TCAD Simulations: Applications at FBK

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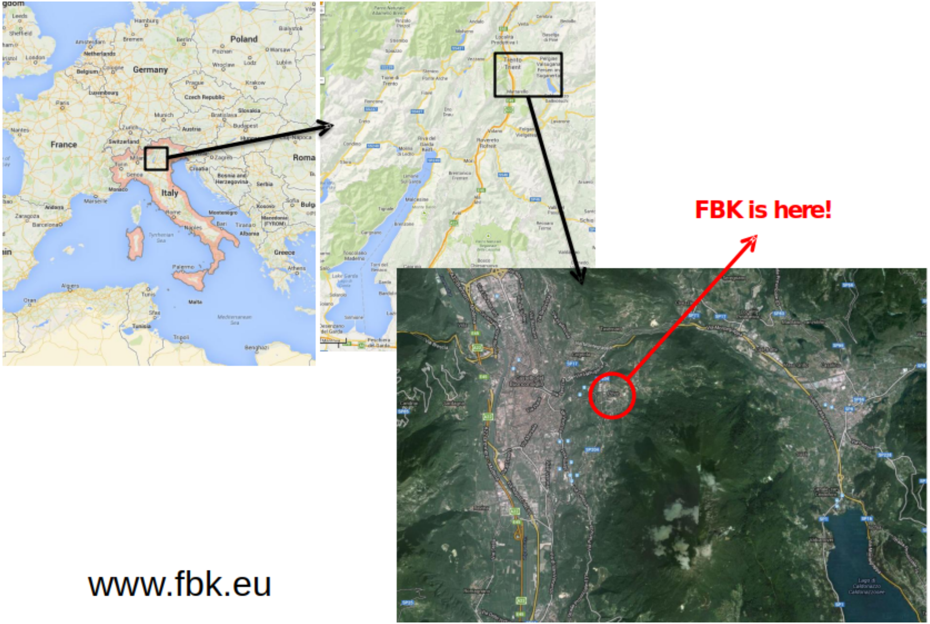
Fondazione Bruno Kessler


FBK is here!
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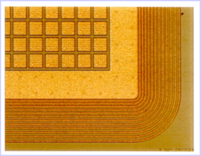
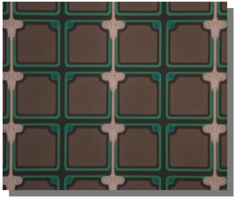
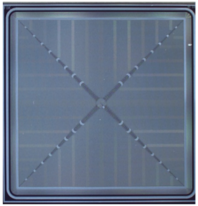
Silicon Detector Technology at FBK



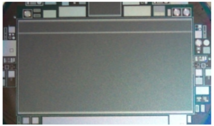
Pixel



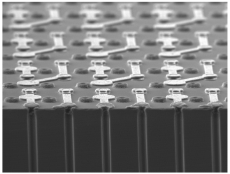
Silicon Photomultipliers



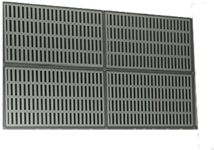
Silicon Drift Detectors



Single and Double Side Microstrip



3D-detectors



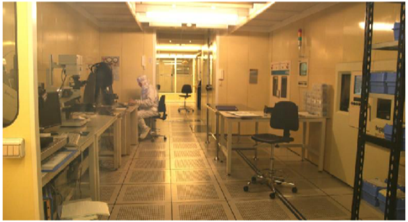
LGAD

Micro Nano Facility

Two separate clean rooms

- 500m^2 of clean room (class 10-100)
- 200m^2 of clean area (class 100-1000) equipped for MEMS technology

6-inch wafers (Si, Quartz, Glass) – 0.35 um processing

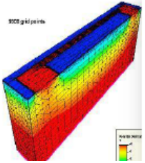


- Dry/wet oxidation
- sputtering Metallization
- Diffusion
- LPCVD
- PECVD
- Projection lithography: CD 2μm
- Stepping lithography: CD 350nm
- Ion Implantation
- Dry/wet etching

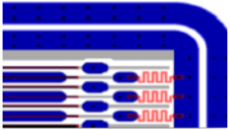
Where does Simulation Fit?

New device concept

TCAD simulation (proof of concept)



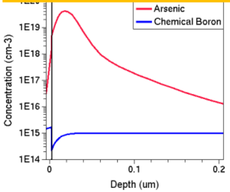
Design



Microfabrication

Testing

Simulation tuning & validation



Why TCAD Simulations?

Powerful tool

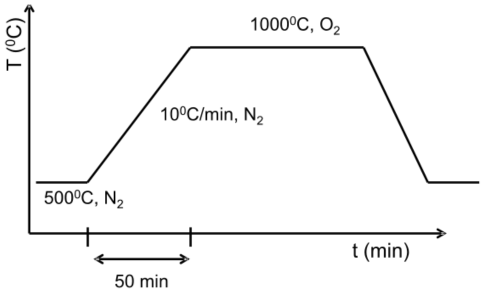
- Design optimization of the device
- Problem solving
- Understanding of the device physics

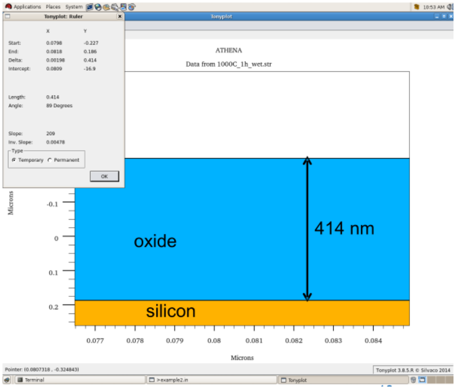
Simulating sensors

- Avoid trivial errors and mistakes
- Reduce the number of splits and iterations during fabrication
  $\Rightarrow$ **save time & money**

Process Simulation Example 1: Oxidation

...well known process, TCAD not strictly required...






```
#
diffus time=50 temp=500 t.final=1000 nitro
#
diffus time=120 temp=1000 dryo2
```

Problem: n-type wafers ($\approx 10^{12}\text{cm}^{-3}$) sometimes behave as p-type after oxidation

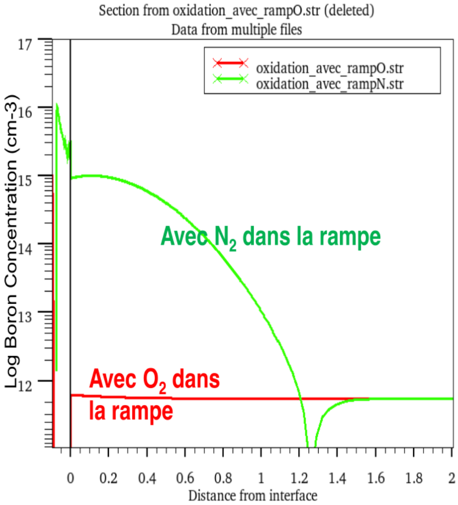
Process Simulation Example 1: Oxidation

Hypothesis test: Boron contamination in the furnace (less than 1 ppm)

```
#
diffus time=50 temp=500 t.final=1000 nitro\
       c.boron=1.0e16
#
diffus time=120 temp=1000 dryo2
```

Test solution: oxidate during ramp
⇒ diffusion barrier

```
#
diffus time=50 temp=500 t.final=1000 dryo2\
       c.boron=1.0e16
#
diffus time=120 temp=1000 dryo2
```



Process Simulation Example 2: Trench Oxidation & LOCOS

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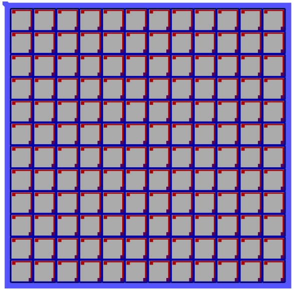
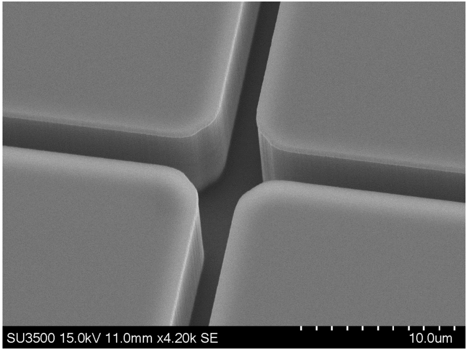
Silicon Photomultipiers (SiPM)

- Light detection with single photon sensitivity
- Array of single photon avalanche diodes (SPAD) connected in parallel
- Geiger mode operation
- Trench isolation to avoid optical cross talk



Trenches between SPAD cells
width < 1 μm, aspect ratio > 5

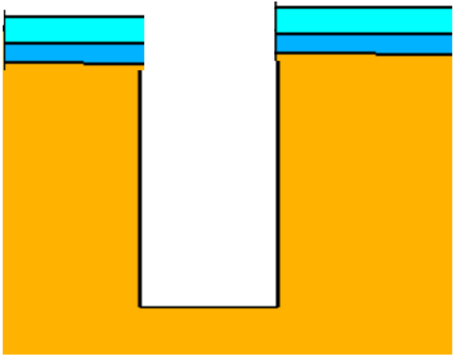


These will be filled with oxide (oxidation + deposition)

Process Simulation Example 2: Trench Oxidation & LOCOS

Trench oxidation:
ideally oxidate only the inside of the trench
$\Rightarrow$ put nitride as diffusion barrier

```
deposit oxide thick=0.02 dy=0.001
deposit nitride thick=0.03 dy=0.001
etch nitride  start x=2.2 y=-0.05
etch cont x=2.8 y=-0.05
etch cont x=2.8 y=0
etch done x=2.2 y=0
etch oxide  start x=2.2 y=-0.05
etch cont x=2.8 y=-0.05
etch cont x=2.8 y=0
etch done x=2.2 y=0
etch silicon  start x=2.2 y=0
etch cont x=2.8 y=0
etch cont x=2.8 y=3
etch done x=2.2 y=3
```



Oxidation in only in some regions:
LOCOS $\rightarrow$ LOCal Oxidation of Silicon

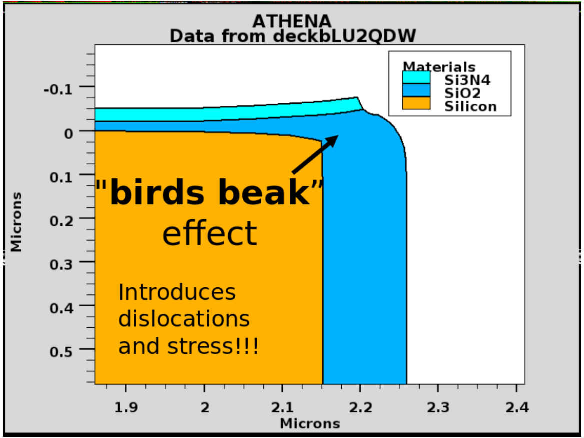
Process Simulation Example 2: Trench Oxidation & LOCOS

Trench oxidation:

```
diffus time=150 temp=1000 dry
```

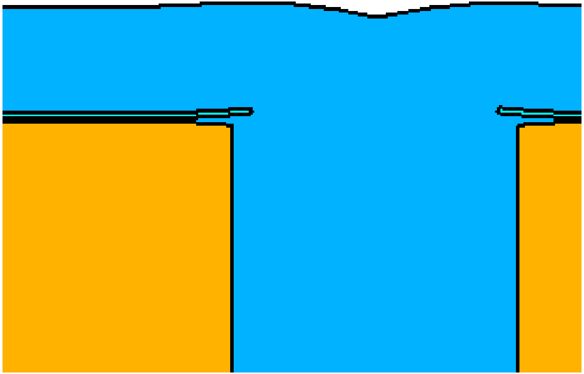
- Beak height depends on initial oxide and nitride thickness
- Higher beak $\Rightarrow$ higher stress and dislocations
  $\Rightarrow$ worse device performance

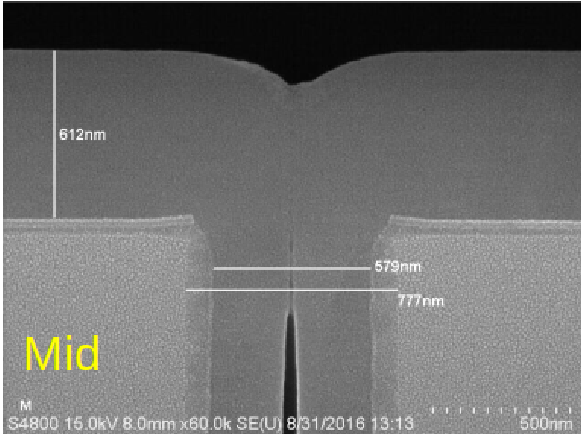
Optimize!



