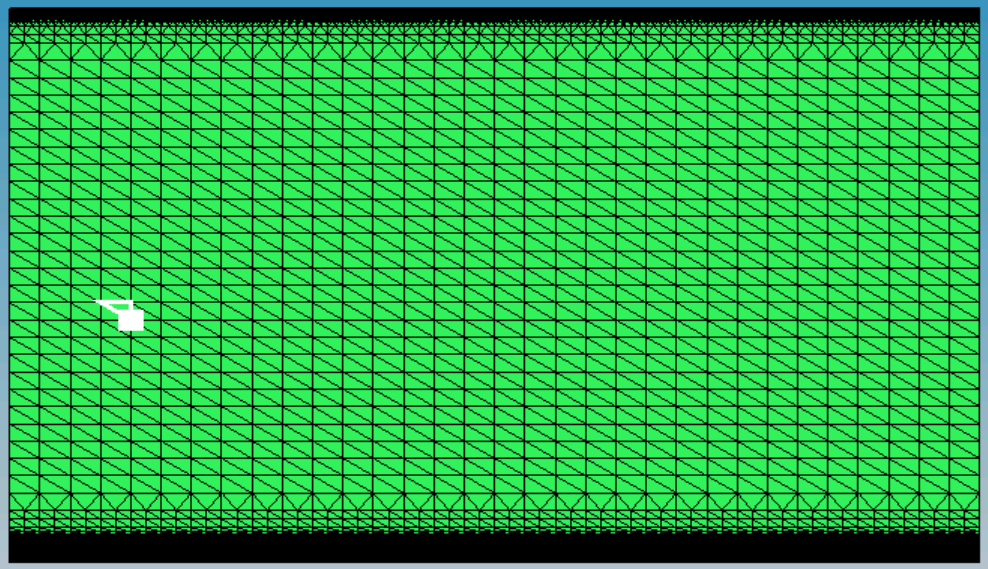
File Edit View Draw Mesh Device Contacts Help

Silicon | base | none | Select Body



```
>(sdedr:append-cmd-file "")
#t
>(sde:build-mesh "snmesh" "-a -c boxmethod" "sdemodel")
Duplicate region/contact names were changed

"Meshing successful"
#t
>
```

2. Simulation

- The input file for the device simulation consists of
  - An input and output file definition
  - An Electrode definition
  - A definition of the used physical models
  - Plot and math selections
  - Spice transformation for capacitance
  - Simulation order 'Voltage ramps'

2.A File input and contacts

- File { * input files
- Grid = "DiodeMesh_msh.tdr"
- Doping = "DiodeMesh_msh.tdr"
- Parameter = "Silicon.par" ← ε,τ
- * output file
- Current = "Diode_des.plt"}

- Electrode {
- {Name = "BPContact" voltage = 0.0 Material = "Aluminum" }
- {Name = "TopContact" voltage = 0.0 Material = "Aluminum" }}
  - Name must be the same than in model!
  - “Barrier=-0.55”

