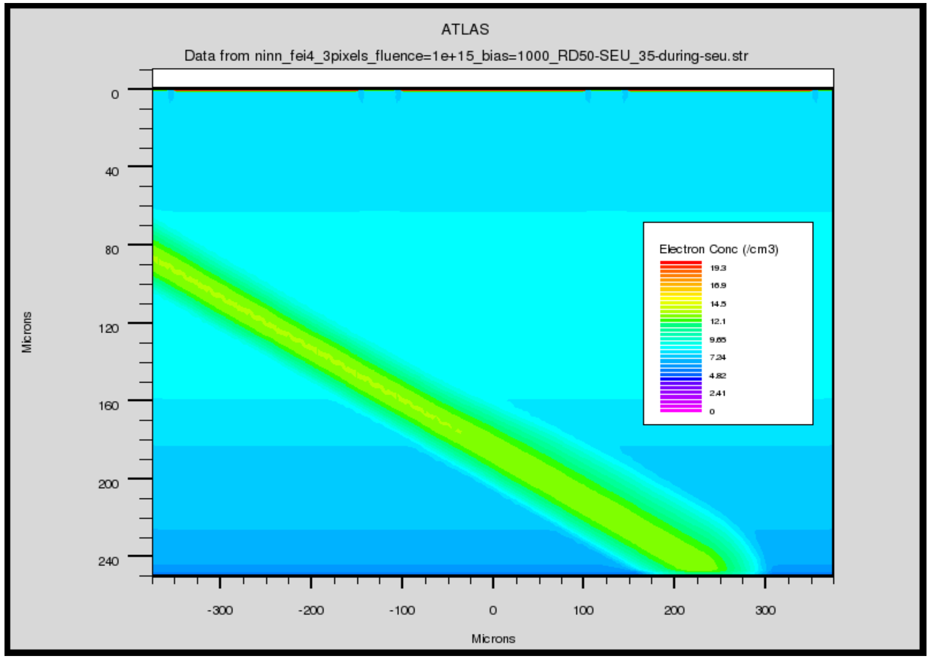
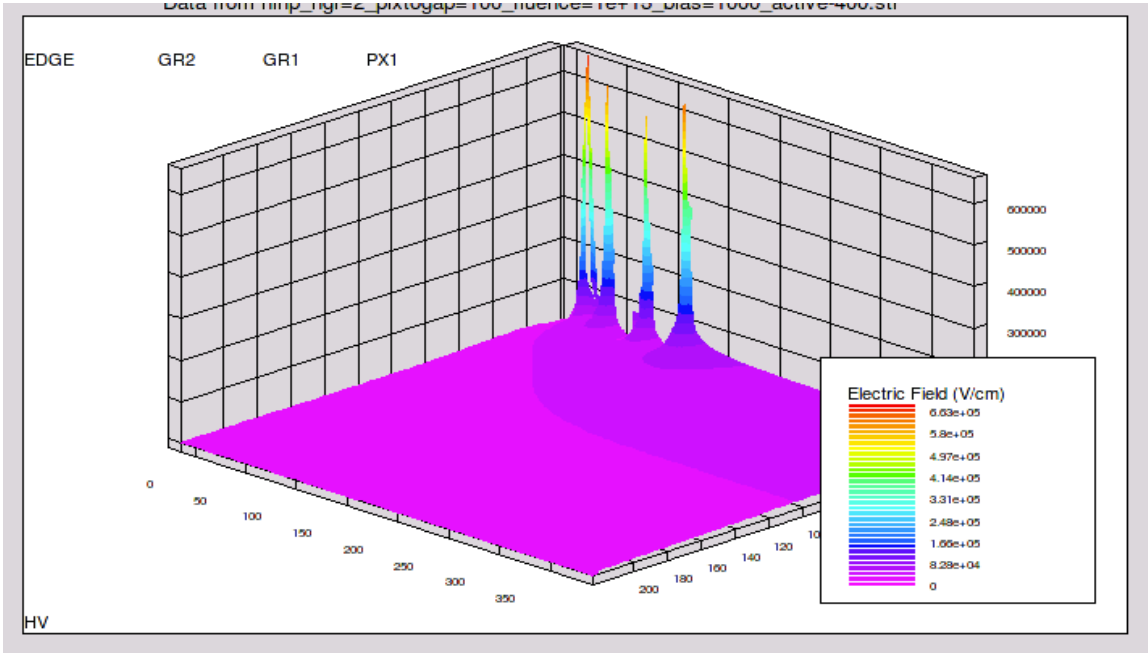
TCAD simulations

for silicon sensors and testbeams





université PARIS DIDEROT PARIS 7

Marco Bomben – UPD & LPNHE (Paris)

LPNHE PARIS

Outline

- Introduction
- Presentation of some of the packages
- Selected results
- Comments and conclusions

SILVACO

INTRODUCTION

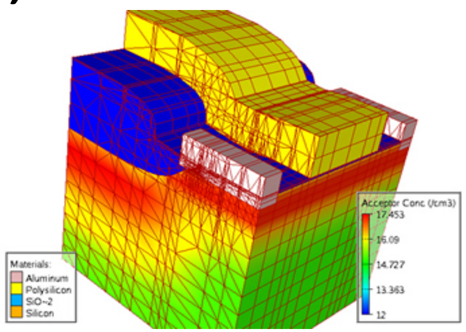
Introduction

- Technology Computer Aided Design - TCAD
- Solve drift/diffusion & Poisson equations for electrons and holes:

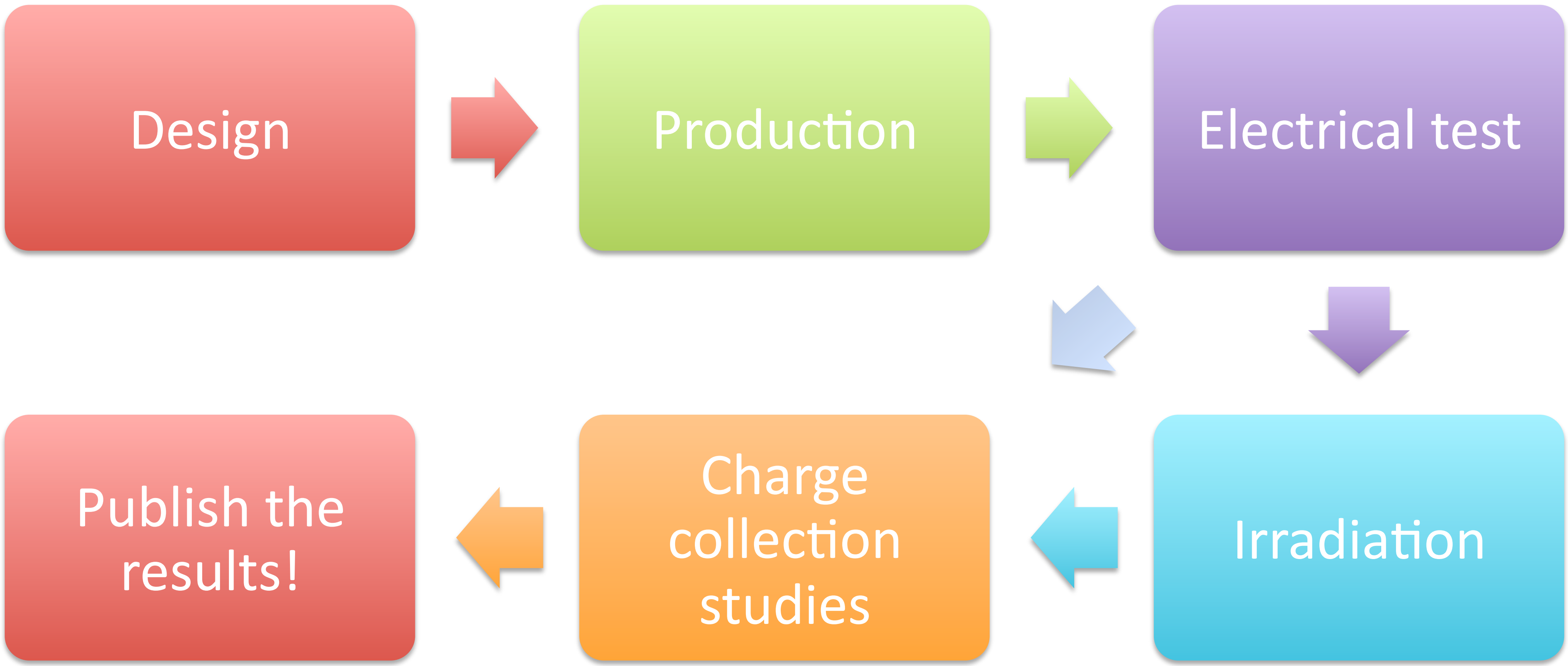
$$J_n = qn\mu_n E + qD_n \frac{\partial n}{\partial x} \qquad J_p = qn\mu_p E - qD_p \frac{\partial p}{\partial x} \qquad \frac{\partial n}{\partial t} = \frac{1}{q}\frac{\partial J_n}{\partial x} + G_n - R_n$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{q}{\epsilon_{Si}\epsilon_0}(N_D + p(x) - n(x) - N_A) \qquad \frac{\partial p}{\partial t} = -\frac{1}{q}\frac{\partial J_p}{\partial x} + G_p - R_p$$

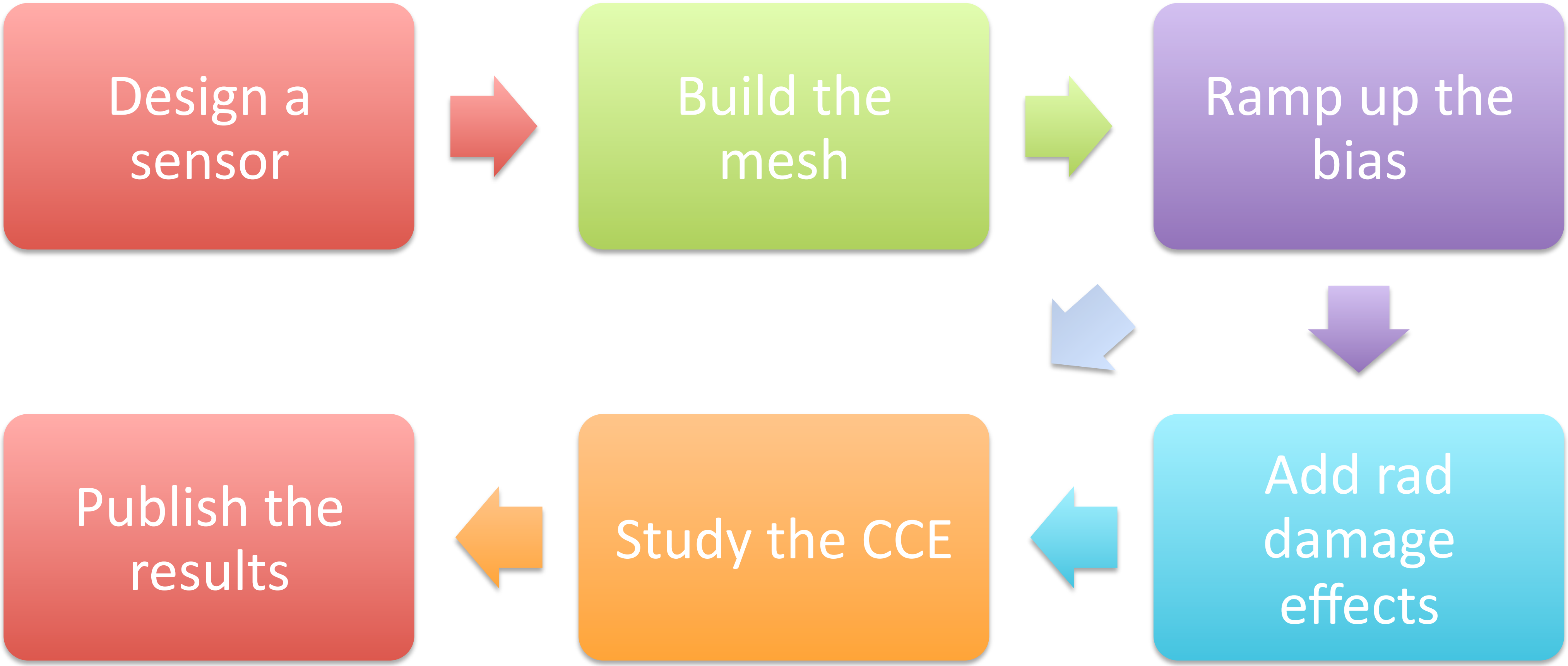
- taking into account boundary conditions
  - Electrodes' potentials, interface charges, etc
- on a grid of points



Normal work flow for a HEP silicon sensors



TCAD simulation work flow



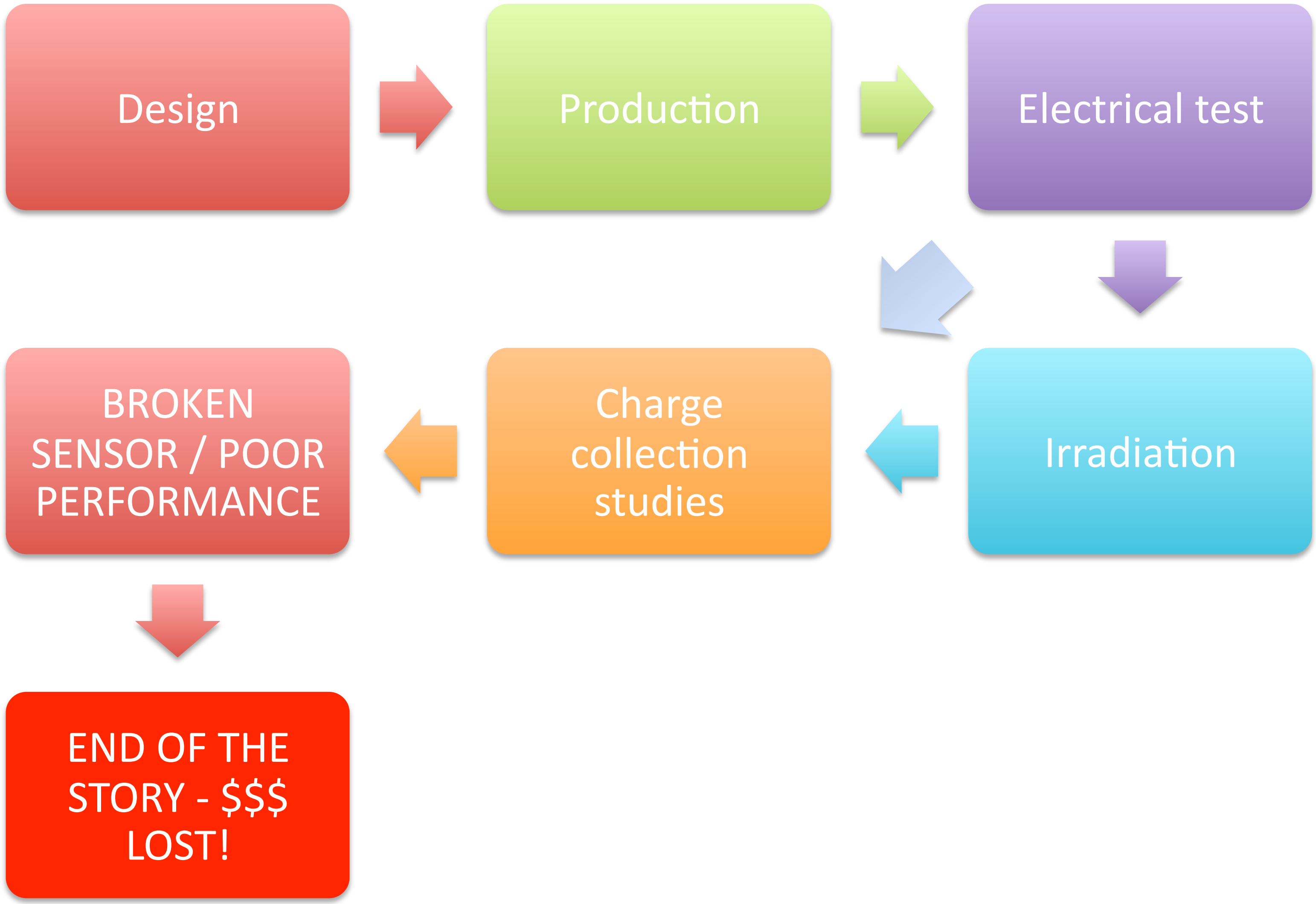
So why bother with simulations?