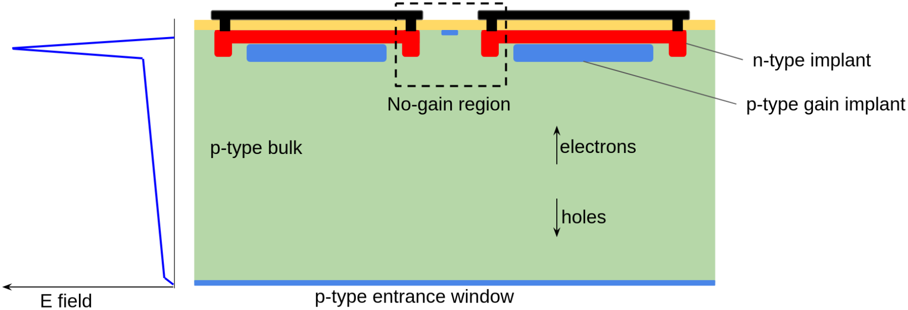
Process Simulation Example 2: Trench Oxidation & LOCOS

Deposit more oxide





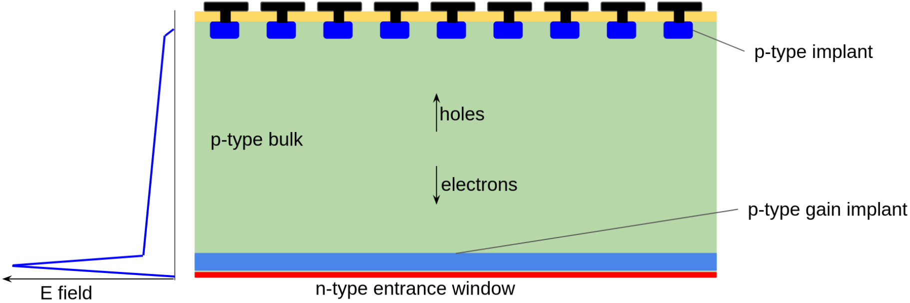
Low Gain Avalanche Detectors



- Silicon detectors with charge multiplication
- Gain ≈ 10
- Gain layer provides high-field region
- Junction Termination Extension improves stability

- **Improve SNR of the system**
  (When the sensor shot noise is not dominating)
- Noise and power consumption
  $\Rightarrow$ low gain

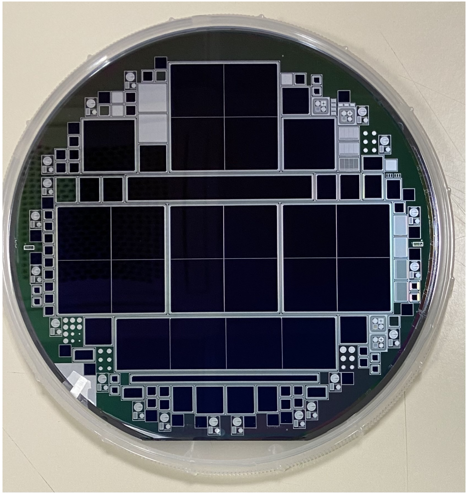
Double Sided LGADs



- Continuous gain area in the active region $\Rightarrow$ 100% fill factor
- Double sided process
- Active thickness is the wafer thickness
- Readout side is ohmic
- Design not optimal for timing applications
- Readout side separated from LGAD side $\Rightarrow$ no restrictions on channel dimensions

[G.F. Dalla Betta et al. NIM A 796 (2015) 154]

Double Sided LGADs for X-rays



- Produced double sided LGADs dedicated to x-rays
- Several strip and pixel sensors geometries
- Different gain structure designs

Two examples: strip sensors signal, gain structure optimization

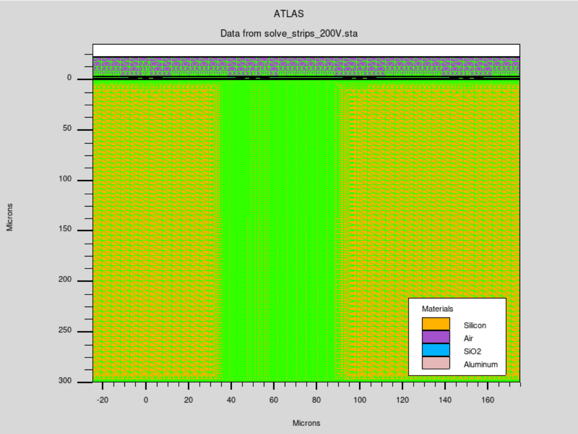
Double Sided LGAD Strip Signals

Aim: determine signal shape and duration at different positions

- Make structure with 4 strips
- Bias it to 200 V
- Generate carriers using photogeneration
- Record signal on the strips
- Repeat at different positions

Two "parts" of the signal:

- Primary ionization
- Multiplication holes



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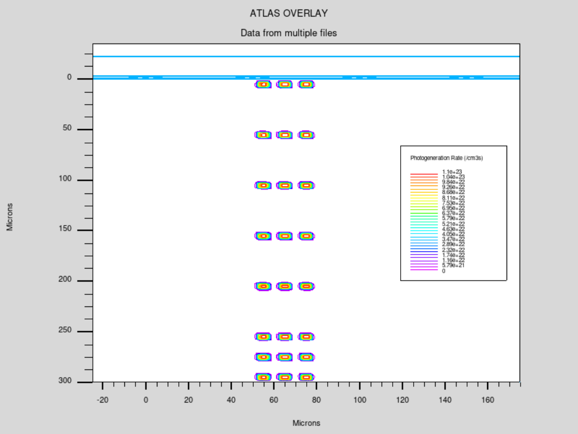
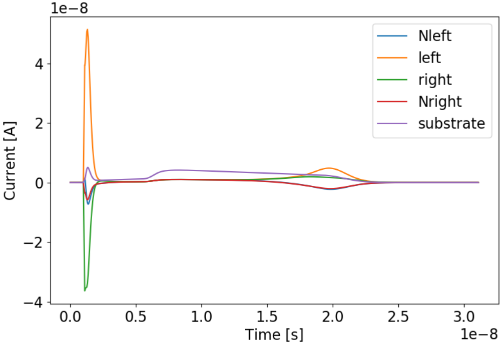


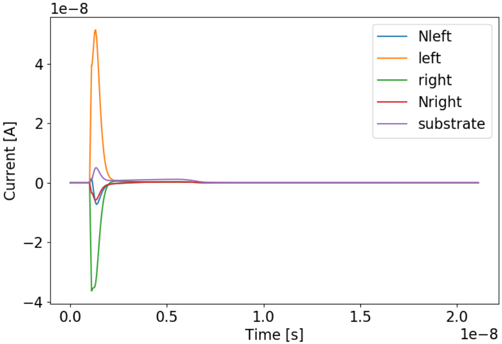
Double Sided LGAD Strip Signals

Photogeneration close to left strip, 200 V bias

Gain



Charge multiplication model turned off



- Same fields in both structures
- Shorter signals for sensor without gain
- With this it is possible to extract gain

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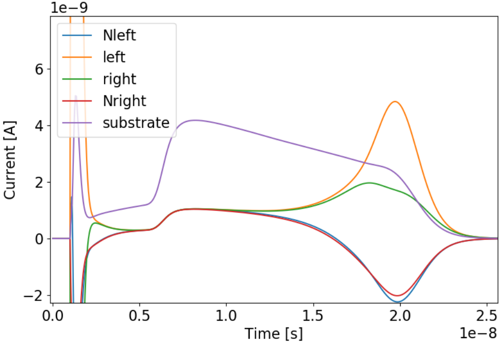
Gain



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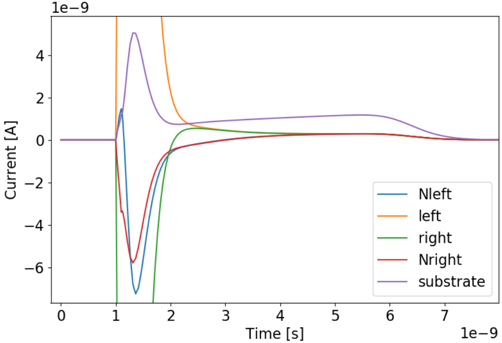

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- Shorter signals for sensor without gain
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Device Simulation Example: Signal in Strip Sensor

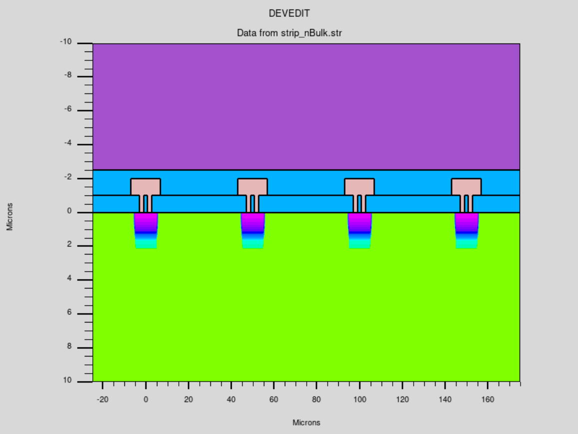
- n-type bulk strip sensor
- Built for didactics $\Rightarrow$ toy implants and geometry
- Similar idea (and code) as the double sided LGAD

Detector building (Devedit)

- make 1/2 strip, mesh and save structure
- load structure
- mirror
- mesh
- save structure
- repeat until 4 strips are present
- assign electrodes names to Al regions
- refine mesh for photogeneration
- save structure

Realistic implant profiles used when needed

Doping density



Preparation for device simulation (Atlas)

Always needed before starting:

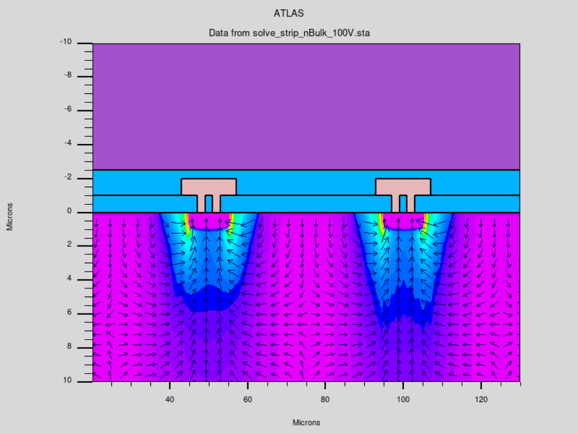
- load structure file
- define material properties (type of material, lifetimes)
- define physical models
- set all electrodes to 0V (neutral)
- define interface properties (charge and surface recombination velocities)

[suasnews]

Bias the detector (Atlas)

- preparation steps
- select output variables
- define numerical methods
- initialize the solution
- first bias points in small steps
  (bias applied to backside)
- ramp up the bias and save solution files for interesting values

E field 100V



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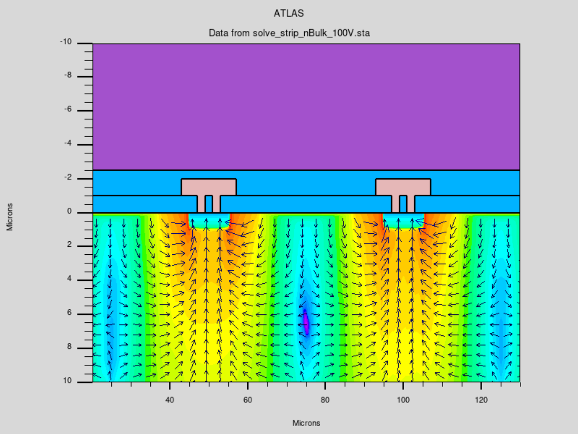
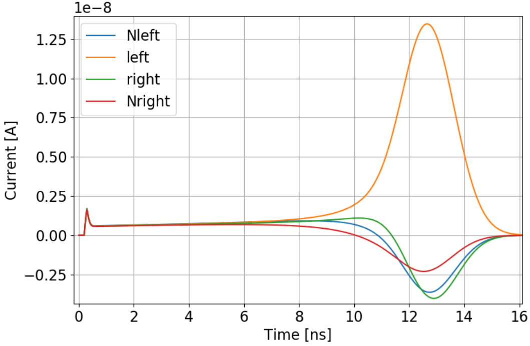
E field 100V log scale



Transient simulation (Atlas)

- preparation steps
- define numerical methods and specify maximum time interval (time discretization)
- load solution file for the bias point
- load photogeneration table
- start the transient simulation
- “flash the light” (beam on and off)
- run the simulation to capture the signal
- optional: save the solution files at various times