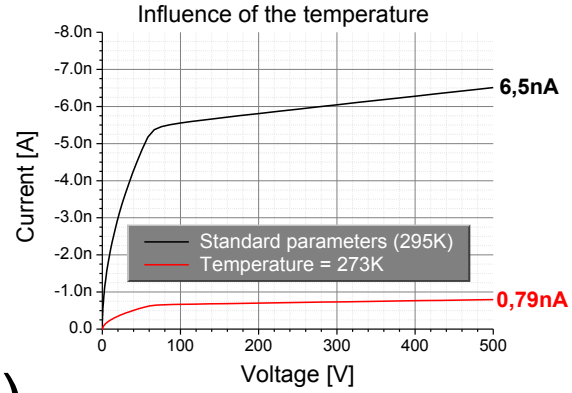
2. B “Standard” physical models

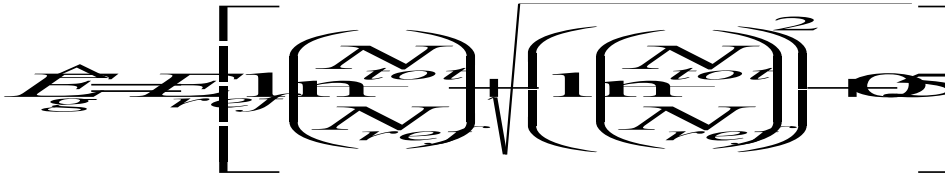
Physics {

Temperature = 295

Fermi #Using Fermi Statistic

EffectiveIntrinsicDensity
(BandGapNarrowining(Slotboom))





2.B Mobility models

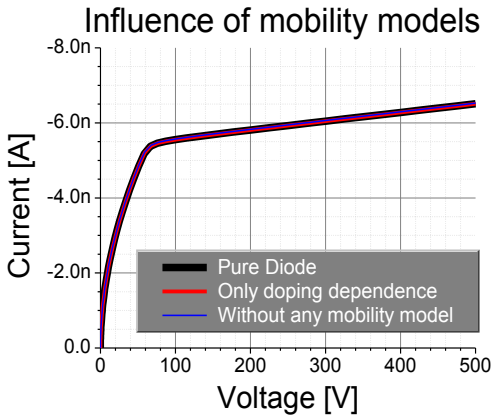
- Mobility (

  DopingDependence

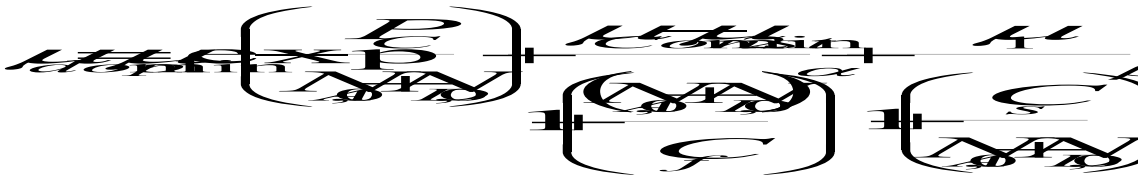
  (HighFieldSaturation)

  CarrierCarrierScattering (ConwellWeisskopf)

  Enormal)