- You repeat all the “steps” of real sensors…

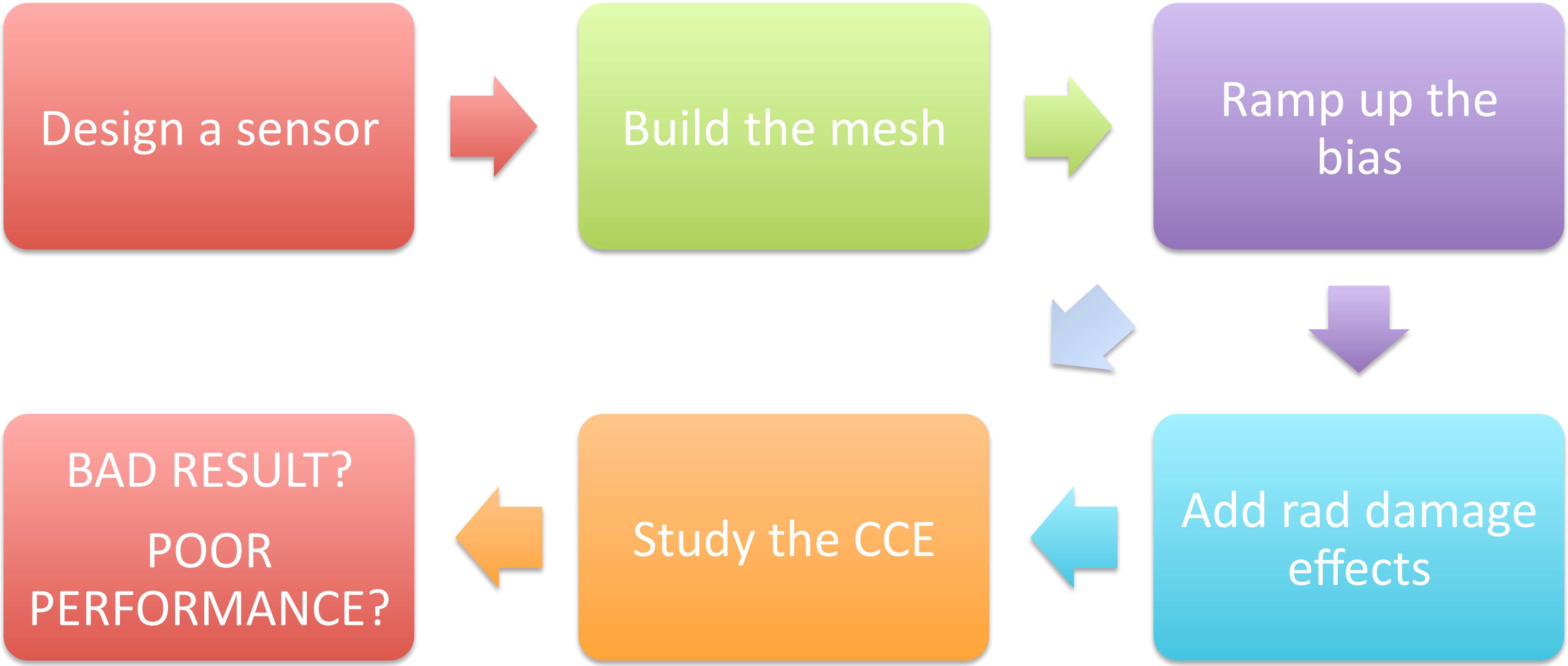
So why bother with simulations?

- You repeat all the “steps” of real sensors…
- It is not true!

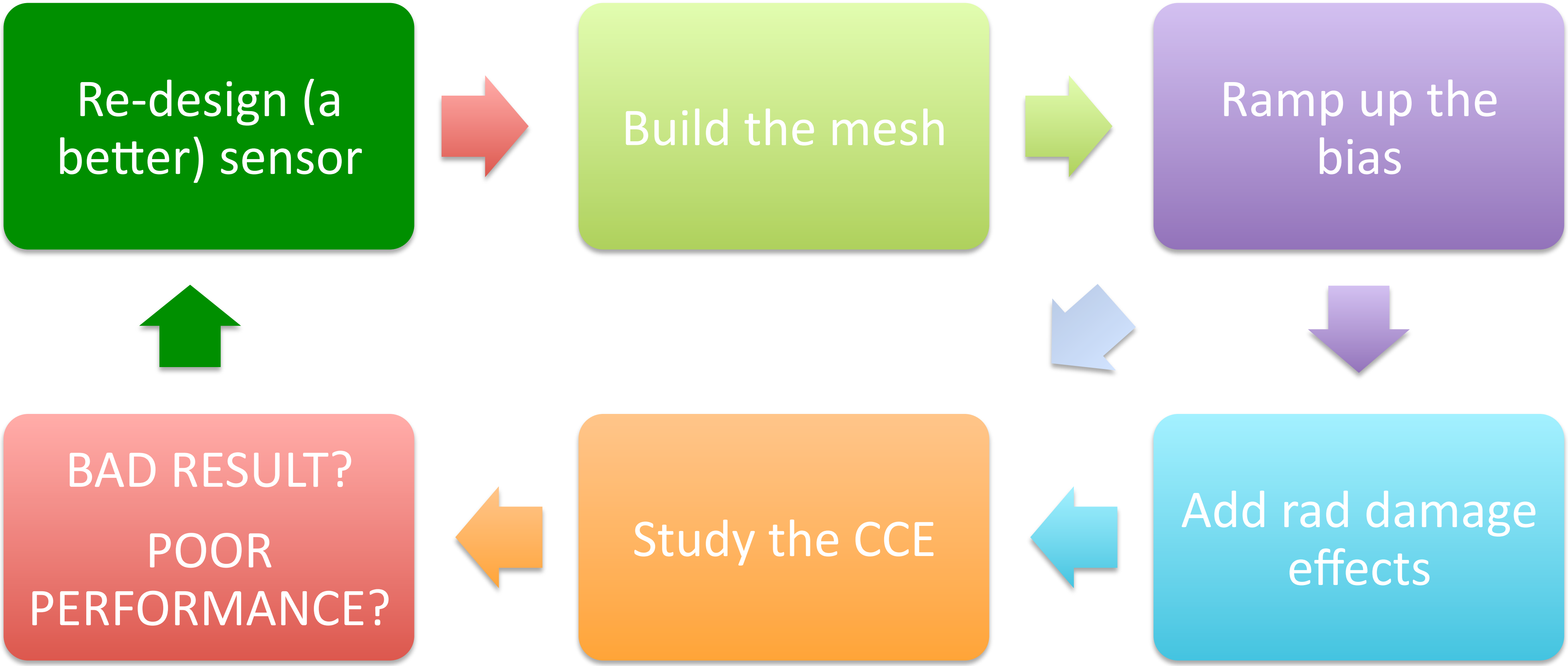
Possible work flow for real sensors



TCAD simulation work flow



TCAD simulation work flow

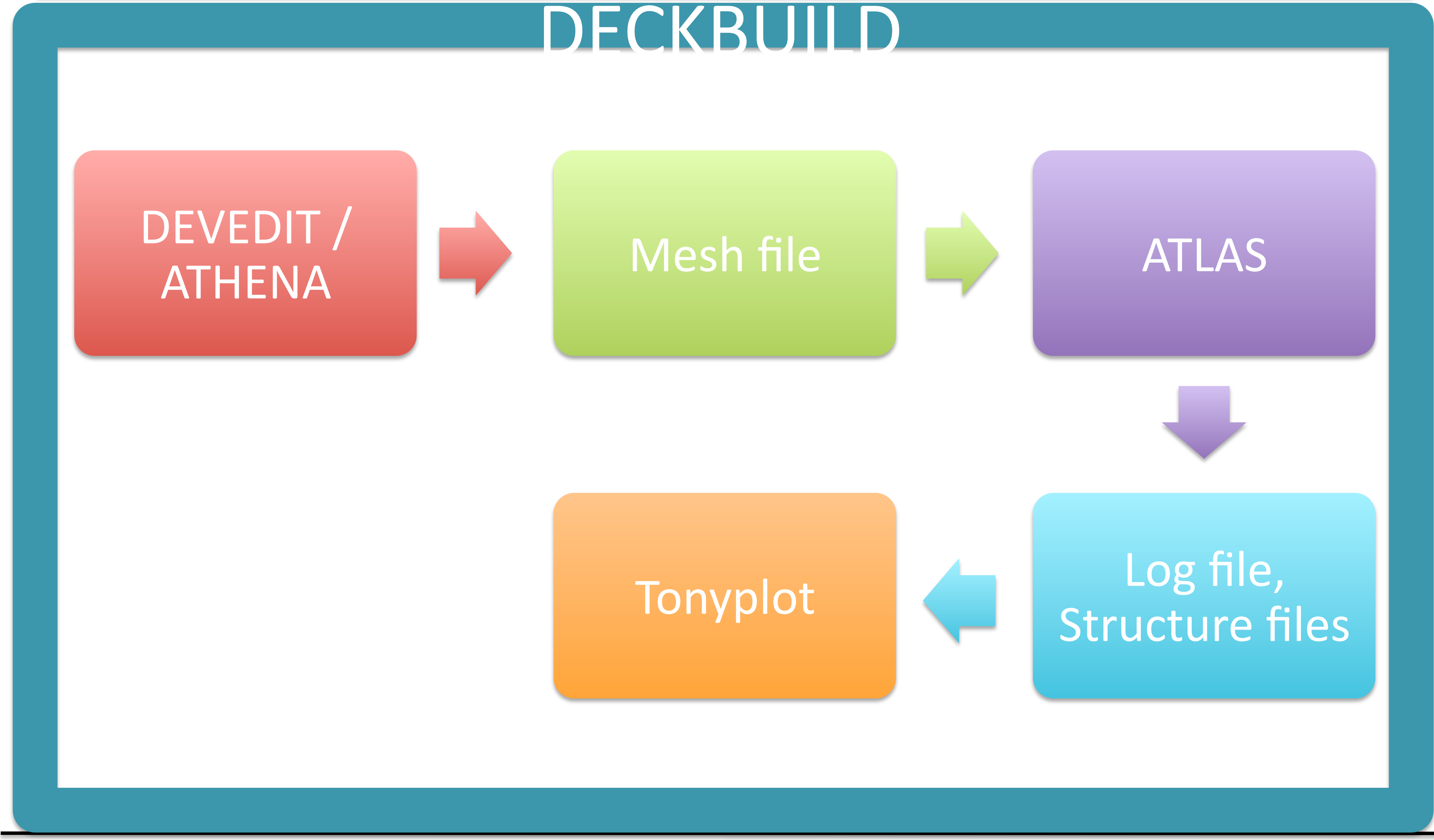


Simulations benefits

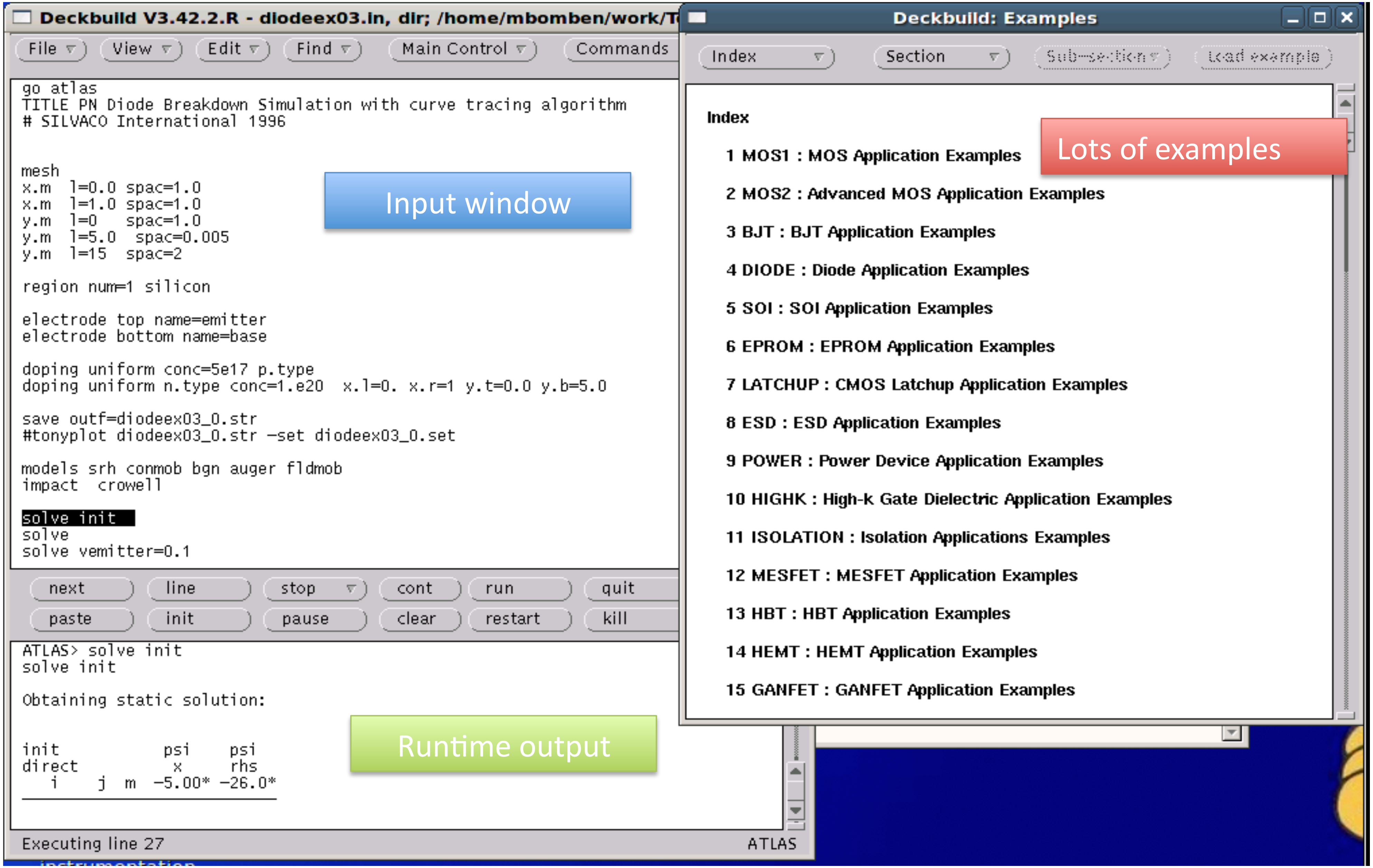
- Simulating sensors helps in saving:
  - ➢ Development time
  - ➢ Number of submissions
  - ➢ Money
- You can learn a lot in terms of:
  - ❑ Physics
    - Study quantities otherwise not accessible!