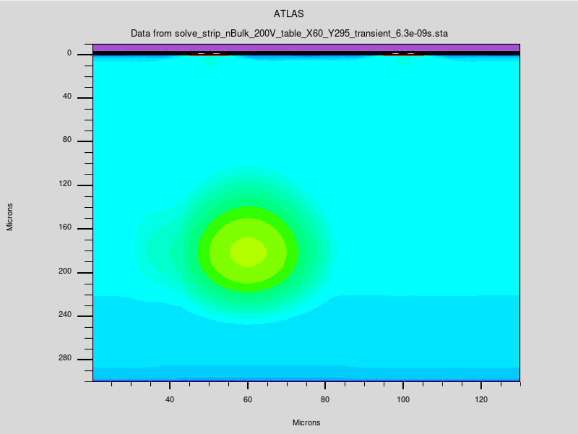
Charge injection close to backside (200V)



Strip Sensor Signals

What we will see:

- Concentration (log scale) of electrons and holes
- Drift
- Diffusion
- Signal current
- Effects of mesh
- Note: the signal start the moment the charge starts to move



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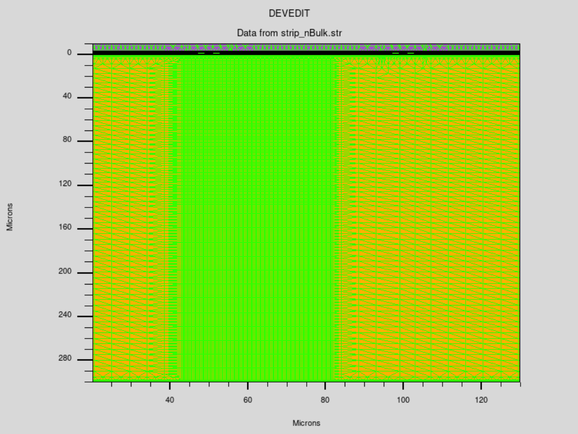
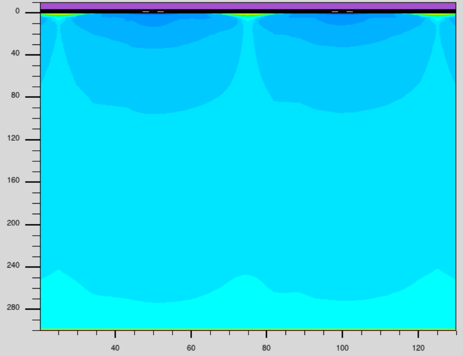


Strip Sensor Bottom Injection

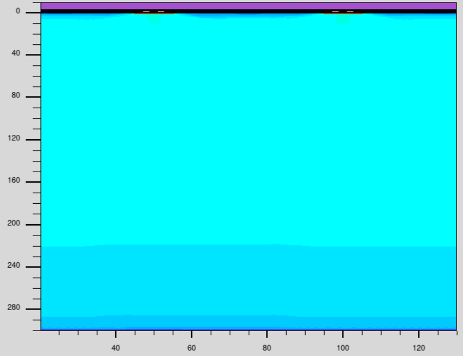
- Bias 200 V
- Charge generated in small volume $\rightarrow$ Similar to x-ray, or red TCT
- Charge deposit $\approx$ 275 eh-pairs $\rightarrow \approx$ 1 keV

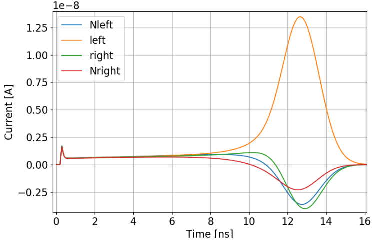
Time 0.2 ns

Electrons

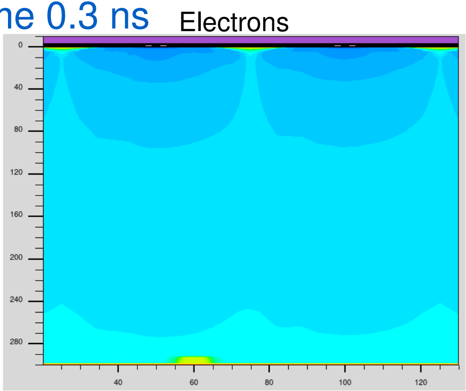


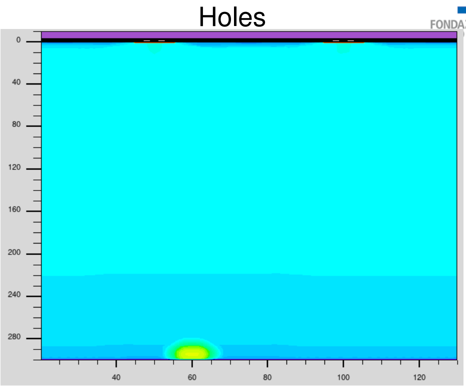
Holes

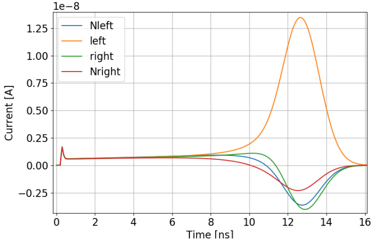




Time 0.3 ns

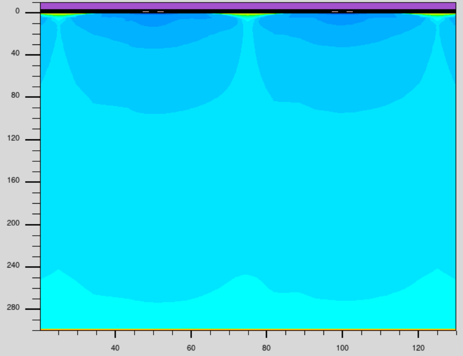

Electrons
0
40
80
120
160
200
240
280
40
60
80
100
120


Holes
0
40
80
120
160
200
240
280
40
60
80
100
120

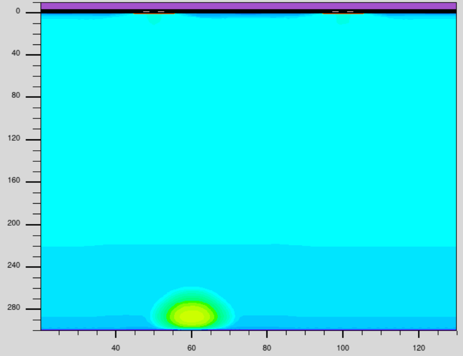

1e−8
Nleft
left
right
Nright
Current [A]
1.25
1.00
0.75
0.50
0.25
0.00
−0.25
0
2
4
6
8
10
12
14
16
Time [ns]