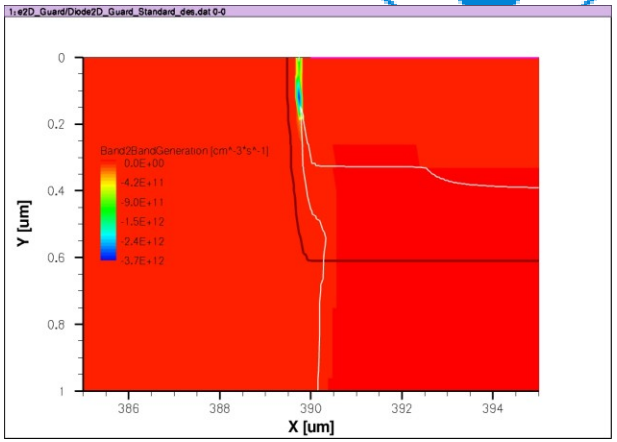


Masetti model



Conwell-Weisskopf-Model

2.B Recombination models



- Recombination (

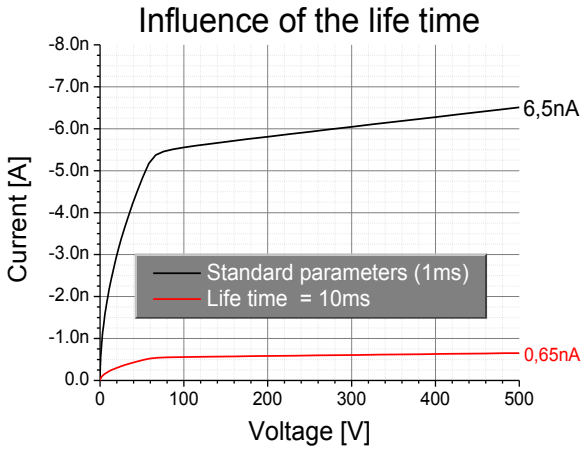
  SRH (DopingDependence TempDependence

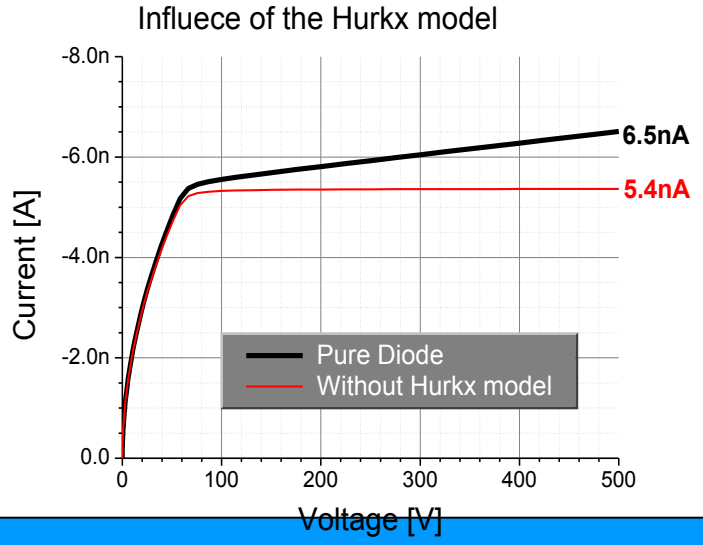
  ElectricField (Lifetime=Hurkx))

  Auger

  eAvalanche (vanOverstraeten) hAvalanche (vanOverstraeten)