SOFTWARE FEATURES

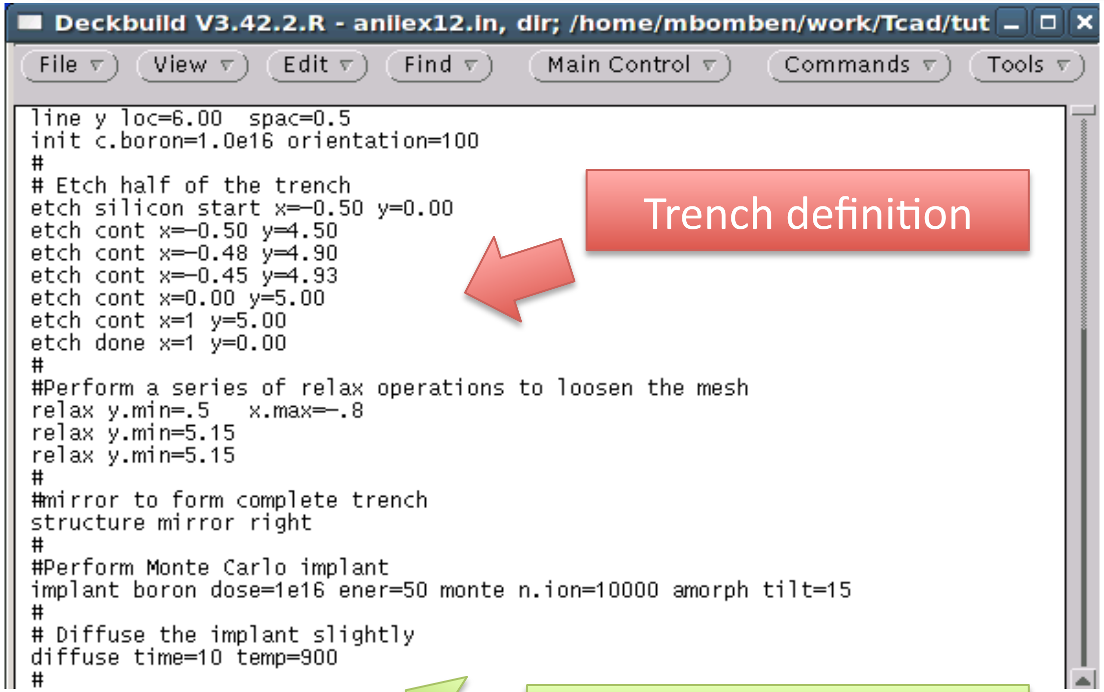
TCAD packages & work flow



A Deckbuild session

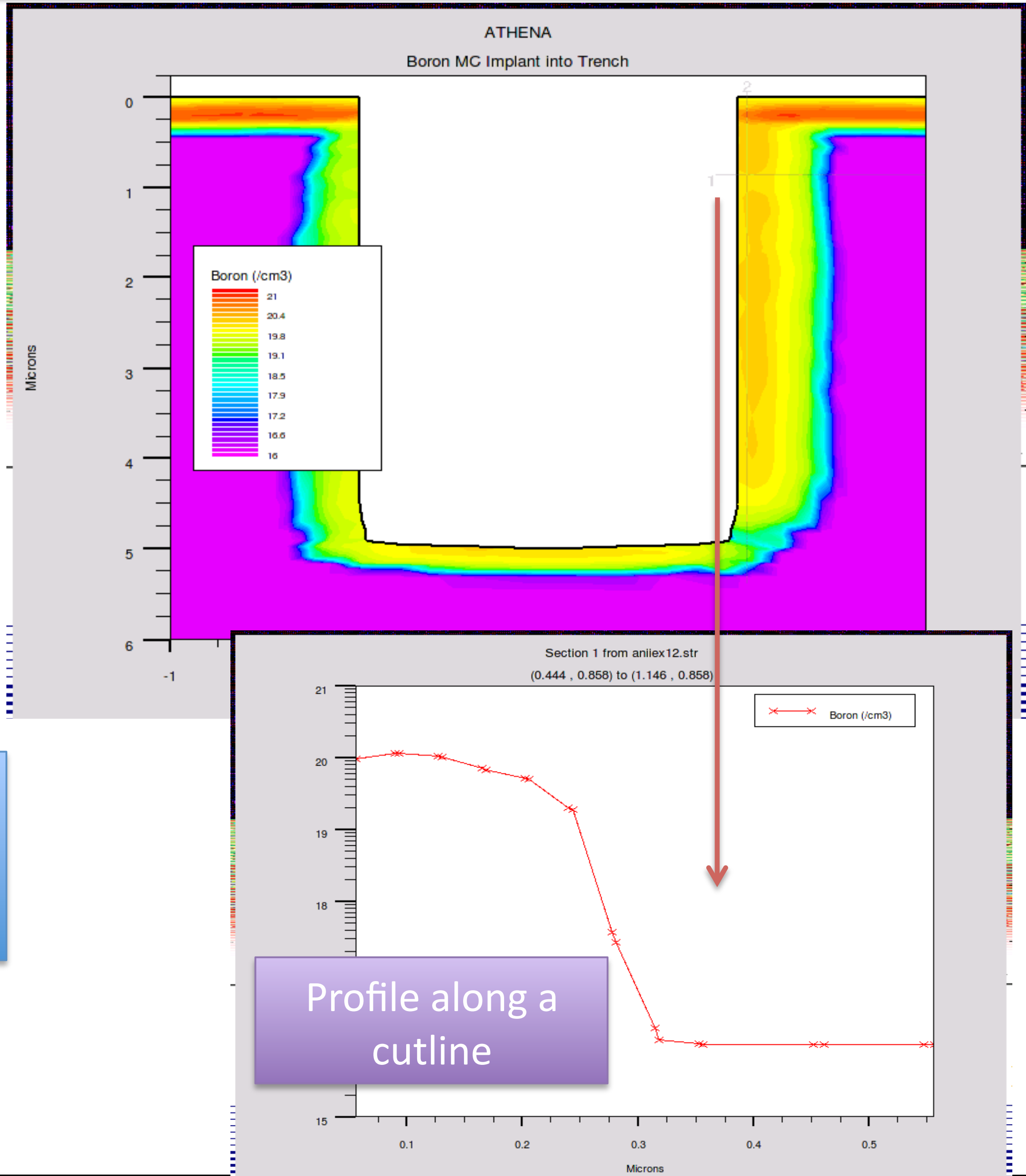


Athena: semiconductor processing simulation



Trench definition

Implant definition



Profile along a cutline

Define implants, trenches, oxidations, ecc using ATHENA

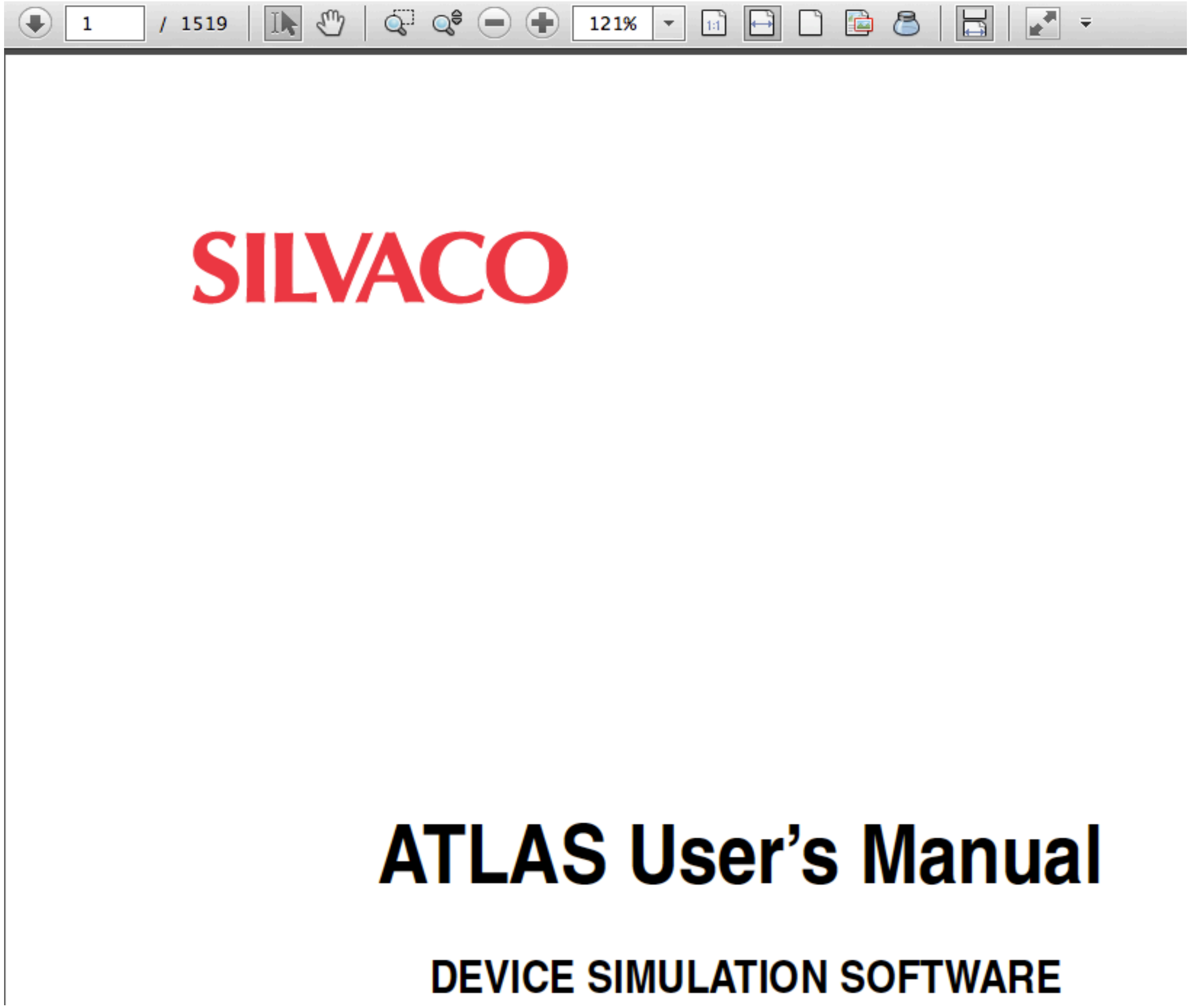
ATLAS: device simulation

- ATLAS provides general capabilities for physically-based two (2D) and three-dimensional (3D) simulation of semiconductor devices.
- Typical simulation program structure →

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
5. Results Analysis	EXTRACT TONYPLOT

ATLAS: main features

- TONS of models:
  - S-Pisces: Silicon Based 2D Simulator
  - 3D Device Simulator
  - Luminous: Optoelectronic Simulator
  - Single Event Upset
  - …
- LOT of options
- HUGE manual



ATLAS: an example

```
ATLAS> trap acceptor e.level=0.495 density=1e+13 degen=1 sign=1e-15 sigp=1e-15

Mesh
 Type:                 non-cylindrical
 Total grid points:  37668
 Total triangles   :  74496
 Obtuse triangles :  0  (0 %)
ATLAS> trap donor e.level=0.48 density=1e+13 degen=1 sign=1e-15 sigp=1e-15
ATLAS> ## else
ATLAS>
ATLAS>    ##    if.end
ATLAS>
ATLAS> ## if.end
ATLAS>
ATLAS>
ATLAS> # MODELS, IMPACT, INTERFACE & METHOD
ATLAS> models bipolar temperature=290 print
ATLAS> impact selb
ATLAS>
ATLAS> interface Qf=3e+12 x.min=1
ATLAS> interface Qf=3e+12 x.max=1
ATLAS> interface S.N=5 S.P=5
ATLAS>
ATLAS>
ATLAS> ### altering default recombination lifetime for bulk
ATLAS> MATERIAL region=2 TAUP0=7.80896e-08 TAUN0=9.43913e-08 ETRAP=0.09
ATLAS>
ATLAS> method gummel newton climit=1e-5
```