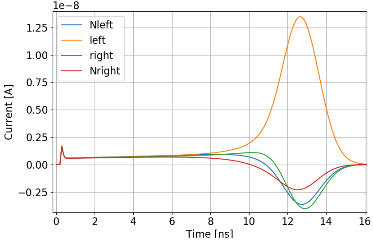
Time 0.8 ns

Electrons



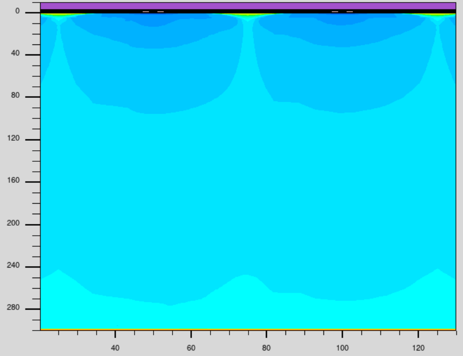
Holes



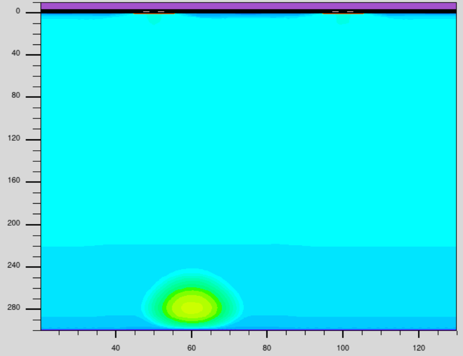


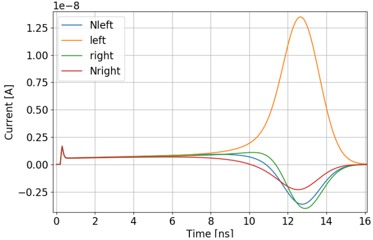
Time 1.3 ns

Electrons



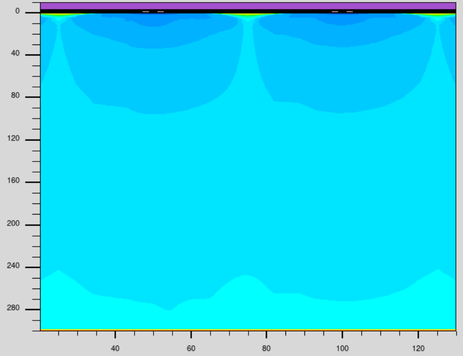
Holes



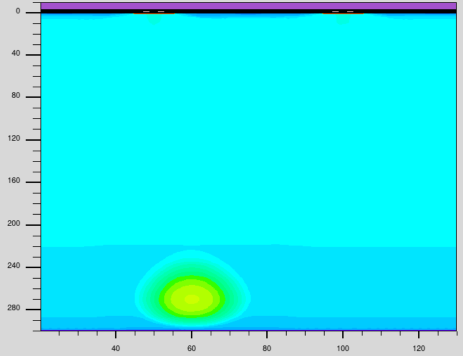


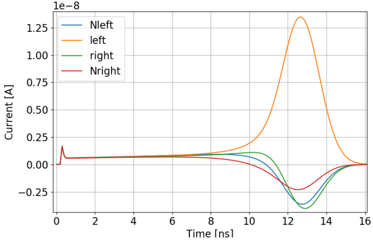
Time 1.8 ns

Electrons



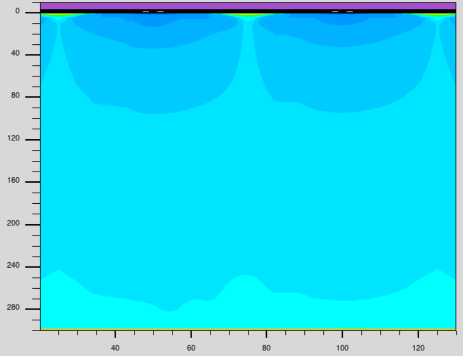
Holes



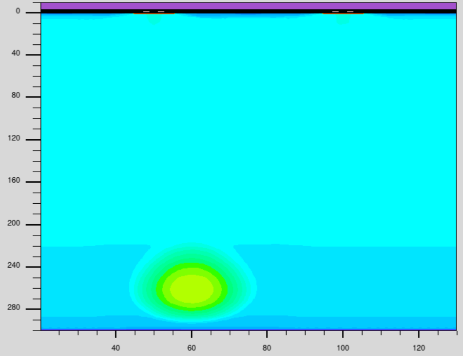


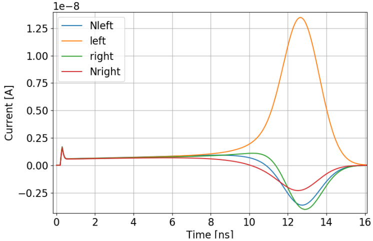
Time 2.3 ns

Electrons



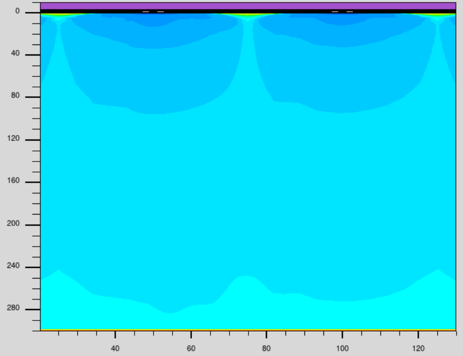
Holes



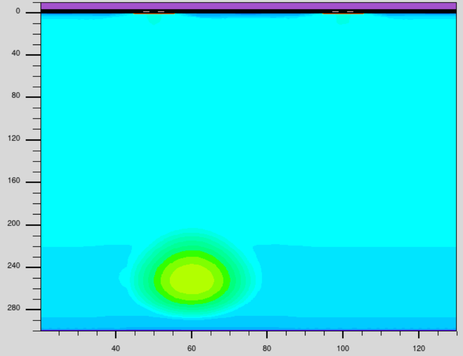


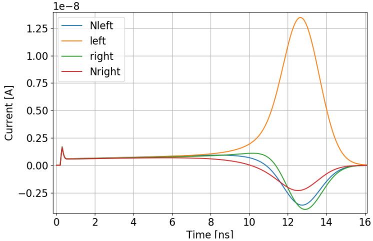
Time 2.8 ns

Electrons



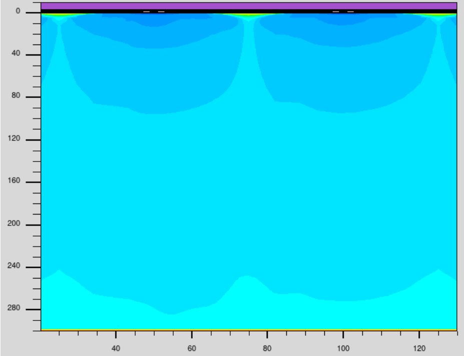
Holes



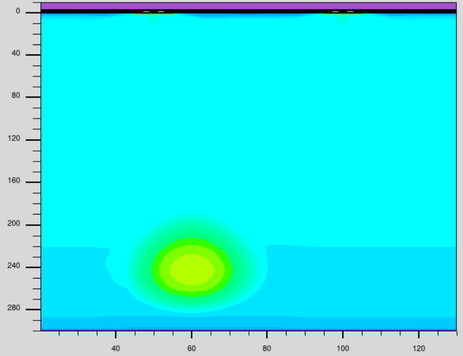


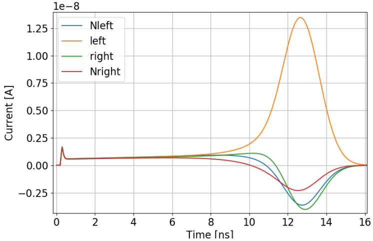
Time 3.3 ns

Electrons



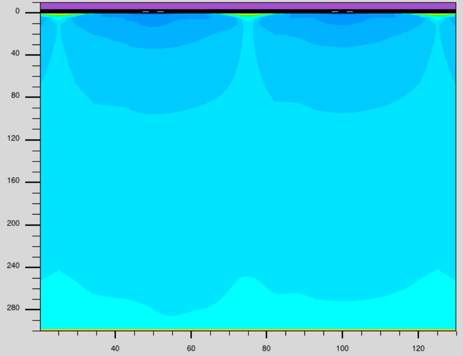
Holes



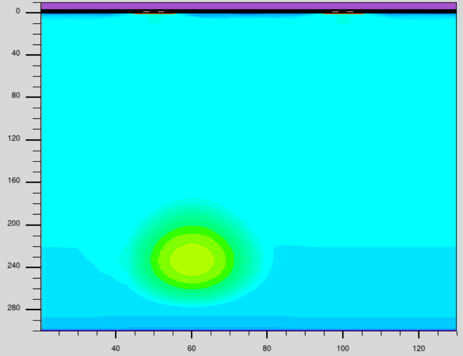


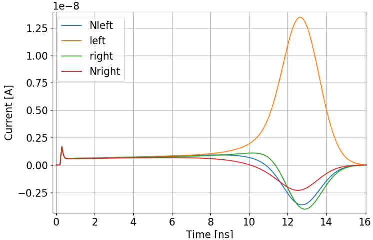
Time 3.8 ns

Electrons



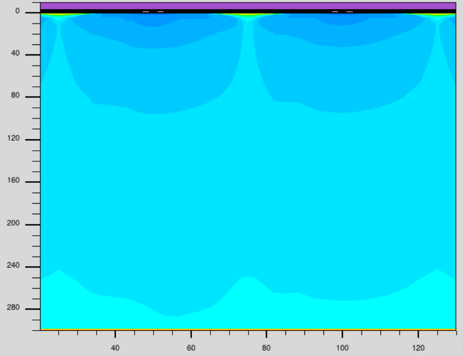
Holes



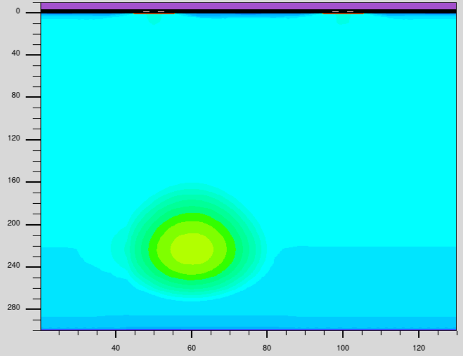


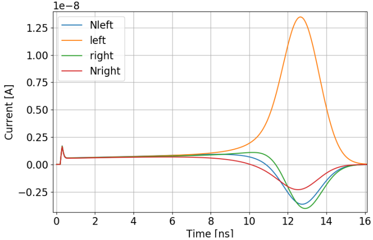
Time 4.3 ns

Electrons



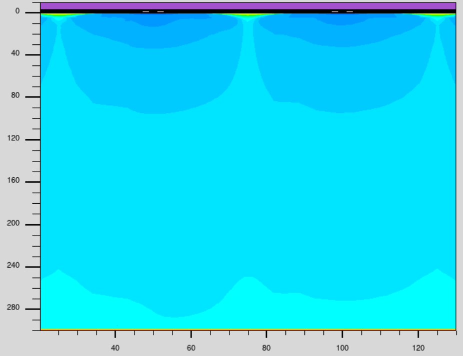
Holes





Time 4.8 ns

Electrons



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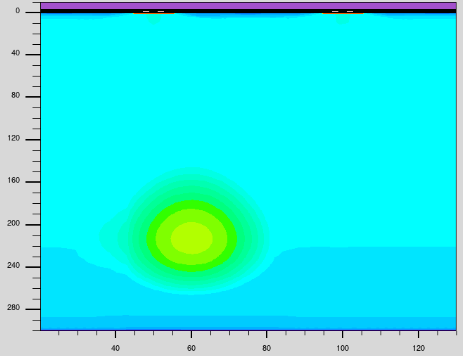
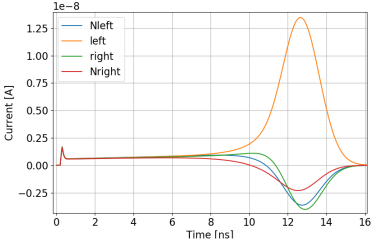
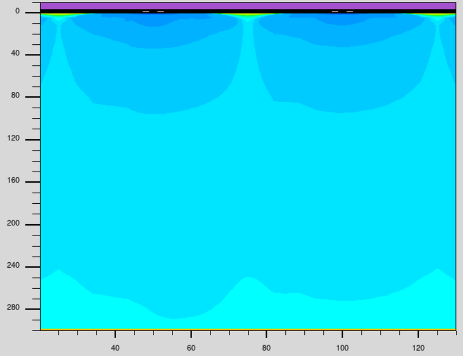




Time 5.3 ns

Electrons



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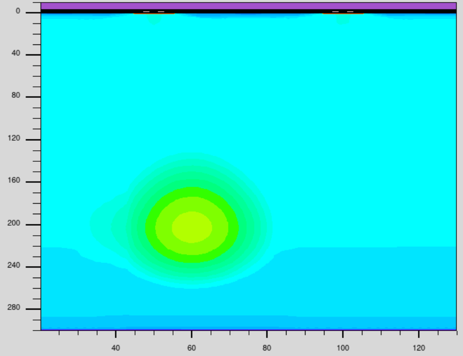
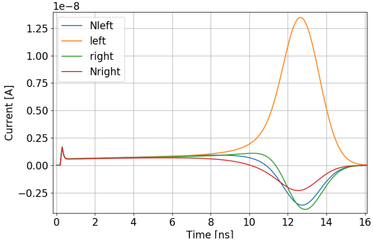
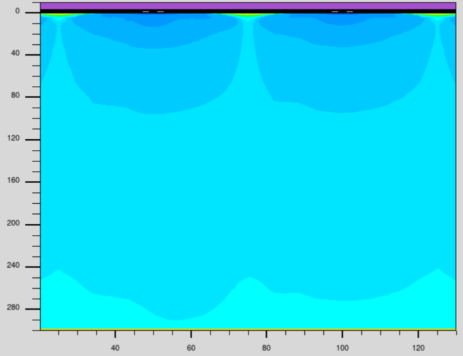




Time 5.8 ns

Electrons



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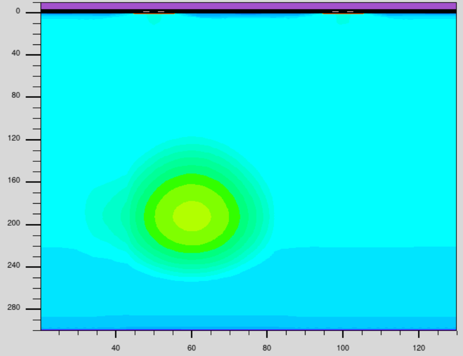
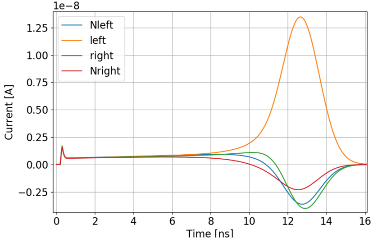
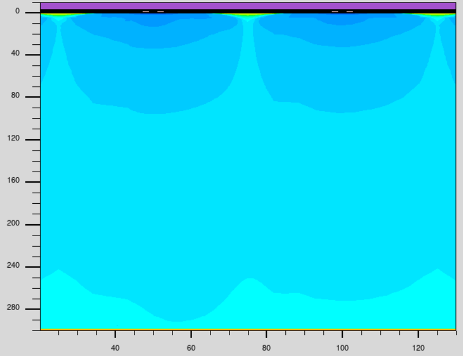