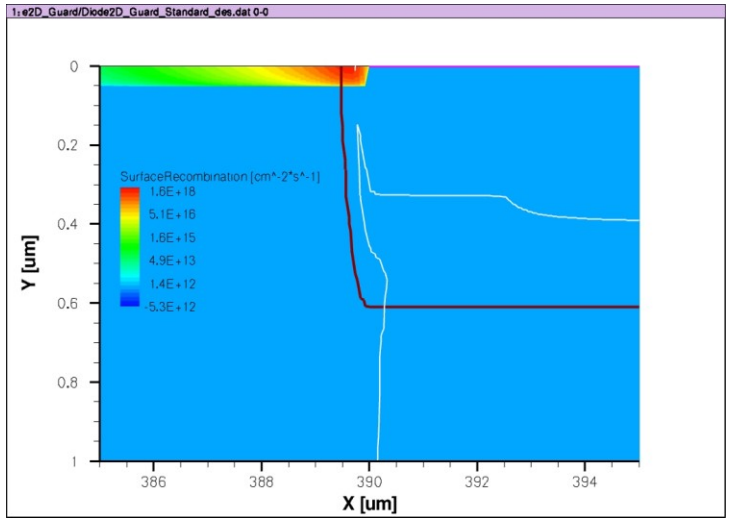
  Band2Band(Hurkx))}

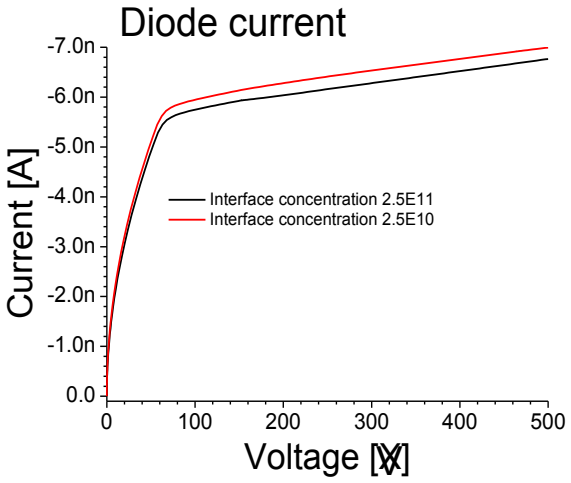


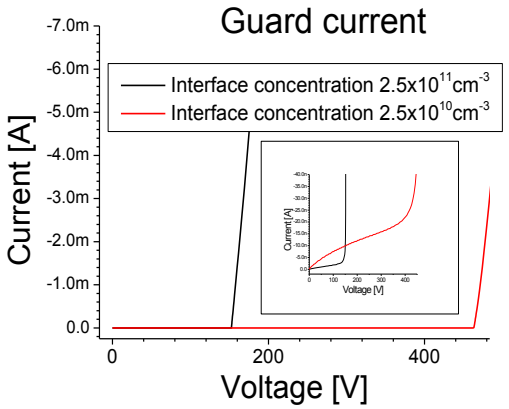


2.B Material Interface

- Physics (MaterialInterface="Silicon/Oxide") {Charge(Conc=1.1e10) Recombination(surfaceSRH)}







2.C Plot selection

- Plot{

  eDensity hDensity eMobility hMobility

  ElectricField/Vector Potential SpaceCharge

*--Generation/Recombination

  SRH Band2Band Auger SurfaceRecombination

  eLifetime hLifetime

* -Driving forces

  eEparallel hEparallel eENormal hENormal

  BandGap BandGapNarrowing}

2.D Math selection

- Math {

  Method = pardiso

  ACMethod = Blocked

  Number_of_Threads = 4

  Derivatives

  RelErrControl

  Iterations = 25}

2.E Spice transformation

- System {

  Diode trans (BPContact=a TopContact=b)