Carriers traps

Models for mobility, recombination, etc

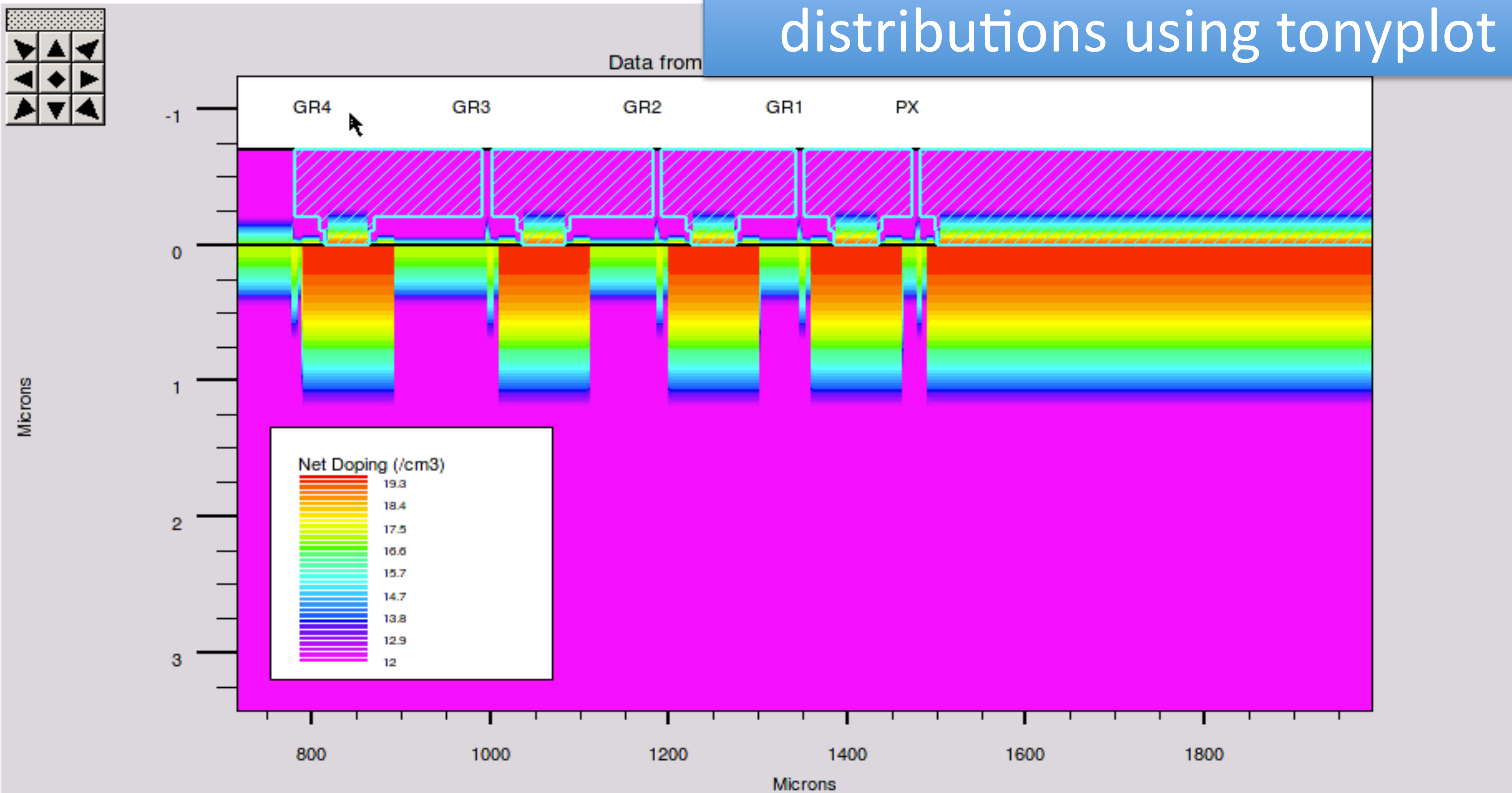
Interface models

Material modifications

Numerical methods

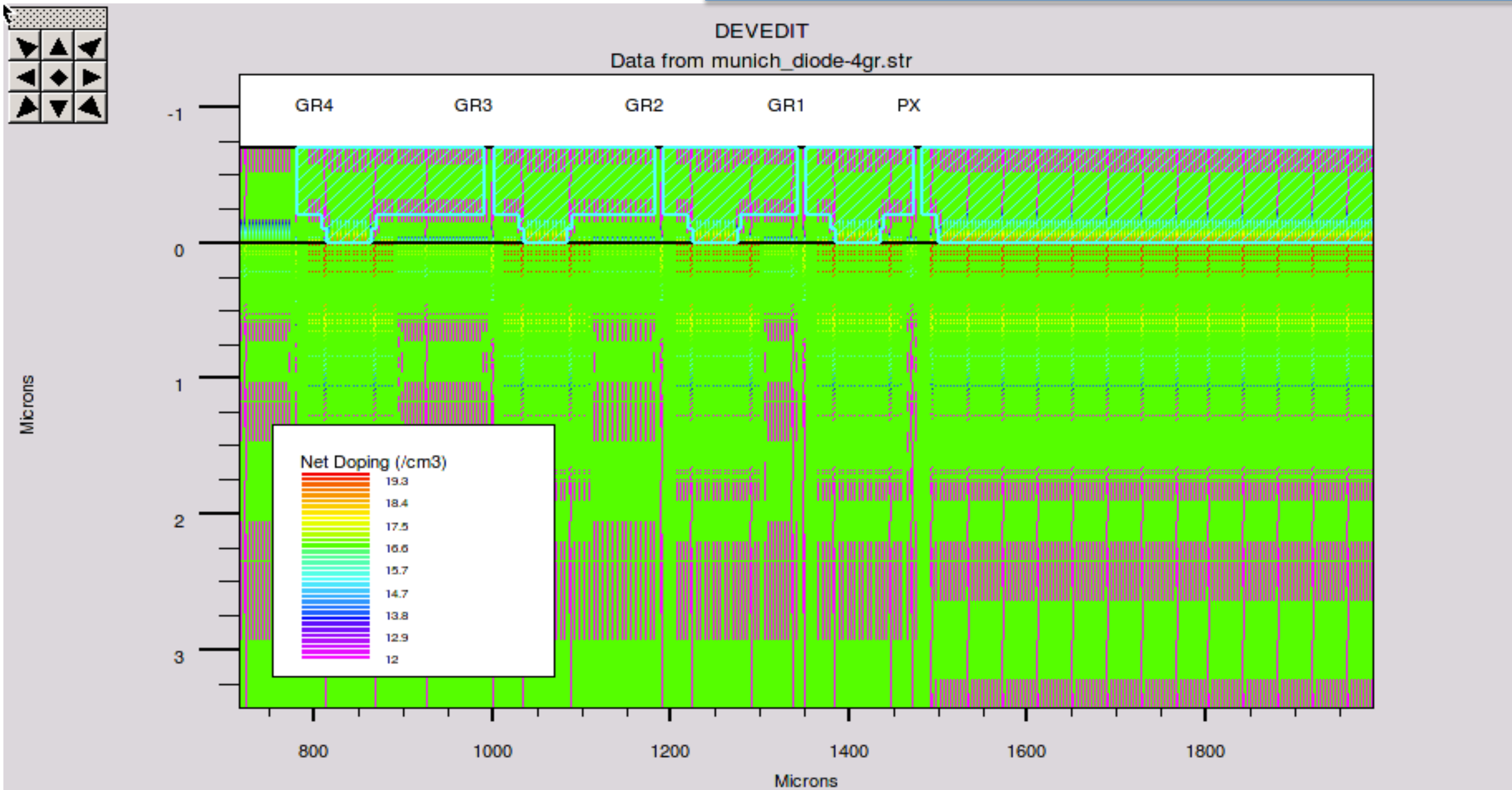
Tonyplot: plotting results

Check curves and 2D/3D distributions using tonyplot



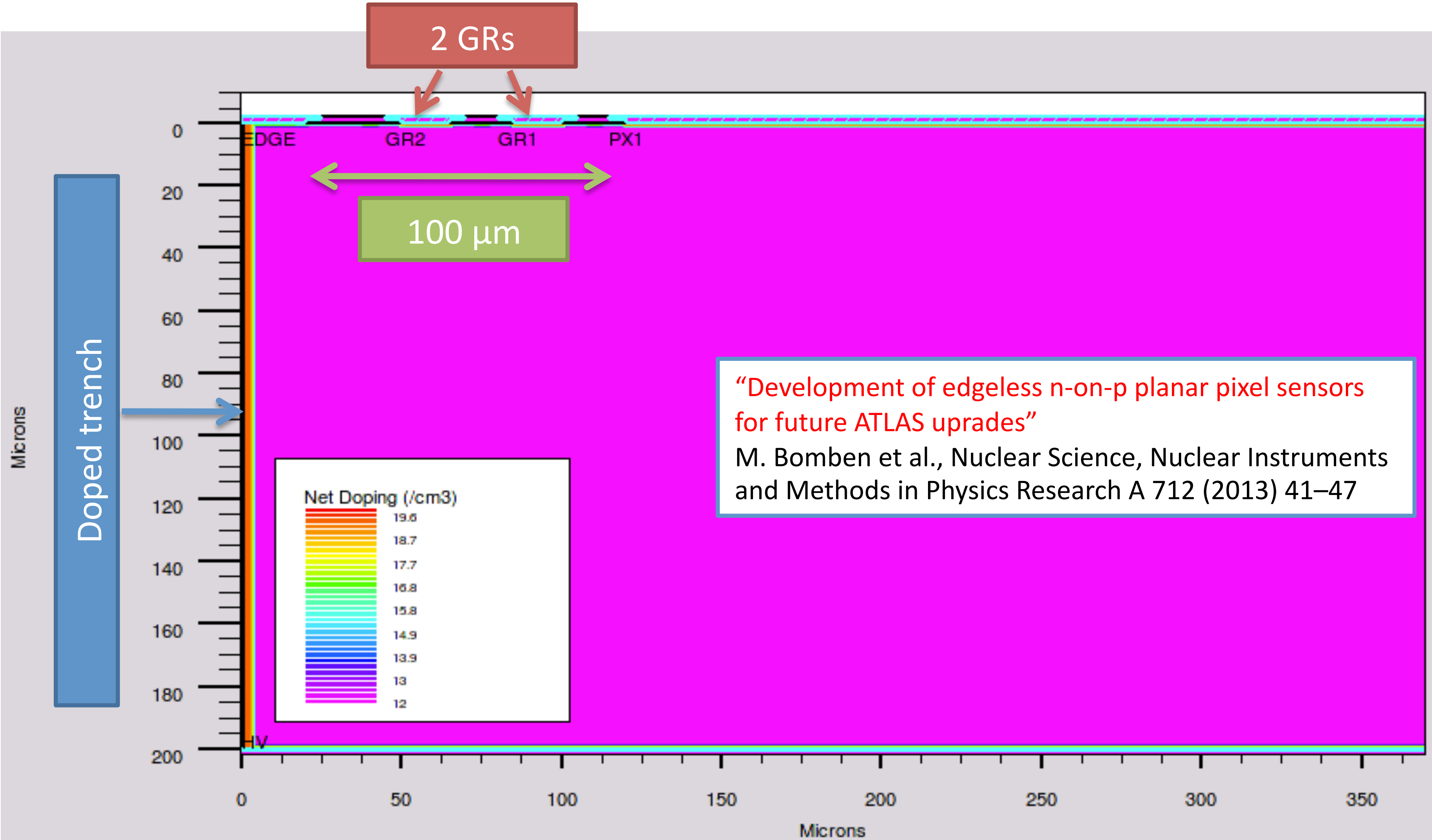
Tonyplot

Mesh structure



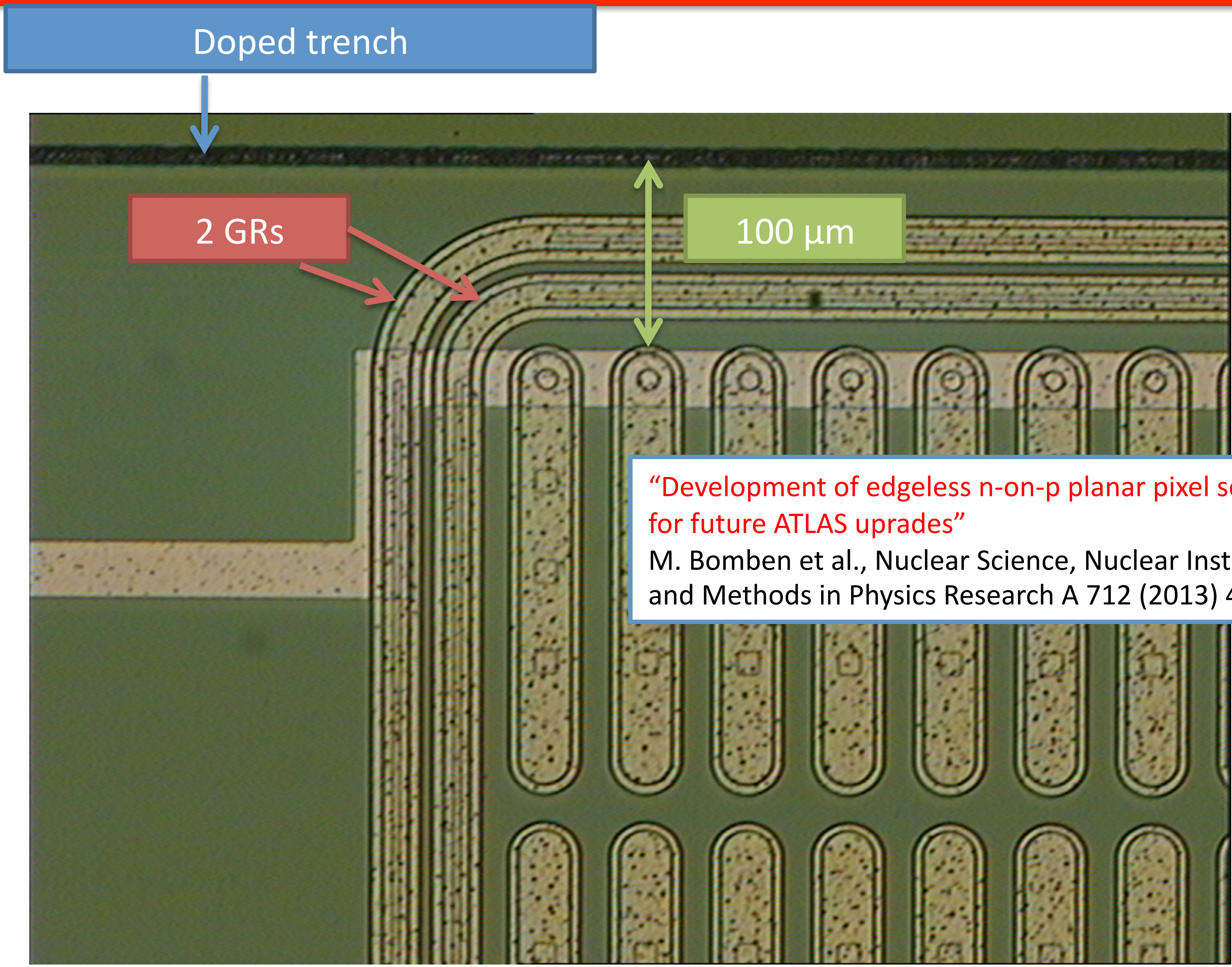
SELECTED RESULTS

A concrete example: Active Edge sensors



"Development of edgeless n-on-p planar pixel sensors for future ATLAS uprades"
M. Bomben et al., Nuclear Science, Nuclear Instruments and Methods in Physics Research A 712 (2013) 41–47