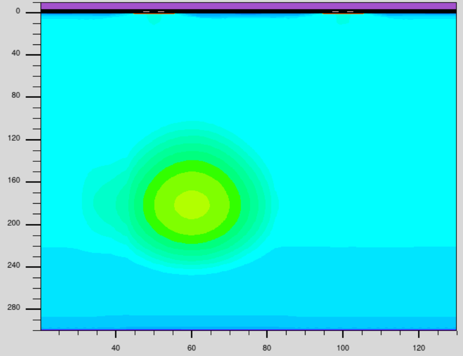


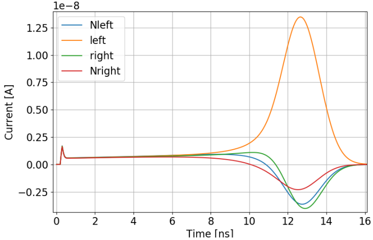
Time 6.3 ns

Electrons



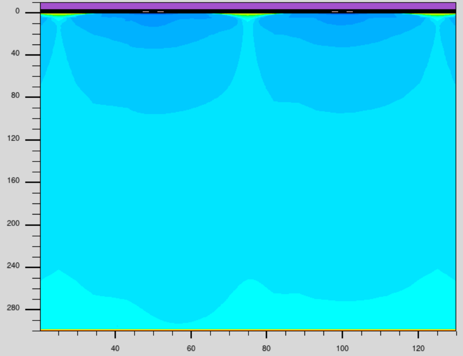
Holes



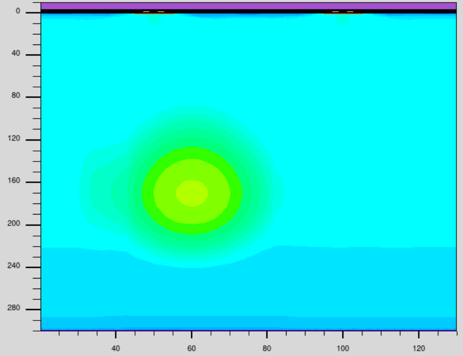


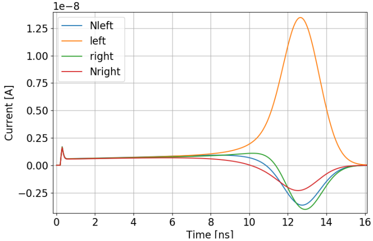
Time 6.8 ns

Electrons



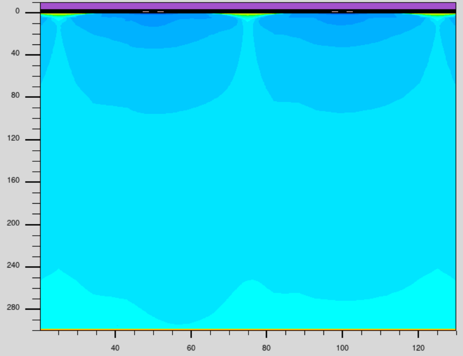
Holes



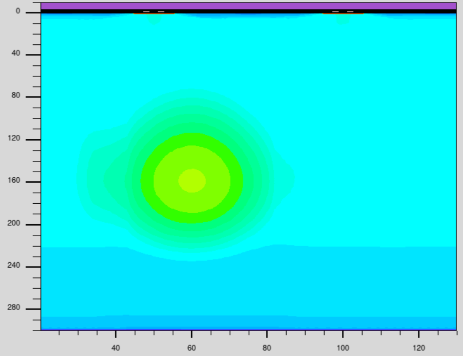


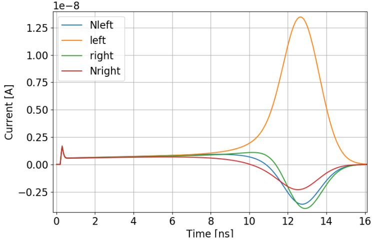
Time 7.3 ns

Electrons

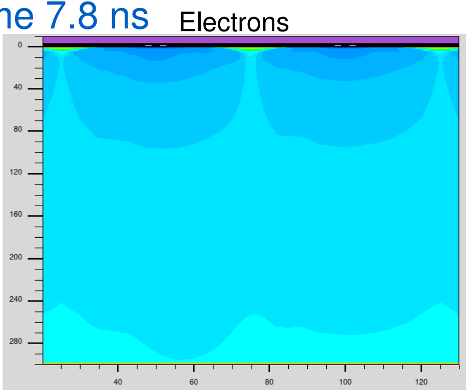


Holes

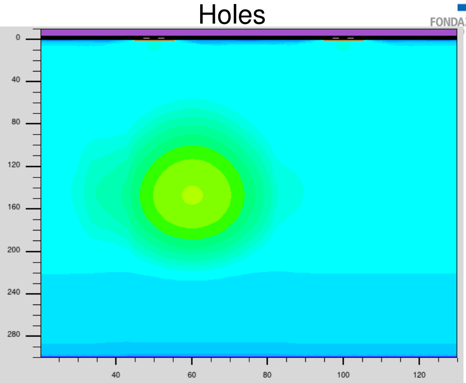




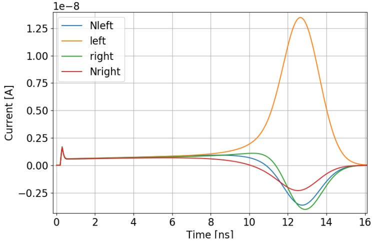
Time 7.8 ns



Electrons
0
40
80
120
160
200
240
280
40
60
80
100
120



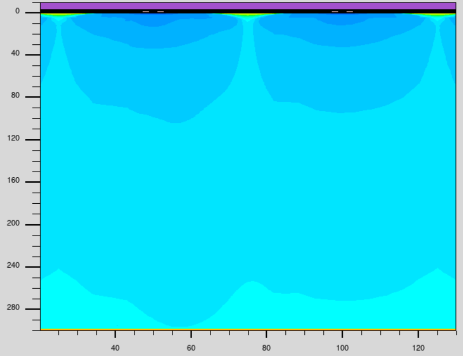
Holes
0
40
80
120
160
200
240
280
40
60
80
100
120



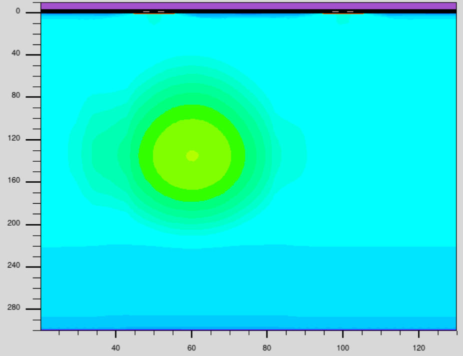
1e−8
Nleft
left
right
Nright
Current [A]
1.25
1.00
0.75
0.50
0.25
0.00
−0.25
0
2
4
6
8
10
12
14
16
Time [ns]