  Vsource_pset vBP (a 0) {dc=0}

  Vsource_pset vTop (b 0) {dc=0}}

Solve

- Solve {

  #-a) Initial

  Poisson

  Coupled { Poisson Electron Hole }

  #-b) ramp IV

  QuasiStationary (

  InitialStep=1e-6 Minstep=1e-10 MaxStep=2e-3

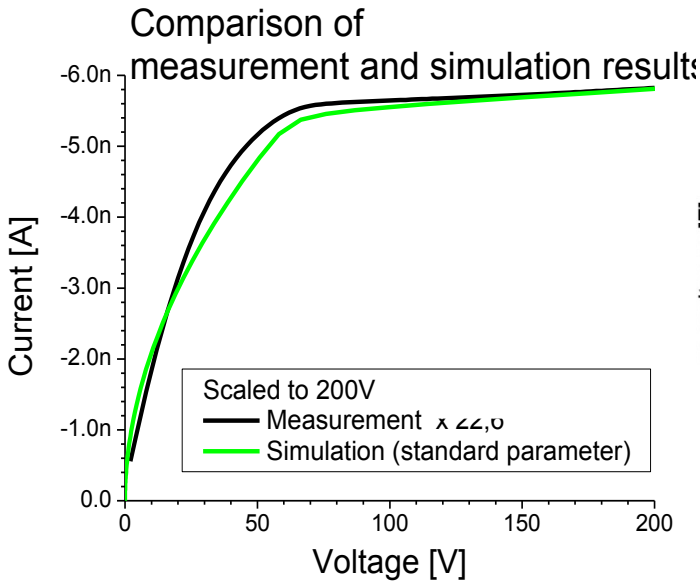
  Increment=1.25 Decrement=4

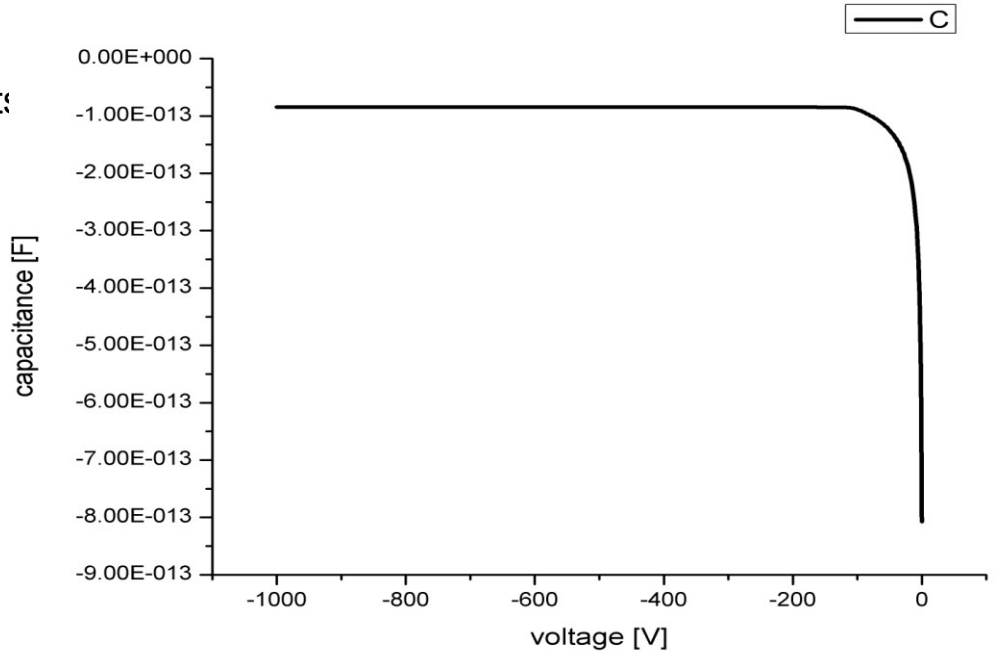
  Goal { parameter =vBP.dc voltage = -1000 })

- #-c) ramp CV

{ACCoupled (
StartFrequency=1e6 EndFrequency=1e6
NumberOfPoints=1 Decade
Node(a b) Exclude(vTop vBP))
{ Poisson Electron Hole }}}

Results


Comparison of
measurement and simulation results
Current [A]
-6.0n
-5.0n
-4.0n
-3.0n
-2.0n
-1.0n
0.0
0
50
100
150
200
Voltage [V]
Scaled to 200V
Measurement x 22,6
Simulation (standard parameter)


C
capacitance [F]
0.00E+000
-1.00E-013
-2.00E-013
-3.00E-013
-4.00E-013
-5.00E-013
-6.00E-013
-7.00E-013
-8.00E-013
-9.00E-013
-1000
-800
-600
-400
-200
0
voltage [V]

	Peak value	Additional Information
Silicon		
Epsilon	1.19E+01	
lifetime[ms]	4	
Poly-Silicon		
Thickness[um]	5	(Mpix)
Oxide		
Oxide charge	1.5	
Charge [cm-3]	1.00E+10	
Metal (Al)		
thickness [um]	1	
Contact barrier	-0.55?	
Doping		
bulk-Doping [cm-3]	1.50E+12	
Pad-Doping [cm-3]	1.00E+19	Gauss, Faktor 0.5
Top-doping thickness[um	1.20E+00	
Backplan-doping[cm-3]	1.00E+19	
Backplane-thickness[um]	1.00E+02	
P-Stop [cm-3]	1.00E+16	???
p-Stop thickness	1	???
p-Stop Width	4	
p-Spray [cm-3]	How ???	
p-Spray thickness	to ???	
p-Spray width	implement ???	

Used Parameters

Conclusions

- TCAD Software is a strong and power full tool for device simulation
- BUT the quality of the output strongly depends of the knowledge of the physical properties of the simulated device

Appendix

Parameter	Electrons	Holes
μ_1	43,4cm^2/Vs	29cm^2/Vs
μ_{min1}	52,2cm^2/Vs	44,9cm^2/Vs
μ_{min2}	52,2cm^2/Vs	0
P_c	0	9,23*10^{16}cm^{-3}
C_f	9,68*10^{16}cm^{-3}	2,23*10^{17}cm^{-3}
Cs	3,43*10^{20}cm^{-3}	6,1*10^{20}cm^{-3}
α	0,68	0,719
β	2	2