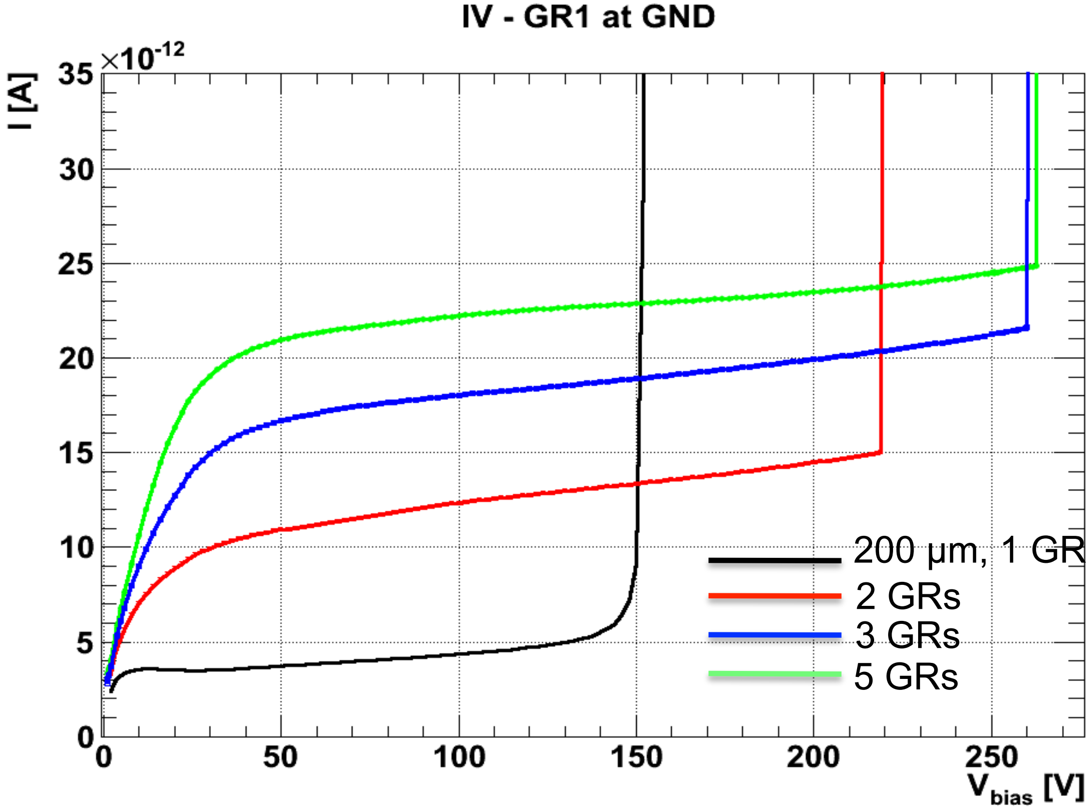
A concrete example: Active Edge sensors



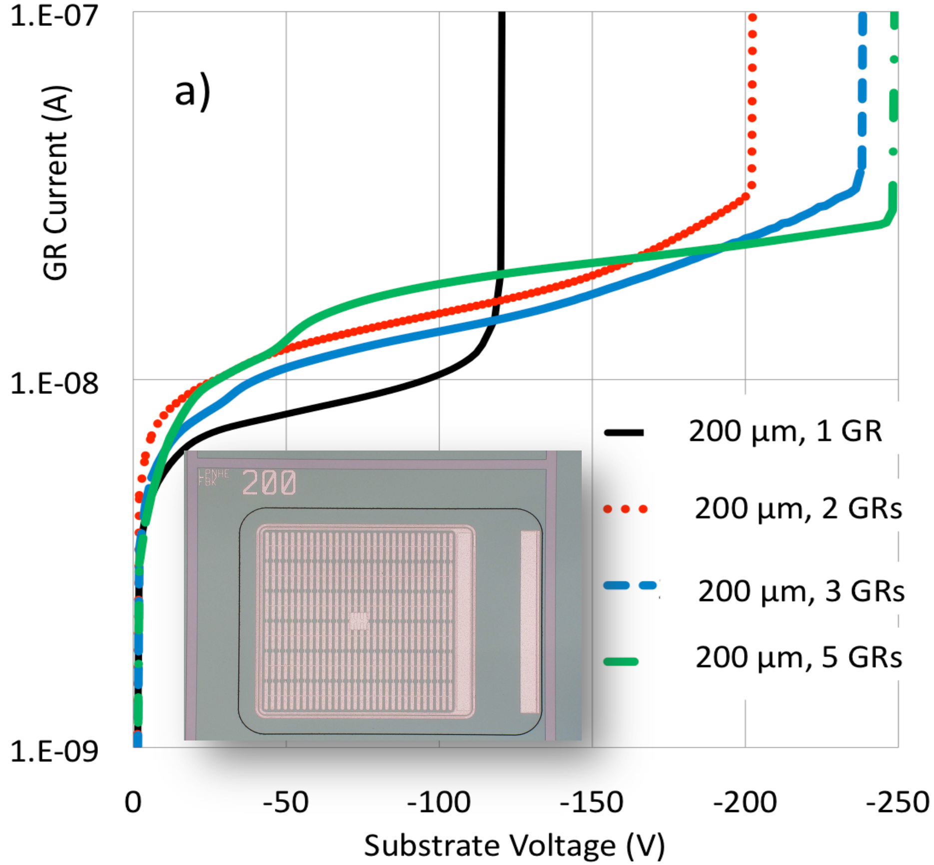
"Development of edgeless n-on-p planar pixel sensors for future ATLAS uprades"
M. Bomben et al., Nuclear Science, Nuclear Instruments and Methods in Physics Research A 712 (2013) 41–47

IV on test structures

SIMULATIONS

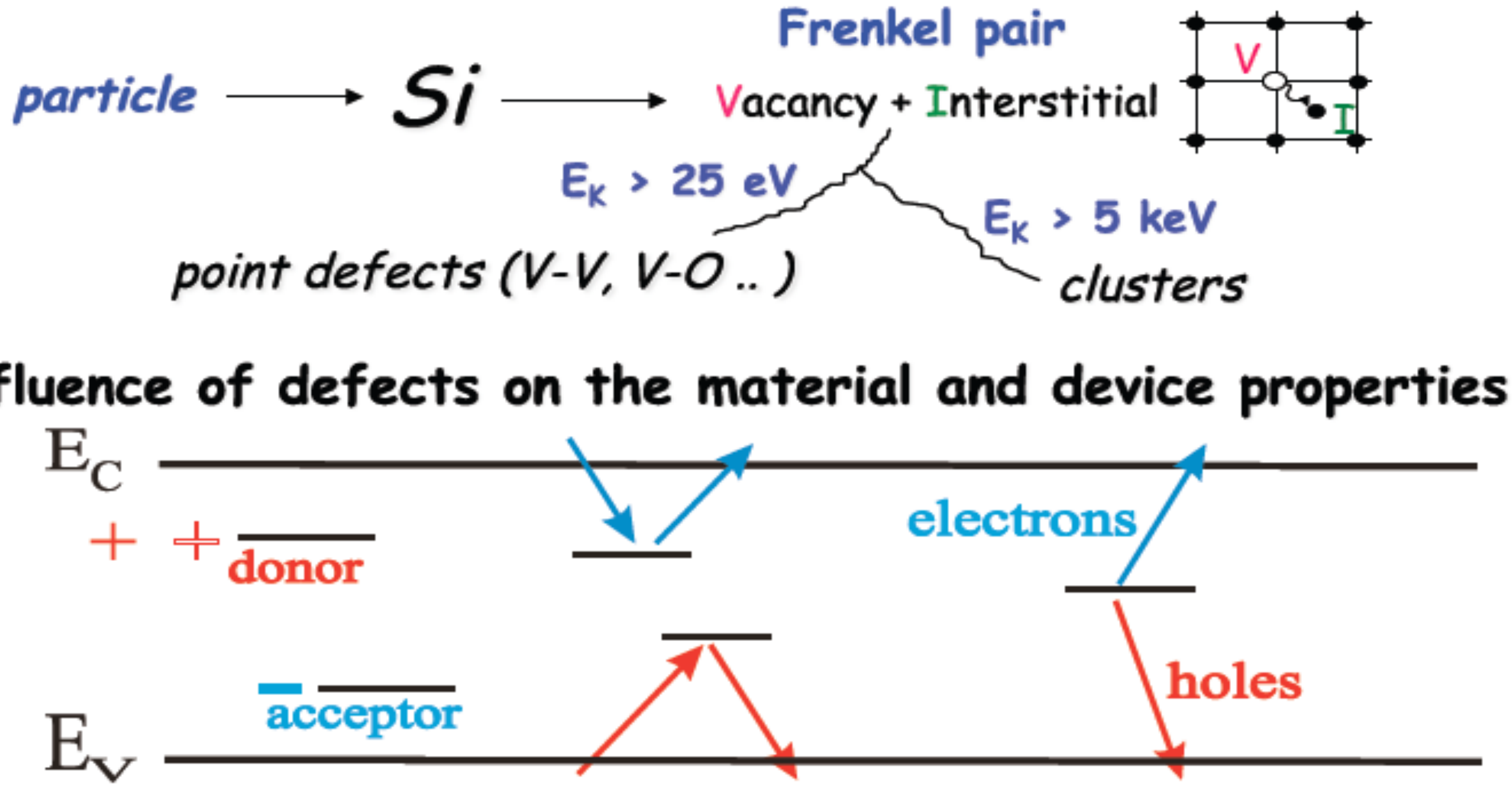


DATA



➢ **BD Voltage: Agreement within 20% or better**

Silicon microscopic damage effects



charged defects
⇒ N_{eff} , V_{dep}
e.g. donors in upper and acceptors in lower half of the band gap

trapping (e and h)
⇒ **CCE**
shallow defects do not contribute at room temperature due to fast detrapping

generation
⇒ **leakage current**
levels close to middle of the bandgap most effective

Panja Luukka, The Fifth International Forum on Advanced Material Science and Technology (IFAMST5 2006)

Radiation damage effects

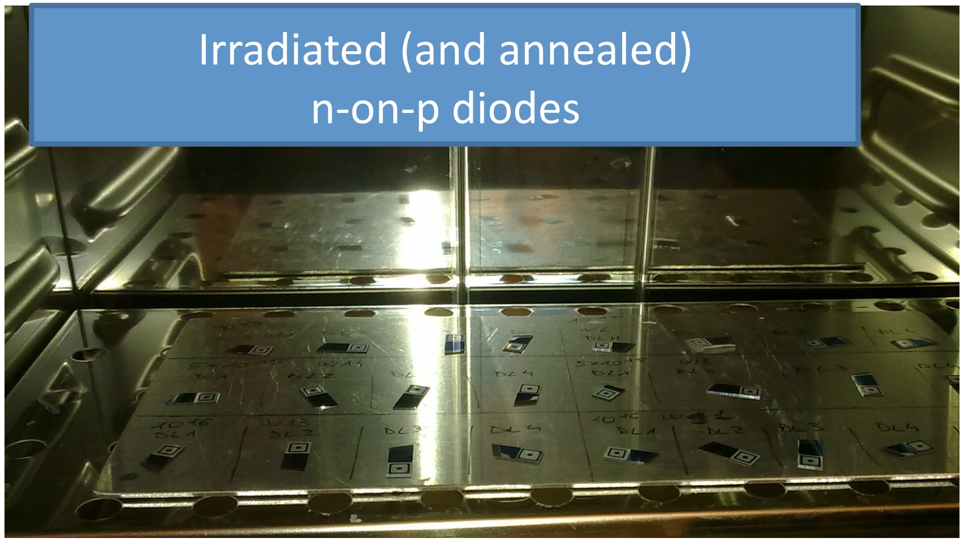
- Implement radiation damage effects via traps in the forbidden gap