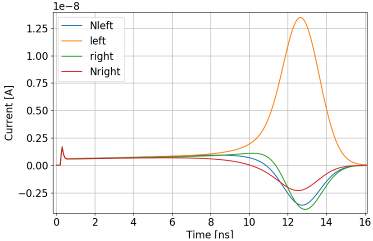
Time 8.3 ns

Electrons



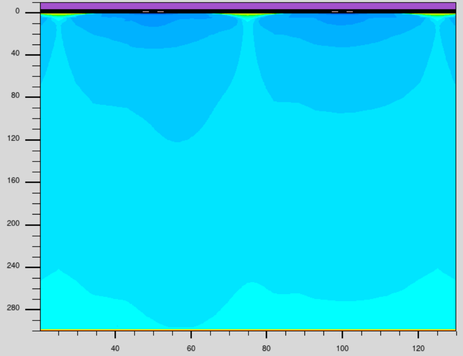
Holes



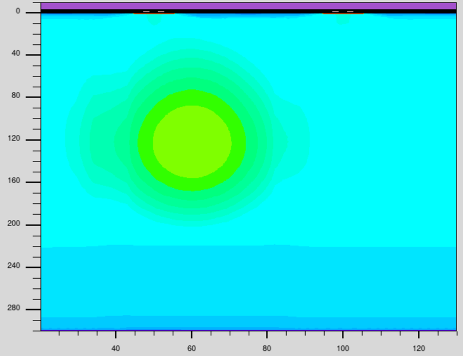


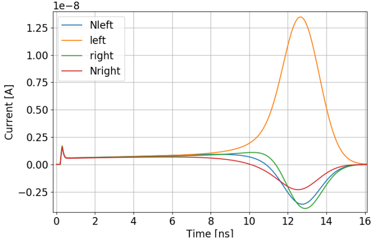
Time 8.8 ns

Electrons



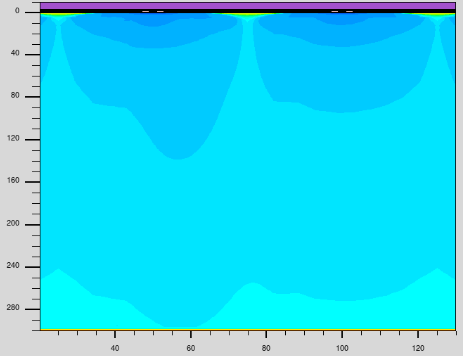
Holes



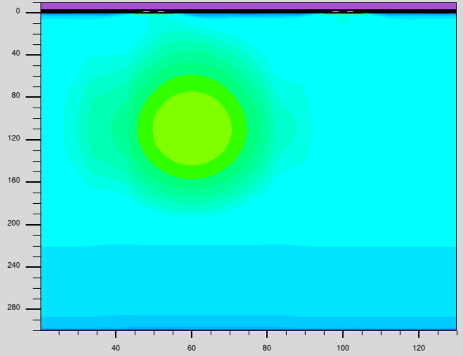


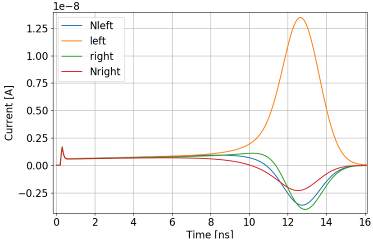
Time 9.3 ns

Electrons



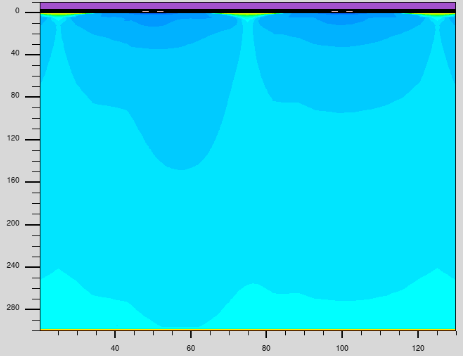
Holes



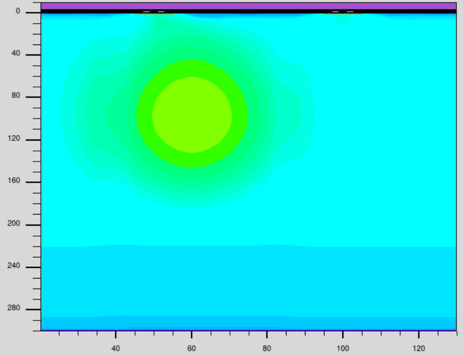


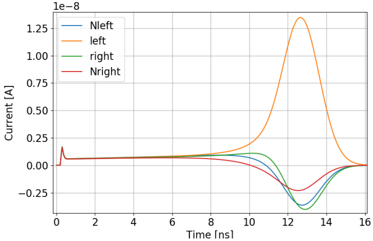
Time 9.8 ns

Electrons



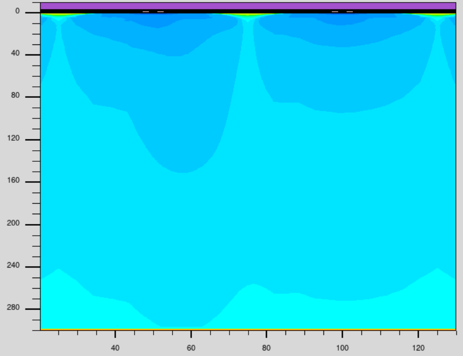
Holes



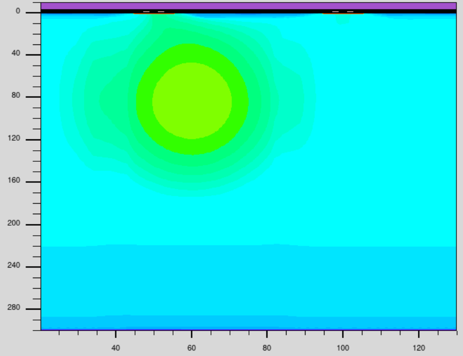


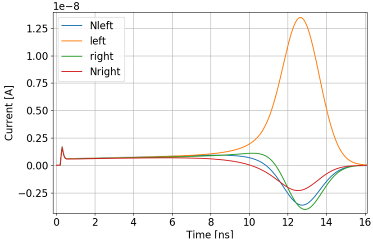
Time 10.3 ns

Electrons



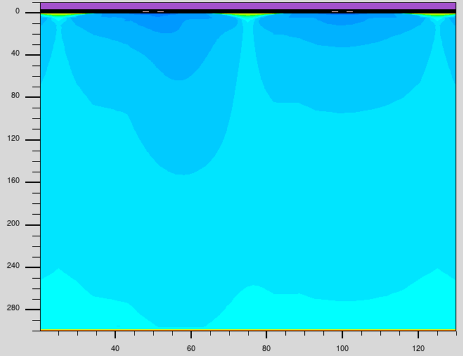
Holes



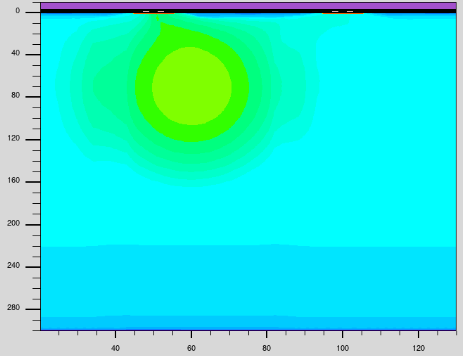


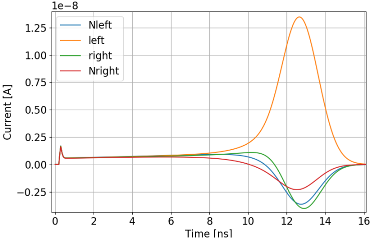
Time 10.8 ns

Electrons



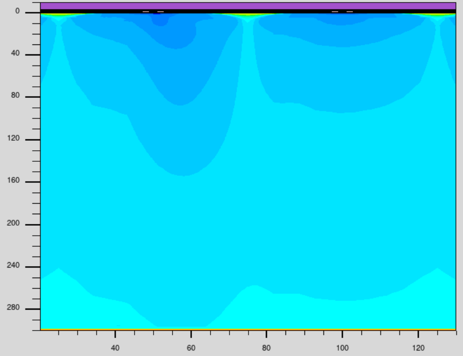
Holes



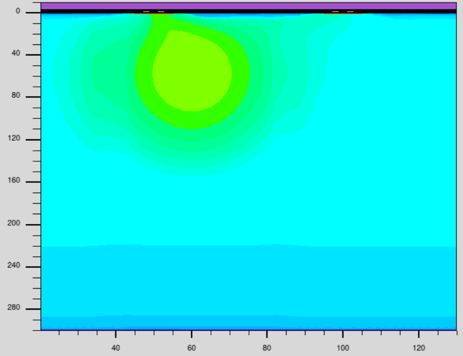


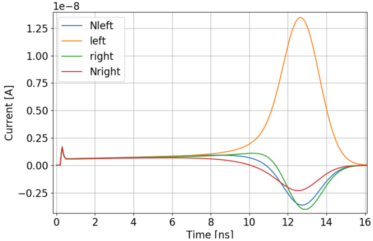
Time 11.3 ns

Electrons



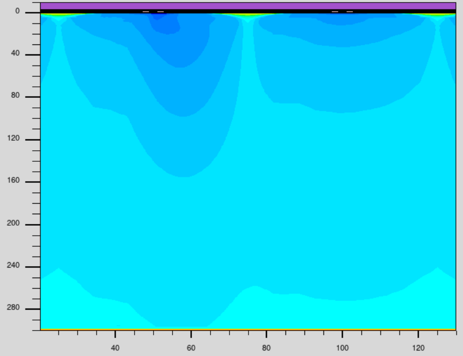
Holes



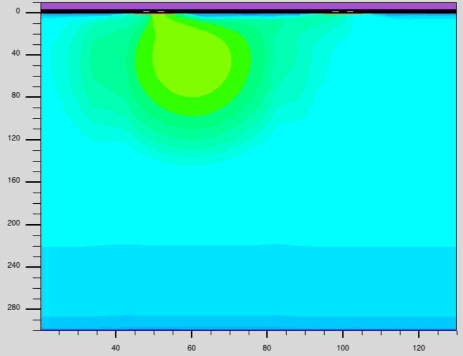


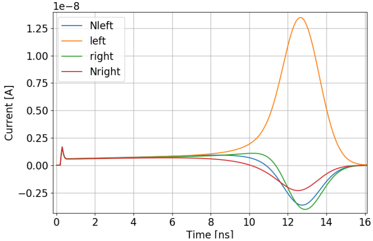
Time 11.8 ns

Electrons



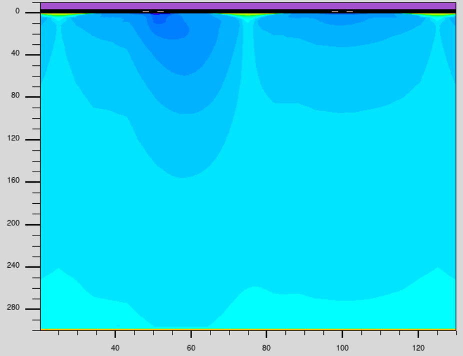
Holes





Time 12.3 ns

Electrons



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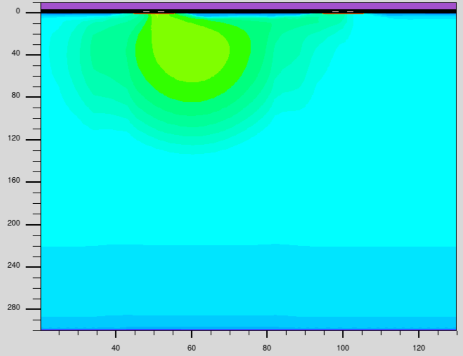
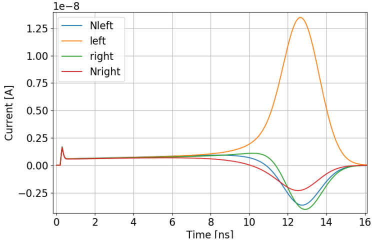
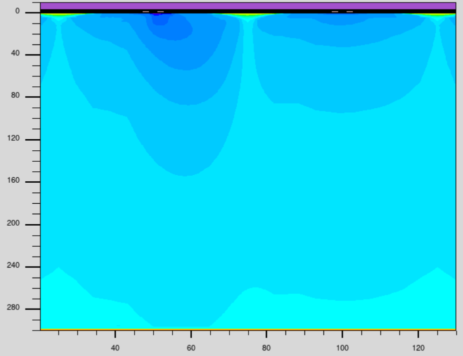




Time 12.8 ns

Electrons



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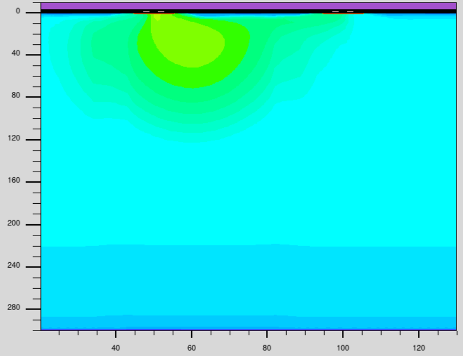
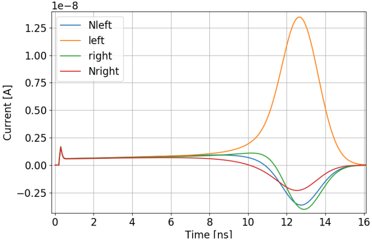
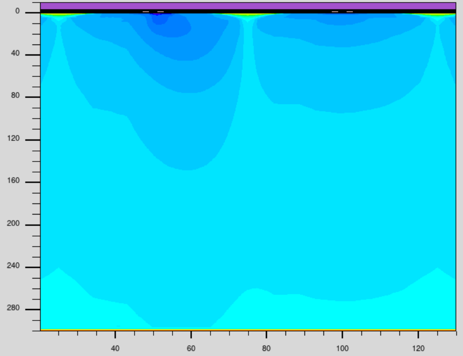




Time 13.3 ns

Electrons



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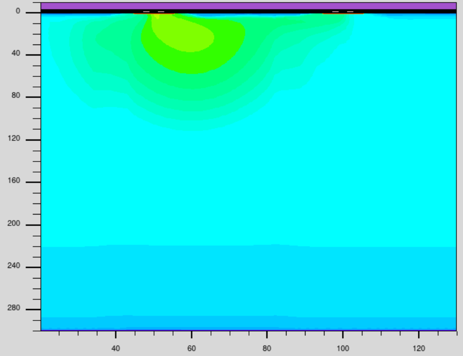
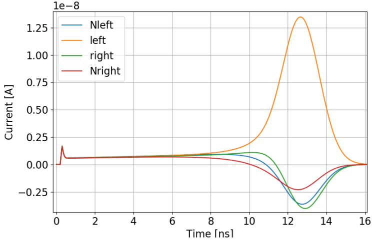
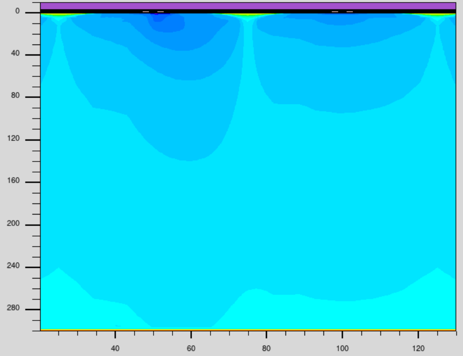




Time 13.8 ns

Electrons



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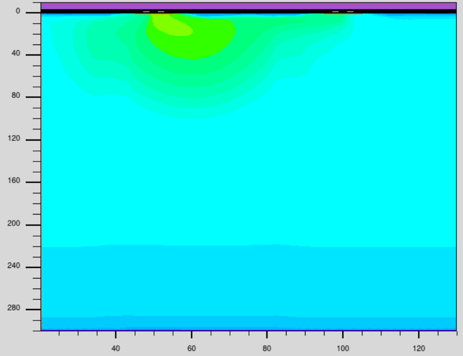
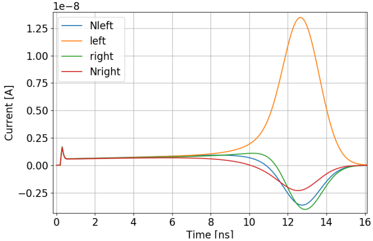
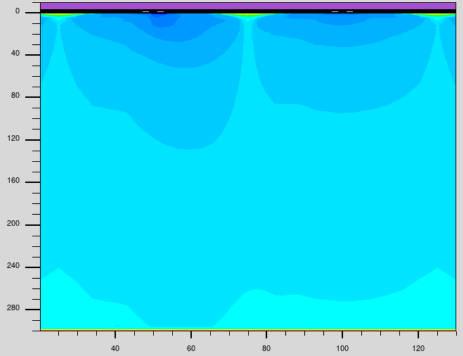