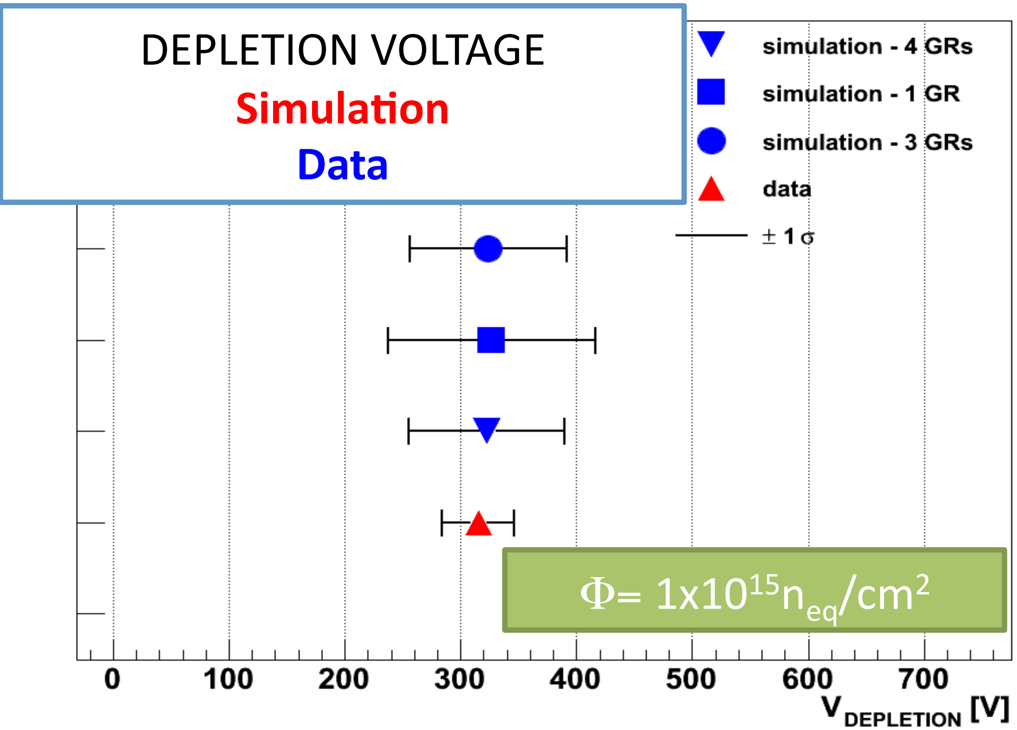
$$N = \eta \times \phi$$

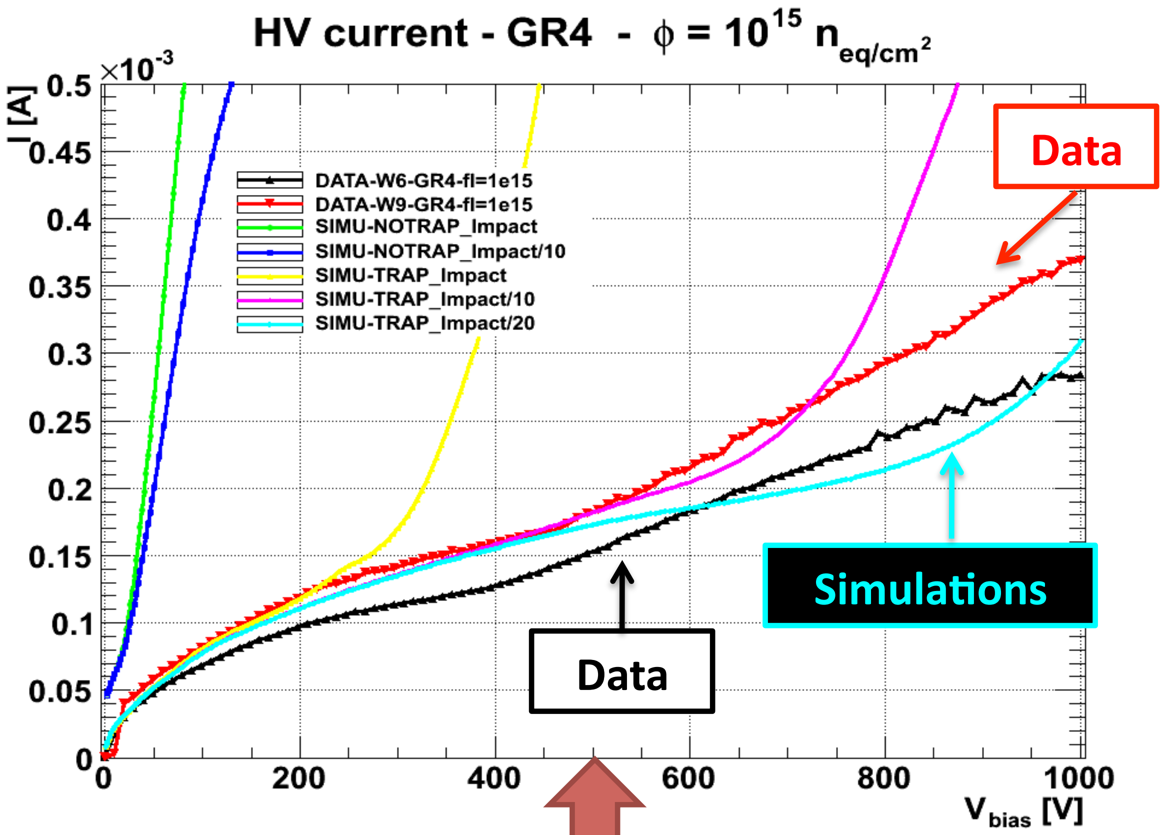
Type	Energy (eV)	$\sigma_e(\text{cm}^2)$	$\sigma_h(\text{cm}^2)$	$\eta(\text{cm}^{-1})$
A	E_C -0.42	9.5×10^{-15}	9.5×10^{-14}	1.613
A	E_C -0.46	5.0×10^{-15}	5.0×10^{-14}	0.9
D	E_V +0.36	3.23×10^{-13}	3.23×10^{-14}	0.9

"Simulations of radiation-damaged 3D detectors for the Super-LHC",
D. Pennicard et al., Nucl. Instrum. and Meth. A 592 (2008) 16-25

Data vs TCAD simulations







A lot of work for impact ionization models and interface traps and charges

Charge collection efficiency with MIP

- We can profit of SEU module to study the drift of charge released along a track

```
# Specify the charge track: normal incidence through the drain
singleeventupset entry="1800.0,0" exit="1800,300" pcunits b.density=1.6e-4 \
                 radialgauss radius=5  t0=2.e-11 tc=0
# Log file for transient
log outf="$'log_file_name'-SEU.log"
```

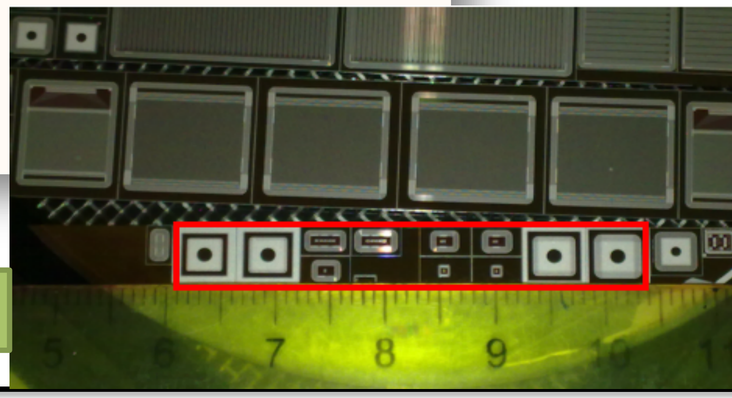
- Entry and exit point
- Charge per length unit
- Track time of arrival

```
# Early transient
method tstep.incr=1.25 dt.max=2.0e-13
solve tfinal=2.0e-12 tstep=2.5e-15 prev
save outf="$'file_name'-before-seu.str"

# SEU peak
#method mestep
solve tfinal=7.0e-12 tstep=2.0e-13 prev
save outf="$'file_name'-during-seu.str"

# Response to particle strike
#method lte.timestep tstep.incr=1.25 dt.max=2.5e-11
solve tfinal=3e-10 tstep=2.0e-13 prev
save outf="$'file_name'-particle.str"
```

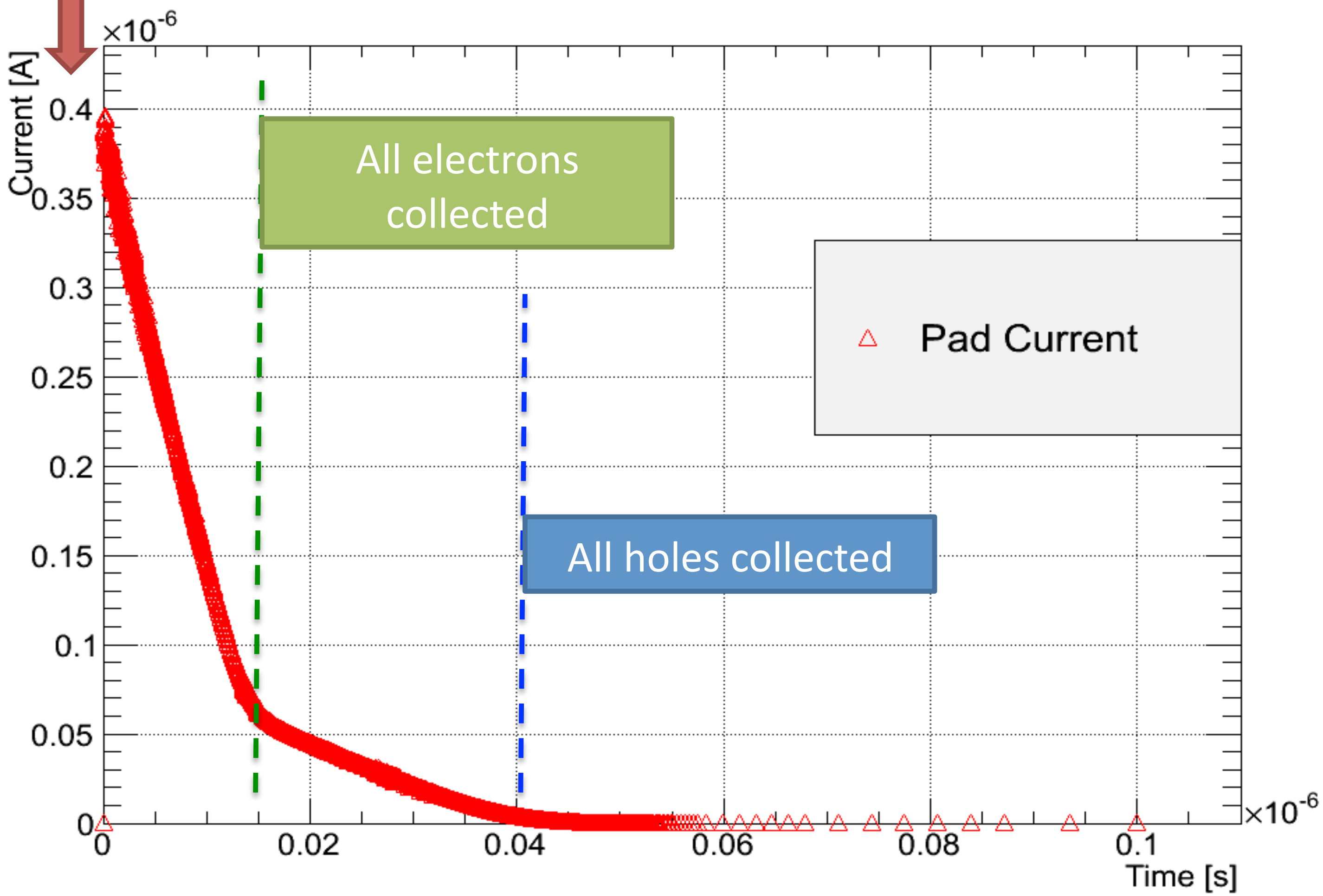
- Solution in the time-domain



In the following: results for n-on-p diodes

Response to a MIP

Expected Initial current ~ $\lambda\,(\langle v_e\rangle+\langle v_h\rangle) = 3.9\times10^{-7}$ A



P-bulk: irradiation models

Petasecca p-bulk

"Numerical Simulation of Radiation Damage Effects in p-Type and n-Type FZ Silicon Detectors,"
Petasecca, M. et al, Nuclear Science, IEEE Transactions on , vol.53, no.5, pp.2971-2976, Oct. 2006,

Type	Energy (eV)	Defect	$\sigma_e(\mathrm{cm}^2)$	$\sigma_h(\mathrm{cm}^2)$	$\eta(\mathrm{cm}^{-1})$
Acceptor	E_C -0.42	VV	2.0×10^{-15}	2.0×10^{-14}	1.613
Acceptor	E_C -0.46	VVV	5.0×10^{-15}	5.0×10^{-14}	0.9
Donor	E_V +0.36	C_iO_i	2.5×10^{-14}	2.5×10^{-15}	0.9

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Donor	E_V +0.36	C_iO_i	3.23×10^{-13}	3.23×10^{-14}	0.9

CCE studies for n-on-p sensors – MPP group

Tested n-in-p Float Zone (FZ) sensors

Max-Planck-Institut für Physik
(Werner-Heisenberg-Institut)

VTT active/slim edges:

- FE-I3 100 μm
- FE-I4 100 μm
- FE-I4 200 μm

CiS production:

- FE-I4 200 μm
- FE-I4 200 μm
- FE-I4 300 μm

Irradiations:

- 5×10^{15} n_{eq}/cm^2 (1@KIT + 4@JSI)
- 5×10^{15} n_{eq}/cm^2 (KIT)
- 6×10^{15} n_{eq}/cm^2 (2@KIT + 4@JSI)
- 7×10^{15} n_{eq}/cm^2 (LANSCE)
- 14×10^{15} n_{eq}/cm^2 (LANSCE)
- 14×10^{15} n_{eq}/cm^2 (LANSCE)

Irradiation facilities:

- JSI: $E \leq 10$ MeV reactor neutrons
- KIT: 25 MeV protons
- LANSCE: 800 MeV protons

S Terzo *et al* 2014
JINST **9** C12029

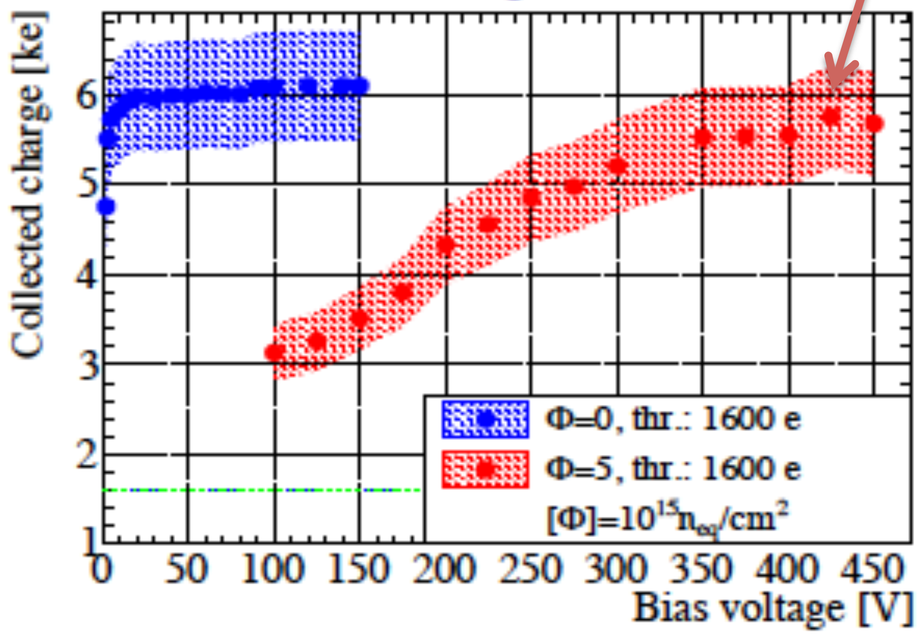
25th RD50 Workshop
19 - 21 November 2014
at CERN

B. Paschen (MPP München) Characterization of thin n-in-p planar pixel sensors

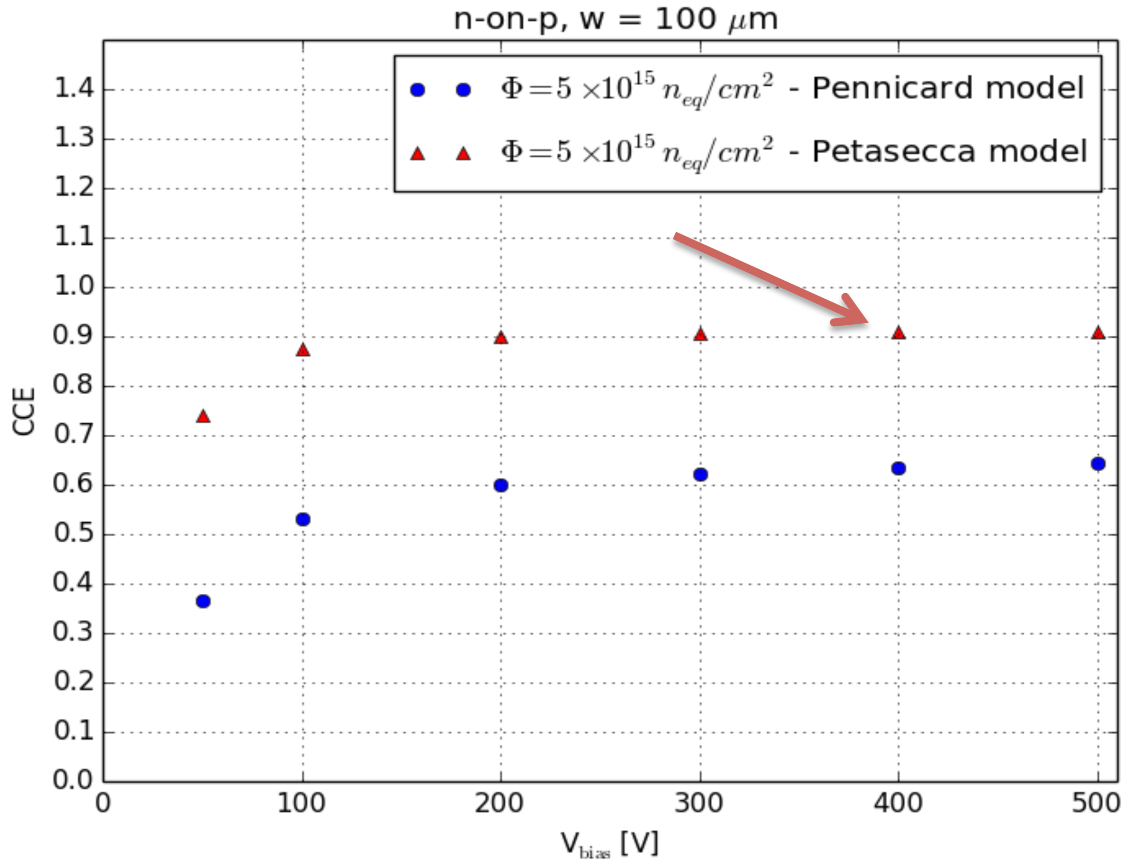
CCE: data-simulation comparison

FE-I4 100 μm

- $5 \times 10^{15}\ n_{eq}/cm^2$ (KIT)



- CCE: (95 ± 13) % at $V_{bias} = 425\ V$



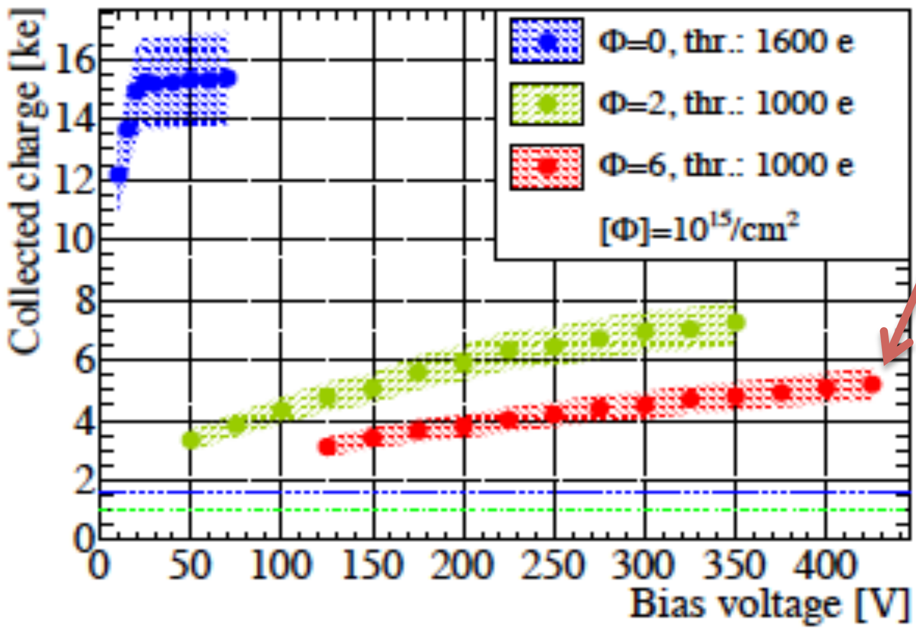
✓ Good agreement with the Petasecca model

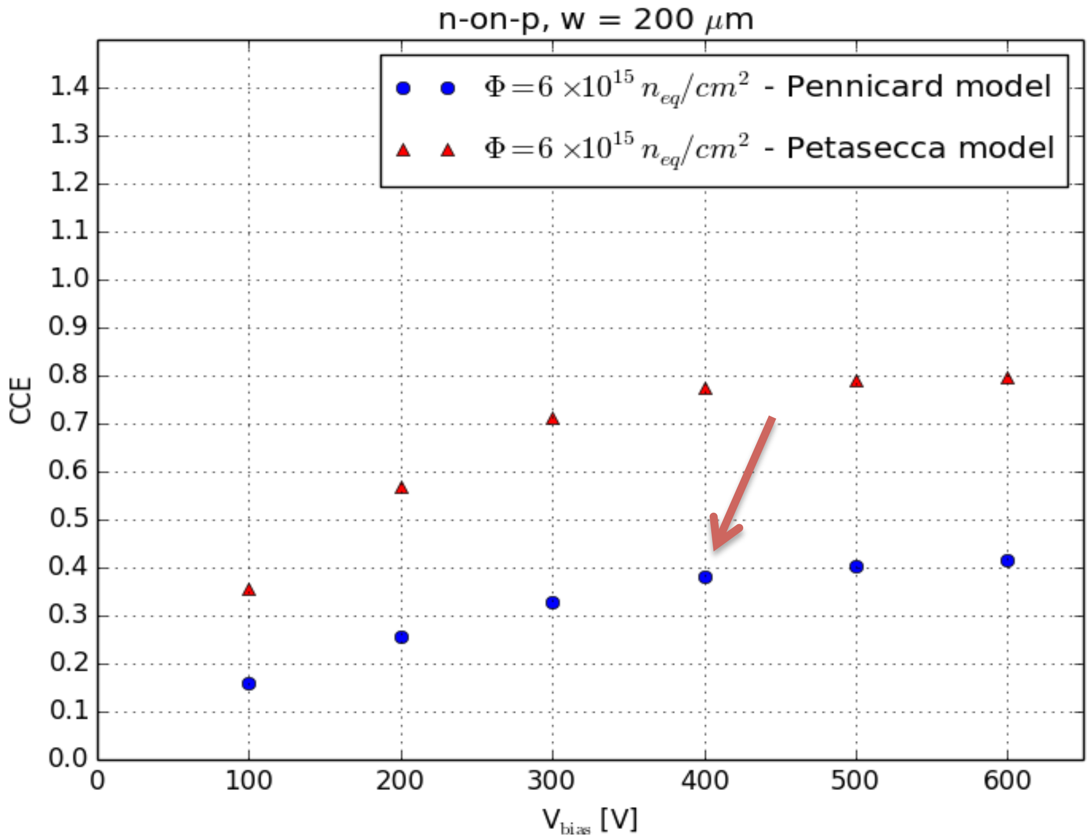
- Pennicard one foresees a too severe trapping

CCE: data-simulation comparison

FE-I4 200 μm

- $6 \times 10^{15}\ n_{eq}/cm^2$ (2@KIT + 4@JSI)

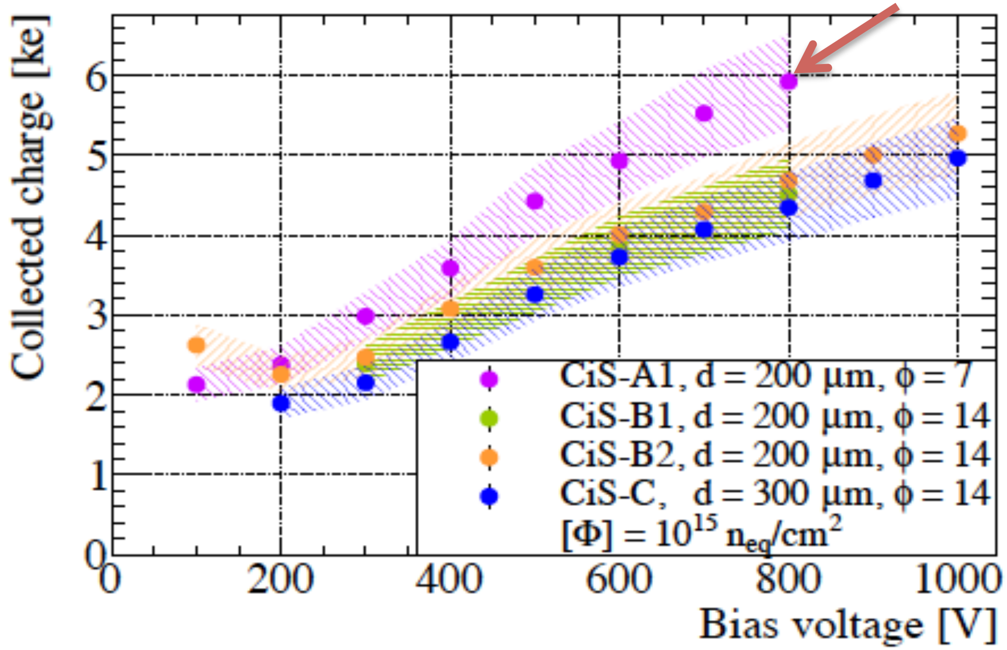


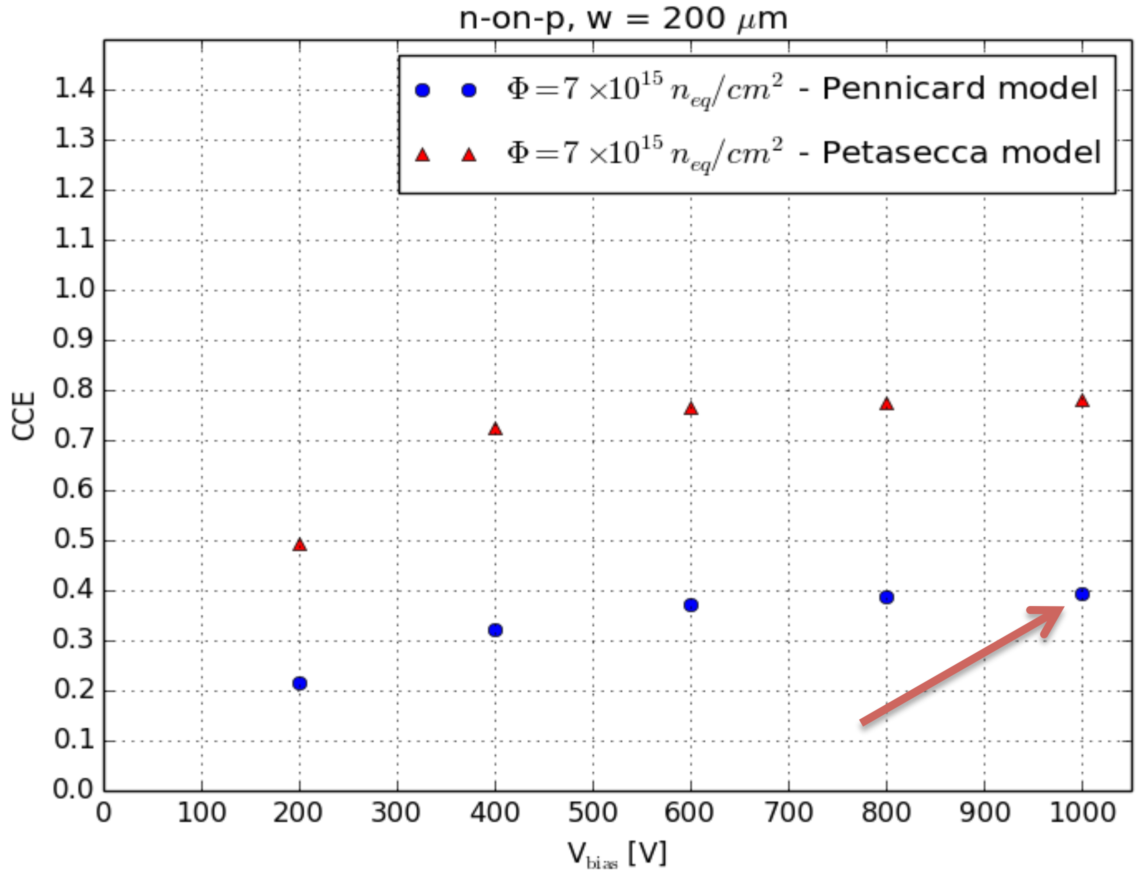


- CCE: (35 ± 5) % at $V_{\text{bias}} = 425\ V$

✓ Good agreement with the Pennicard model
▪ Petasecca one foresees a less severe trapping
? Annealing effect? Mixed irradiations effect?

CCE: data-simulation comparison



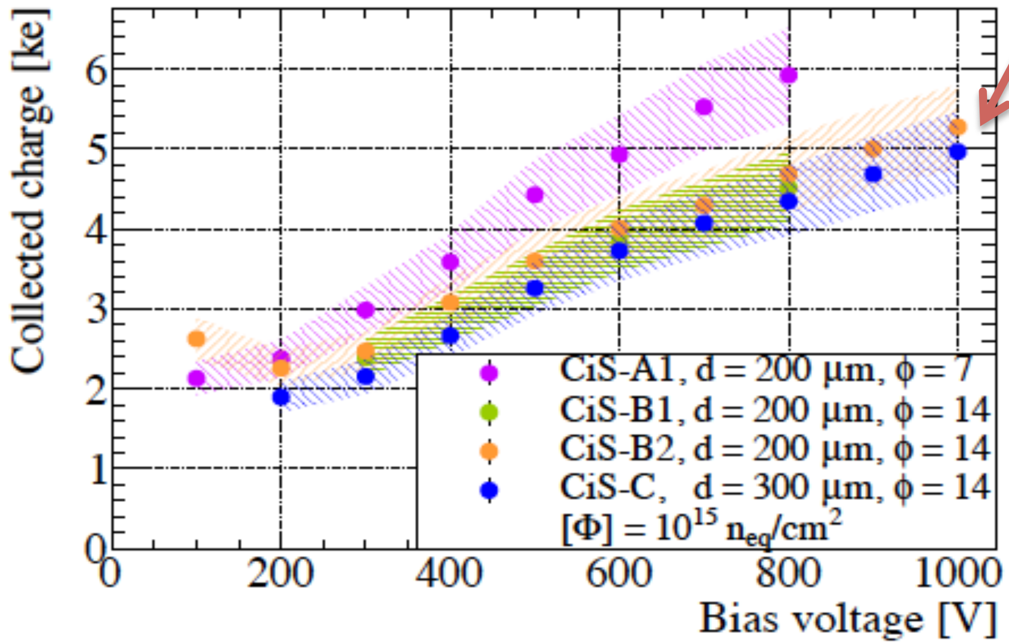


CCE of 200 μm sensors:

- $7 \times 10^{15}\ \mathrm{n_{eq}/cm^2} \rightarrow (45 \pm 6)$ %
- $14 \times 10^{15}\ \mathrm{n_{eq}/cm^2} \rightarrow (35 \pm 5)$ %
- LANSCE: 800 MeV protons

✓ Good agreement with the Pennicard model
▪ Petasecca one foresees a less severe trapping
? Annealing effect? Non unform irradiations effect?