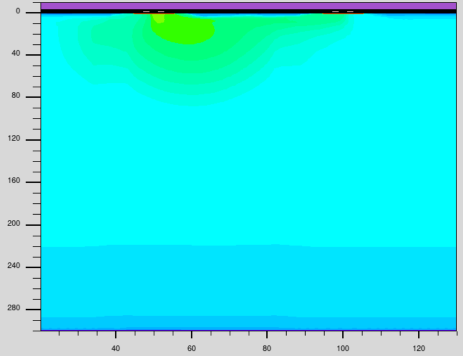


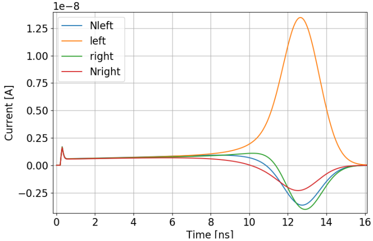
Time 14.3 ns

Electrons



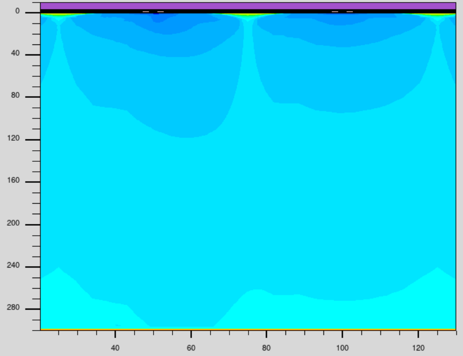
Holes



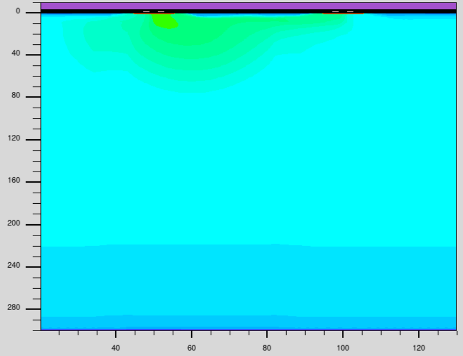


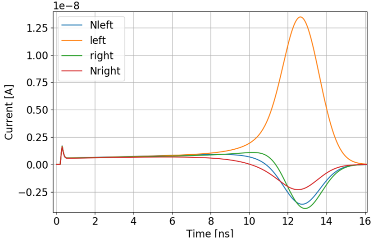
Time 14.8 ns

Electrons



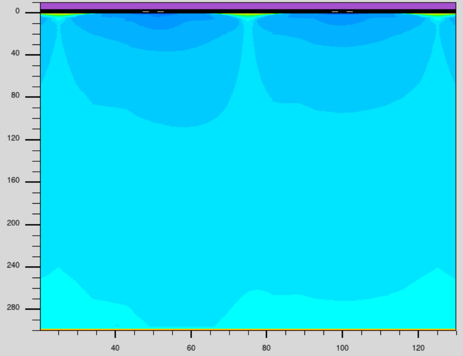
Holes



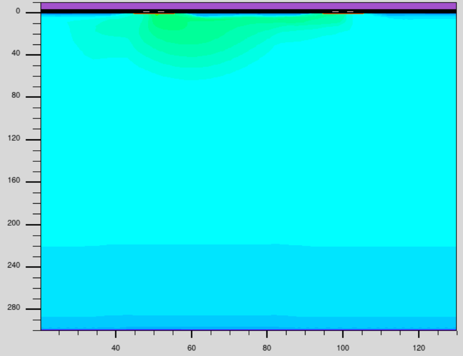


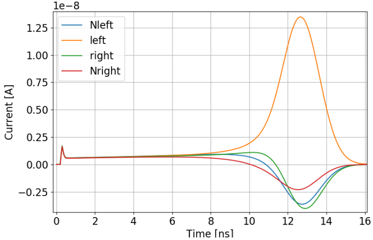
Time 15.3 ns

Electrons



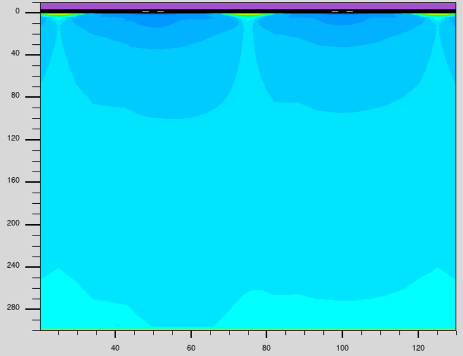
Holes



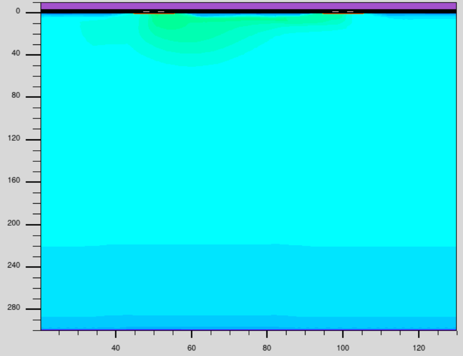


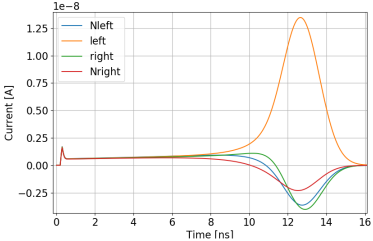
Time 15.8 ns

Electrons

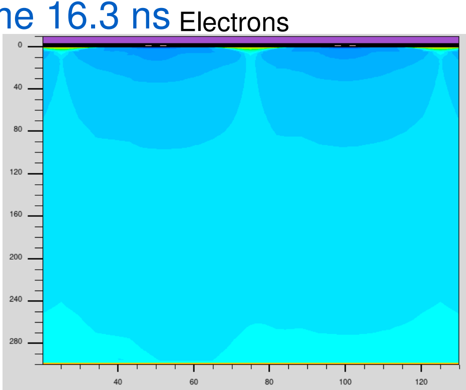


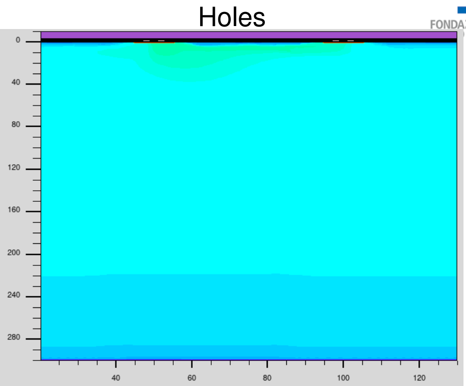
Holes

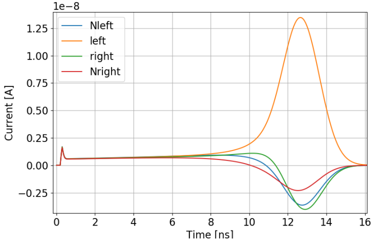




Time 16.3 ns

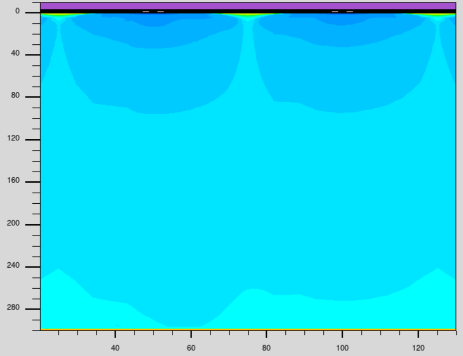

Electrons
0
40
80
120
160
200
240
280
40
60
80
100
120


Holes
0
40
80
120
160
200
240
280
40
60
80
100
120

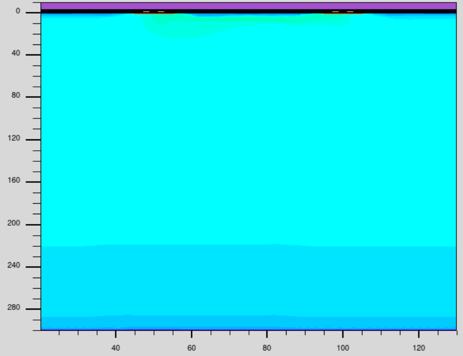

1e−8
Nleft
left
right
Nright
Current [A]
1.25
1.00
0.75
0.50
0.25
0.00
−0.25
0
2
4
6
8
10
12
14
16
Time [ns]

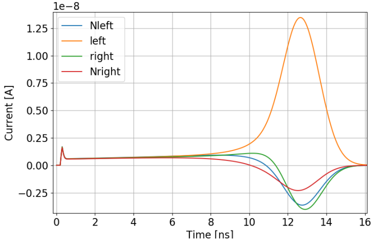
Time 16.8 ns

Electrons



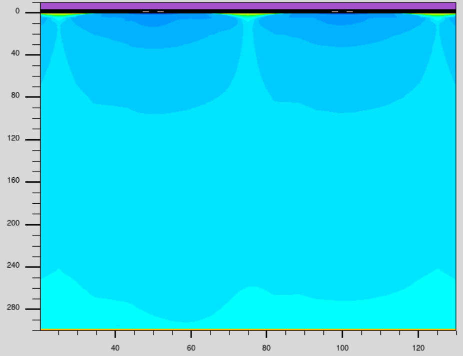
Holes



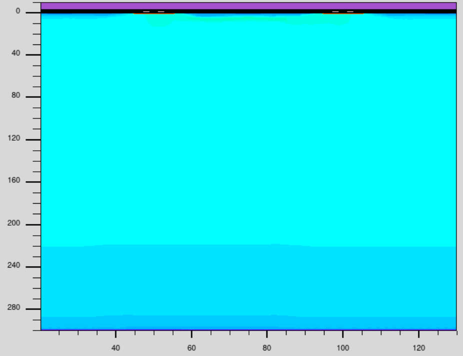


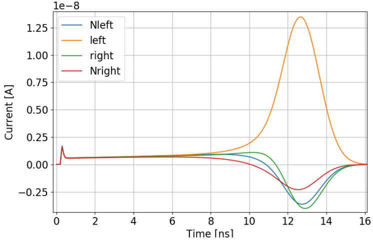
Time 17.3 ns

Electrons



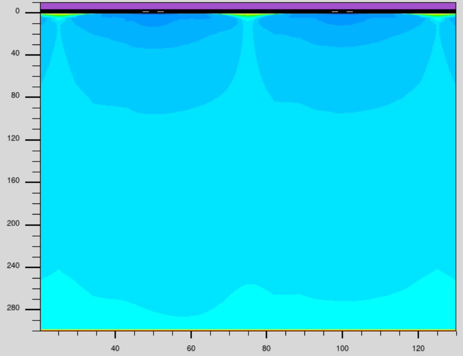
Holes



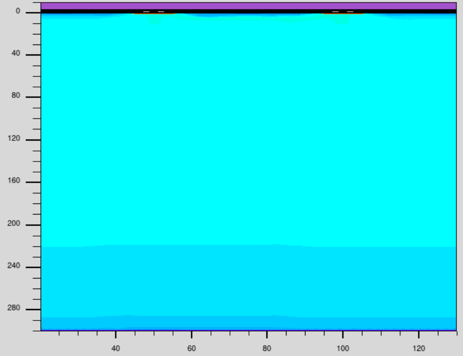


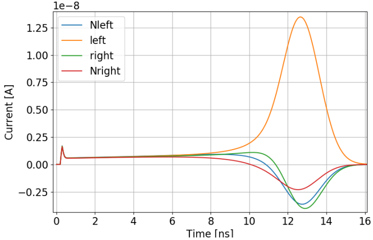
Time 17.8 ns

Electrons



Holes



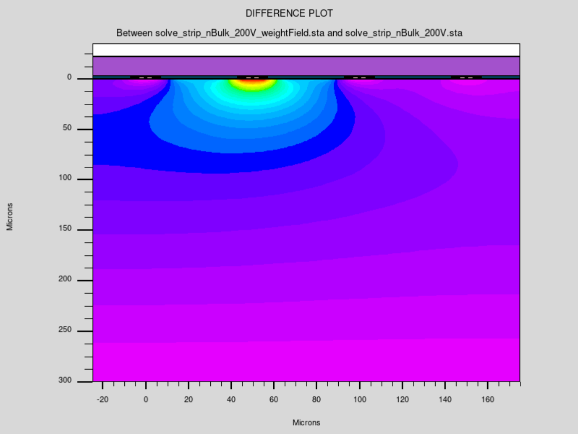


Extract the weigthing field and potential (Atlas + Tonyplot)

- preparation steps
- load solution file for bias point
- raise the potential of the interested electrode by 1V (same steps as for biasing)
- save solution file
- difference in potential between files
  $\Rightarrow$ weighting potential
- difference in electric field between files
  $\Rightarrow$ weighting field

Note: it is not necessary to use 1V, but other values need normalization afterwards

Weighting potential (200V, left strip)



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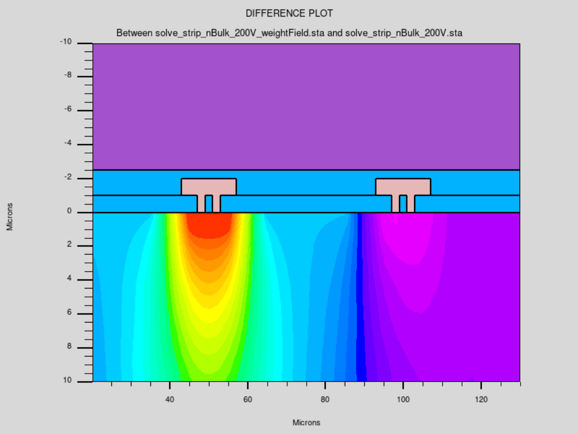

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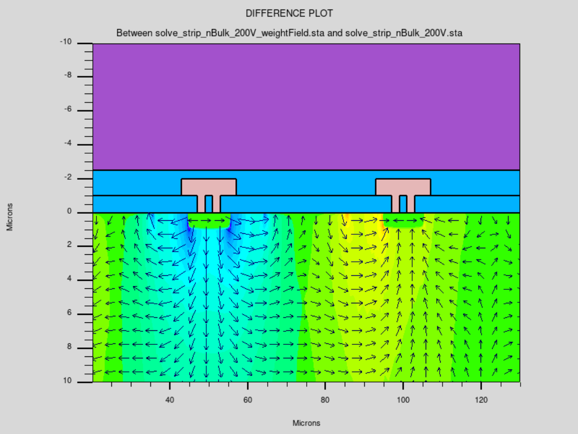
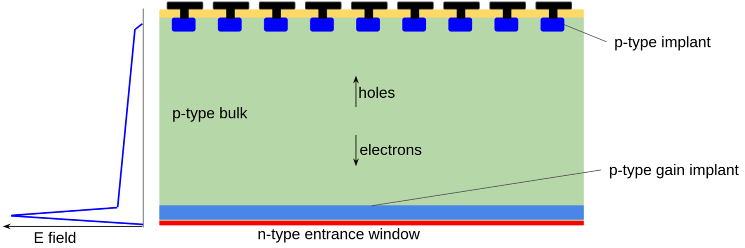
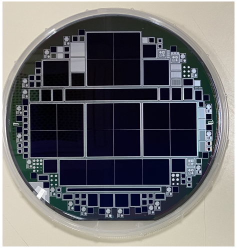


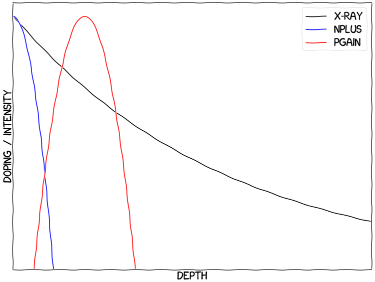
Process & Device Simulation Example: Gain Layer Optimization

- Optimization for x-ray applications
- Gain dose to be adjusted for device thickness
- Implants dose and energy to be adjusted for different process splits
- **Provide a starting point for the process split table**

Double Sided LGADs for X-rays







- Optimization for x-rays
- One possibility: gain structure as narrow as possible
- Few variations in the batch

Gain Extraction

“Analitical”

- α, β from bias simulation
- Gain calculation using McIntyre 1966

$$M(x) = \frac{\exp\left[-\int_x^w \alpha - \beta \, dx'\right]}{1 - \int_0^w \alpha \exp\left[-\int_{x'}^w \alpha - \beta \, dx''\right] dx'}$$

- Ideal case, low injection
- Faster simulation $\Rightarrow$ more attempts

Fully simulated

- Simulate same structure with and without gain
- Transient or steady state simulations with photogeneration
- Ratio of integrated signals / currents

- More realistic: diffusion, density effects...
- Computing intensive

The “analytical” path was choosen

Simulation Workflow

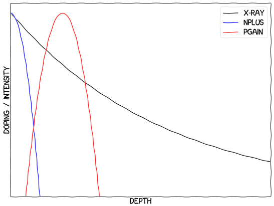
For each process variation:

Process Simulation (Athena)

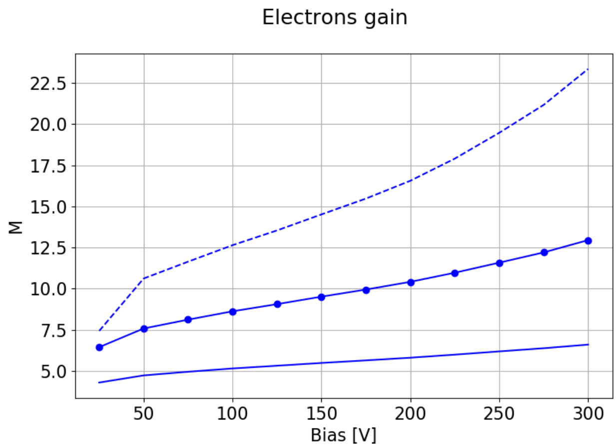
- Make mesh
- Create substrate
- Backside implant (bulk contact)
- Screen oxide
- Implants
- Annealing
- Remove oxide
- Save structure file

Device Simulation (Atlas)

- Make mesh
- Create substrate
- Declare electrodes
- Import doping from structure file
- Preparation steps
- Bias
- Extract α, β at given bias values



Gain



Quite sensitive to:

- Gain layer position
- Doping contentration
  (left: ≈ 2% dose variation)
- Impact ionization model

Summary

Process Simluations

- Problem solving
- Process optimization

Device Simulations

- Estimation of detector properties
- Understanding the detector structure

- **TCAD is a useful tool in detector fabrication**
- Reduce the number of splits and iterations during fabrication
  $\Rightarrow$ save time & money

Not everything can be simulated:
process variations are still necessary to explore the phase space

Backup Material

Weighting Field

Math construct that relates charge movement to induced current on electrodes

- Determines the signal shape
- Depends on the sensor geometry
- Concept from vacuum tubes
- Shockley (1938) Ramo (1939)
- Extensions in recent years to account for different effects

For the i-th electrode

$$i_i(t) = Nq_e \vec{E}_{w,i} \cdot \vec{v}$$

$$Q_i = \int_{t_0}^{t} i_i(t')dt' = Nq_e[\phi_{w,i}(\vec{r}(t)) - \phi_{w,i}(\vec{r}(t_0))]$$

$$\vec{E}_{w,i} = -\vec{\nabla}\phi_{w,i} \qquad \vec{v} = \frac{d\vec{r}}{dt}$$

To calculate:

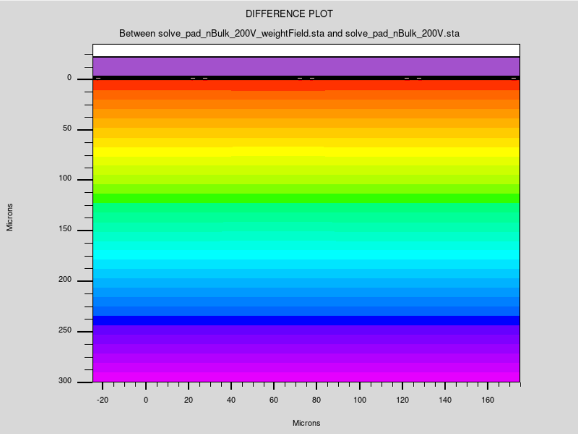
- Set all electrodes to 0V
- Set electrode of interest to 1V
- Solve equations (disregard space charge)

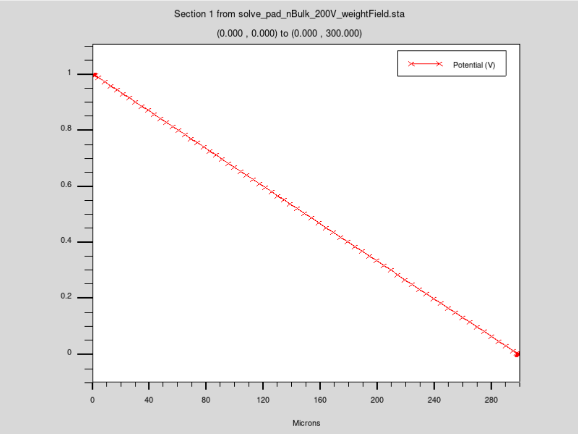
- $\vec{E}_{w,i}$ with $\vec{v}$ determine signal shape
- $\Delta\phi_{w,i}$ determines the induced charge
- $[\vec{E}_{w,i}]$ = cm^{-1}
- $[\phi_{w,i}]$ = dimensionless

Note: these are NOT the fields determining carrier movement

Weighting Field Pad Diode (Top Electrode)

Weighting Potential

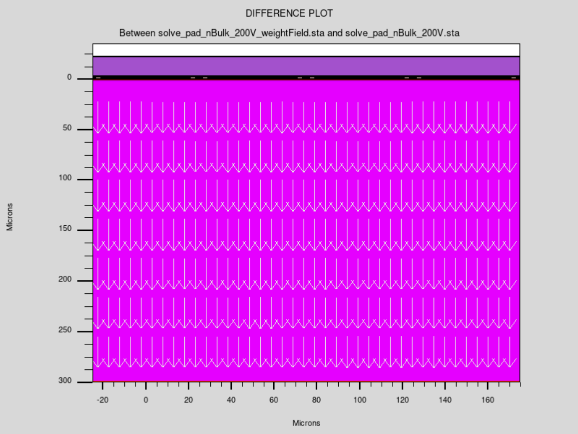


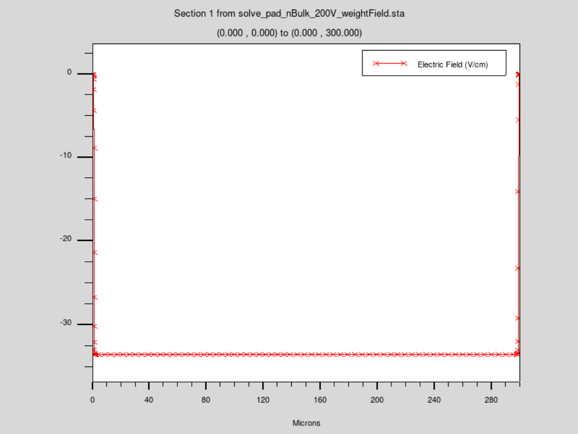


- Simple geometry
- Linear potential $\Rightarrow$ Charge proportional to path
- Constant field $\Rightarrow$ Current proportional to $|\vec{v}|$

Weighting Field Pad Diode (Top Electrode)

Weighting Field





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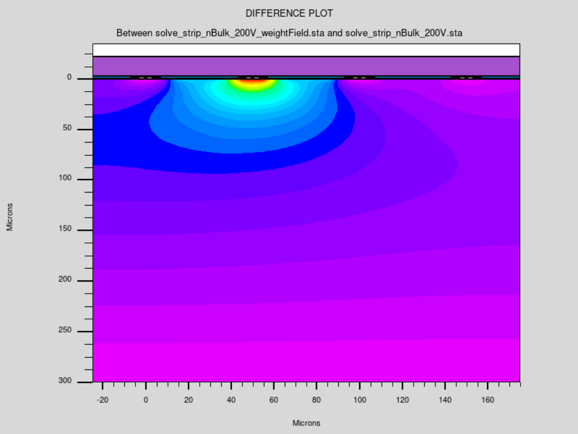
Weighting Field Strip Sensor

Weighting Potential

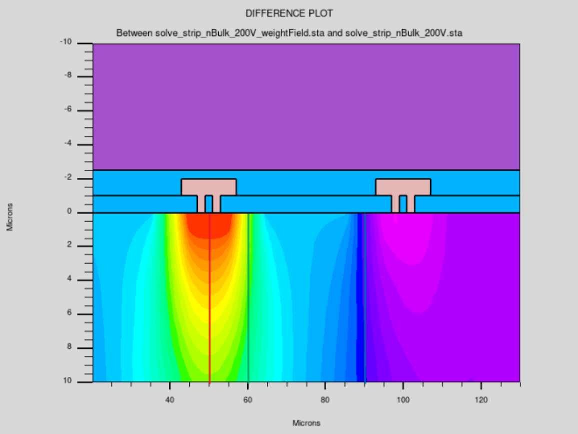


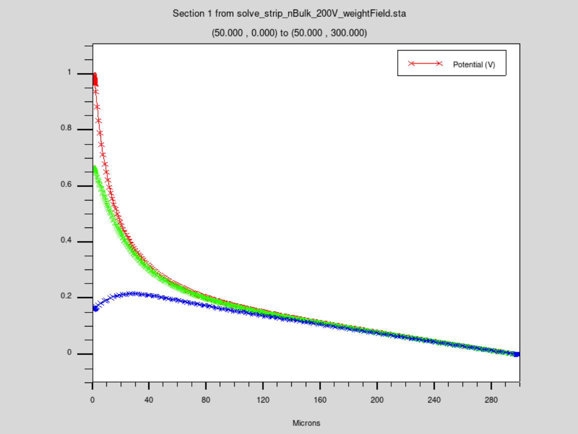
- Weighting potential for strip L
- Asymmetry due to boundary conditions

- Peaked potential toward strip side $\Rightarrow$ most of charge induced in the space closest to the strip
- Different sign of field $\Rightarrow$ Different sign of signal possible $\rightarrow$ Bipolar signals on some strips

Weighting Field Strip Sensor

Weighting Potential

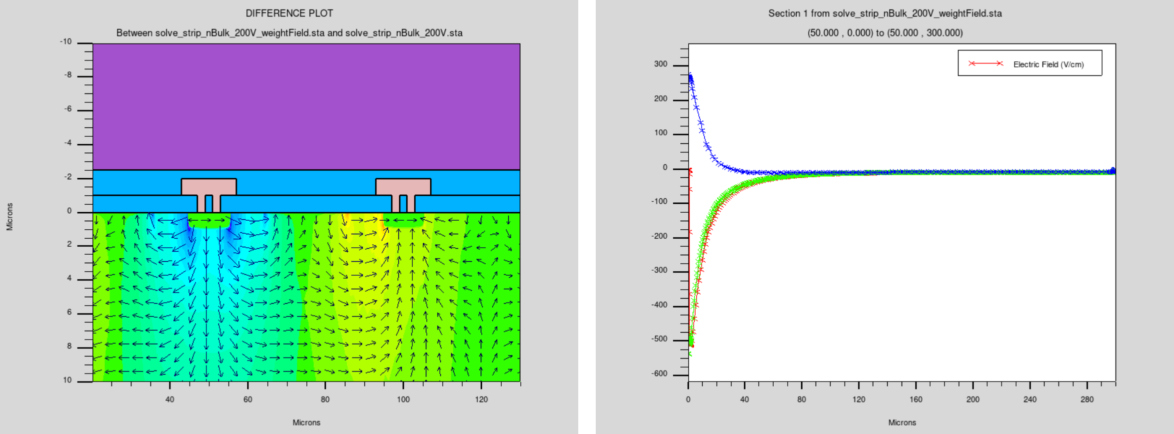




- Peaked potential toward strip side ⇒ most of charge induced in the space closest to the strip
- Different sign of field ⇒ Different sign of signal possible → Bipolar signals on some strips

Weighting Field Strip Sensor

Weighting Field



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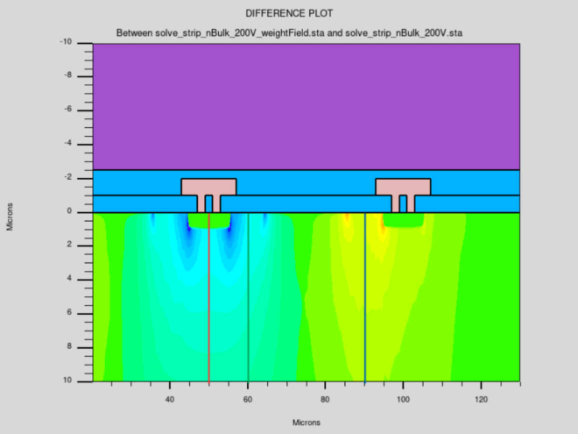
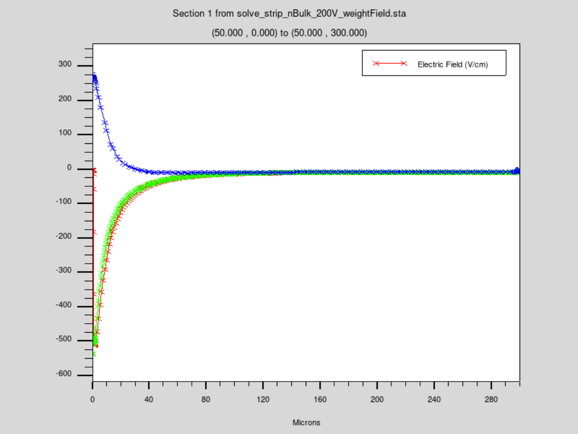
Weighting Field Strip Sensor

FONDAZIONE BRUNO KESSLER

Weighting Field





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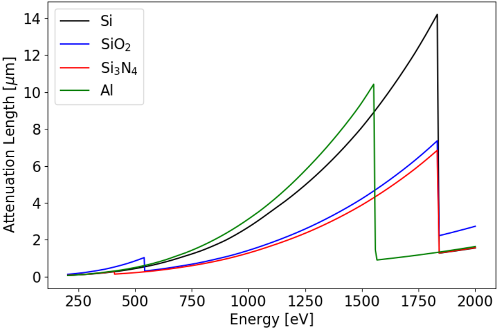
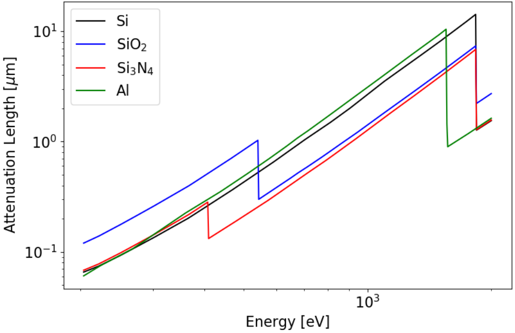
X-ray Attenuation Length





http://henke.lbl.gov/optical_constants/atten2.html