CCE: data-simulation comparison



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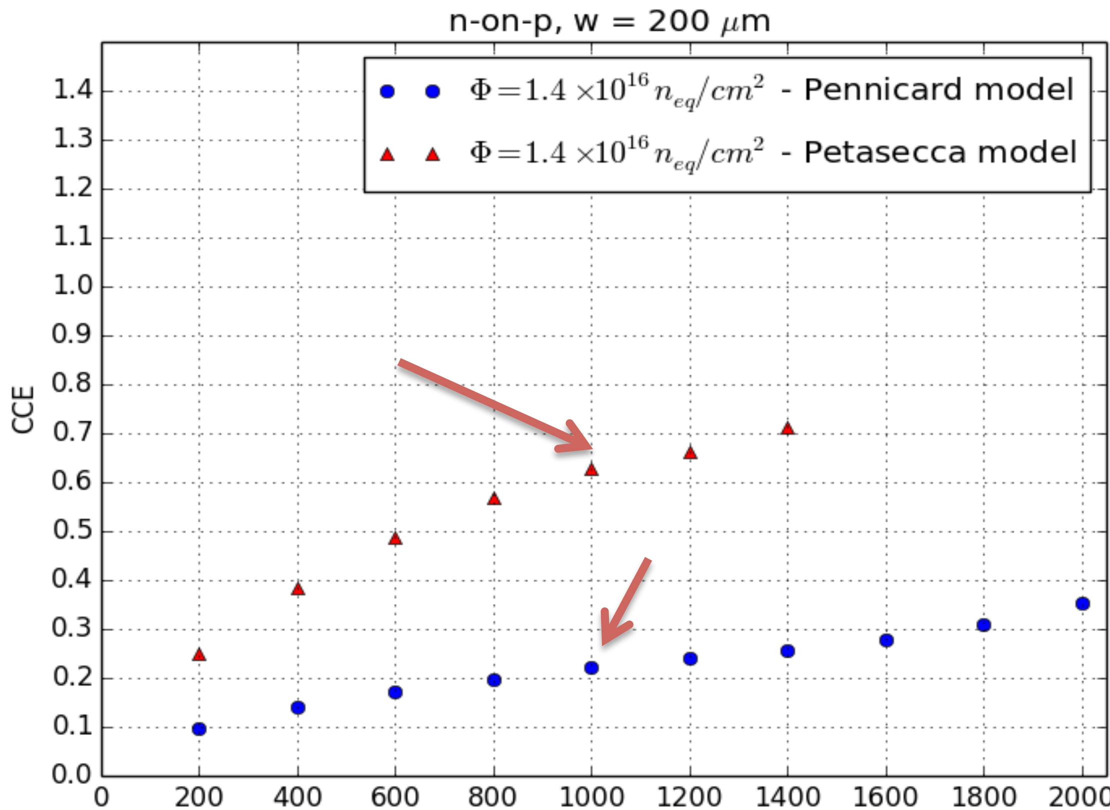


▪ None of the model gives a reasonble prediction for the CCE

➢ Need to develop a better model

?Annealing effect?

?Non uniform irradiation effects?

➢ **These questions can be addressed using simulations**

Extract electric field from TCAD sims & tb data

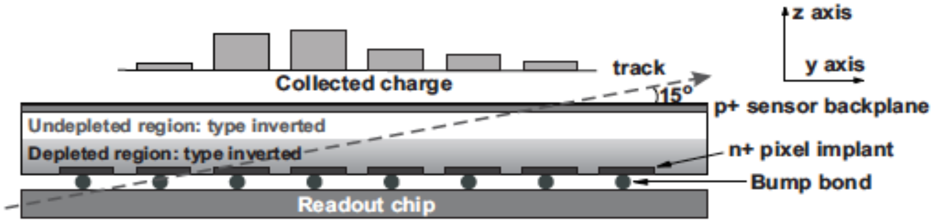
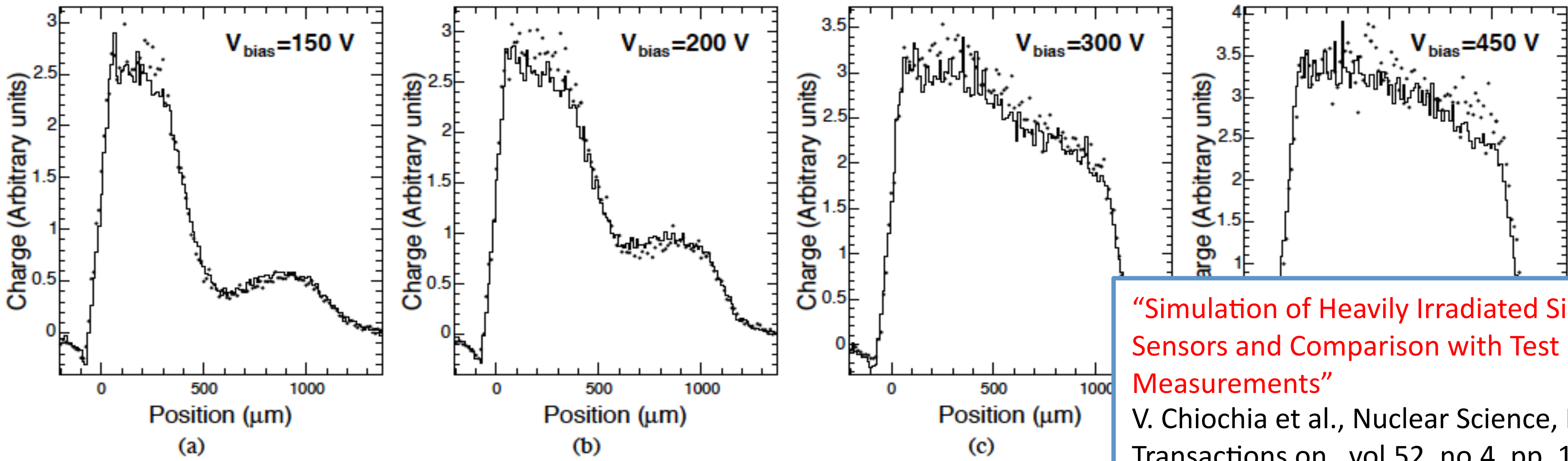


Fig. 2

THE GRAZING ANGLE TECHNIQUE FOR DETERMINING CHARGE COLLECTION PROFILES. THE CLUSTER LENGTH IS PROPORTIONAL TO THE DEPTH OVER WHICH CHARGE IS COLLECTED.

- Study of Charge Collection as a function of charge deposition depth
- Parameterization of the Electric Filed in simulations
- Comparison data/simulation



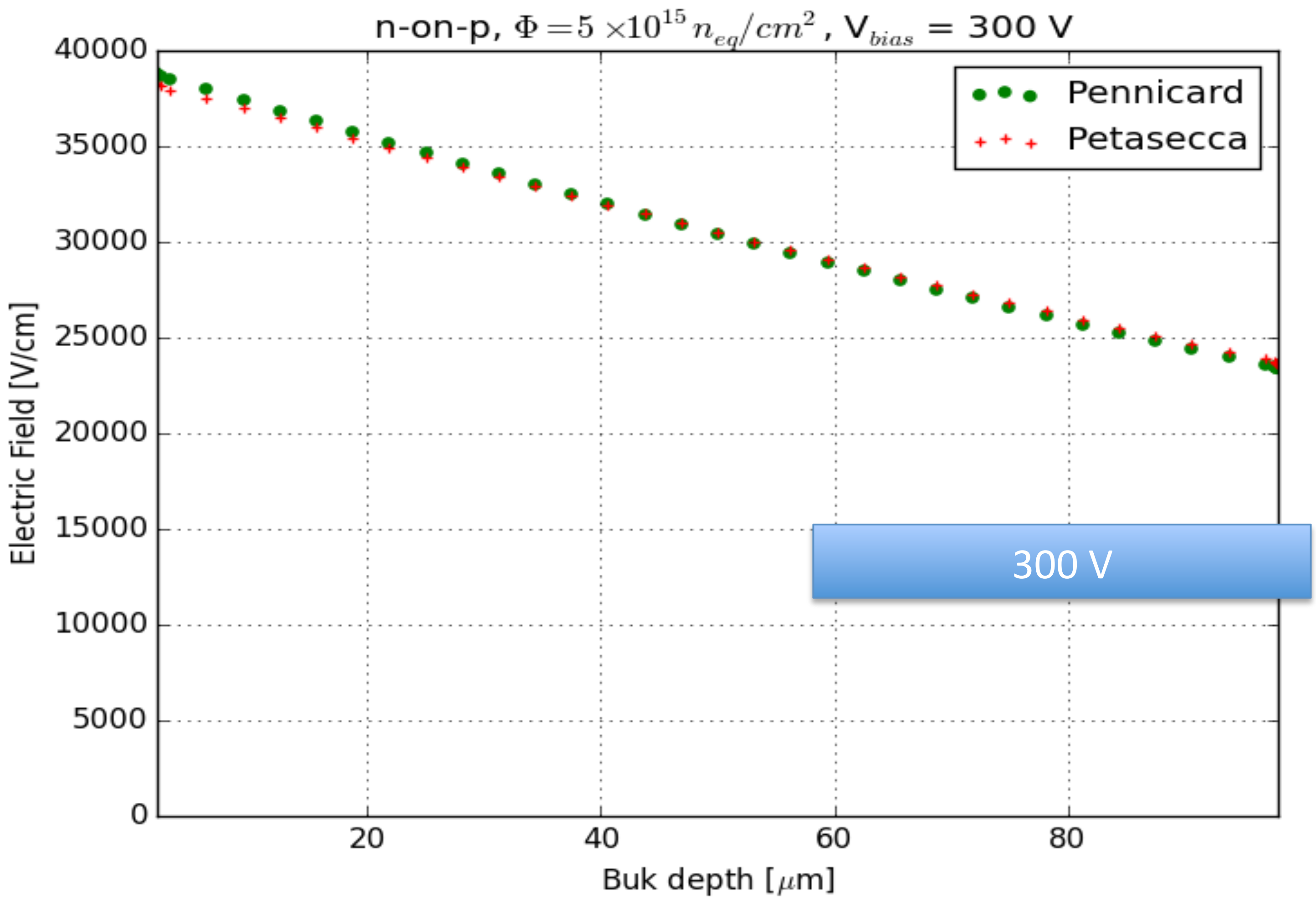
"Simulation of Heavily Irradiated Silicon Pixel Sensors and Comparison with Test Beam Measurements"
V. Chiochia et al., Nuclear Science, IEEE Transactions on , vol.52, no.4, pp. 1067- 1075, Aug. 2005

Fig. 10

THE MEASURED CHARGE COLLECTION PROFILES AT BIAS VOLTAGES OF 150 V, 200 V, 300 V, AND 450 V ARE SHOWN AS SOLID DOTS FOR FLUENCES OF 6×10^{14} N_{eq}/CM^2. THE BF SIMULATION IS SHOWN AS THE SOLID HISTOGRAM IN EACH PLOT.

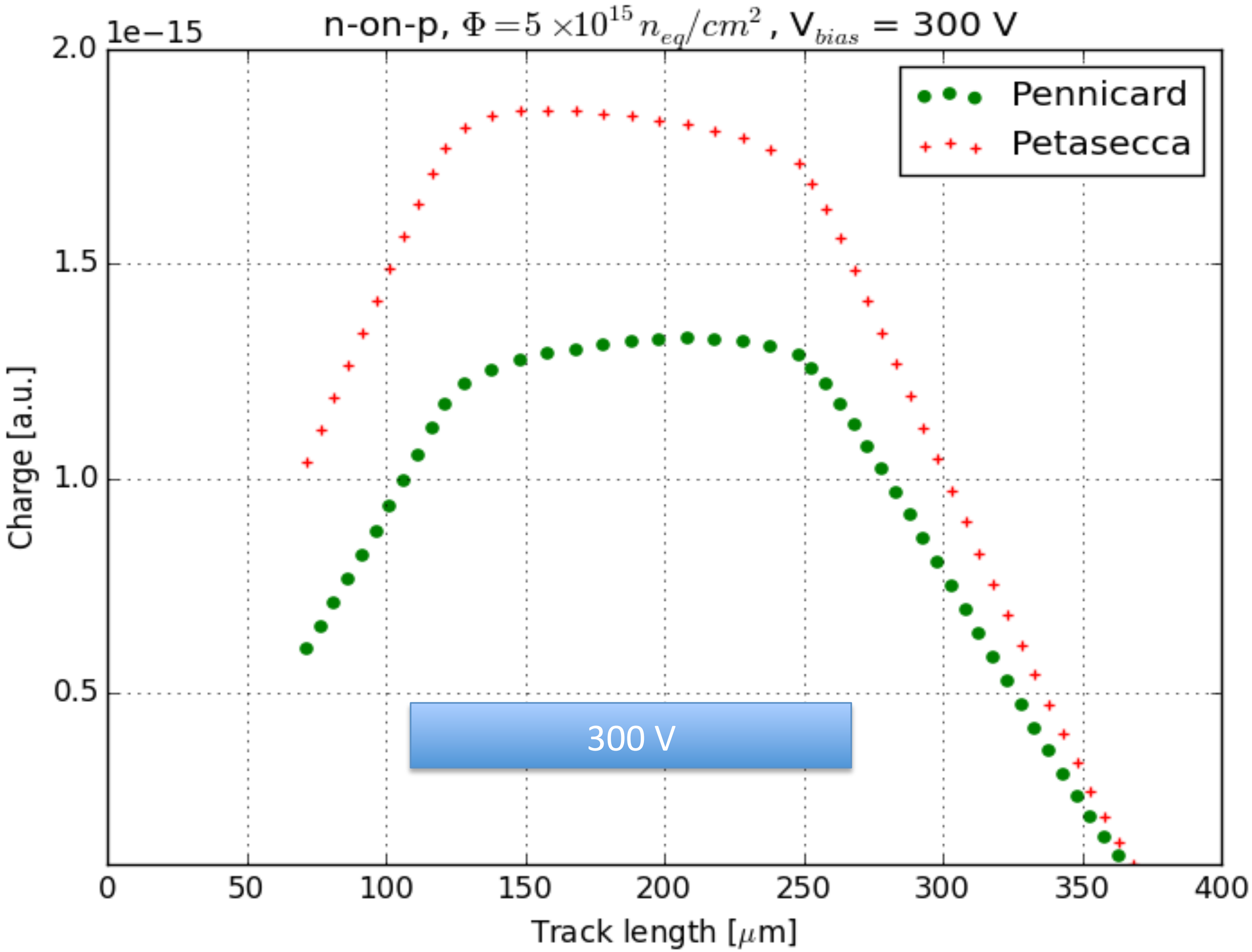
Electric field distribution

Similar predictions from the 2 models

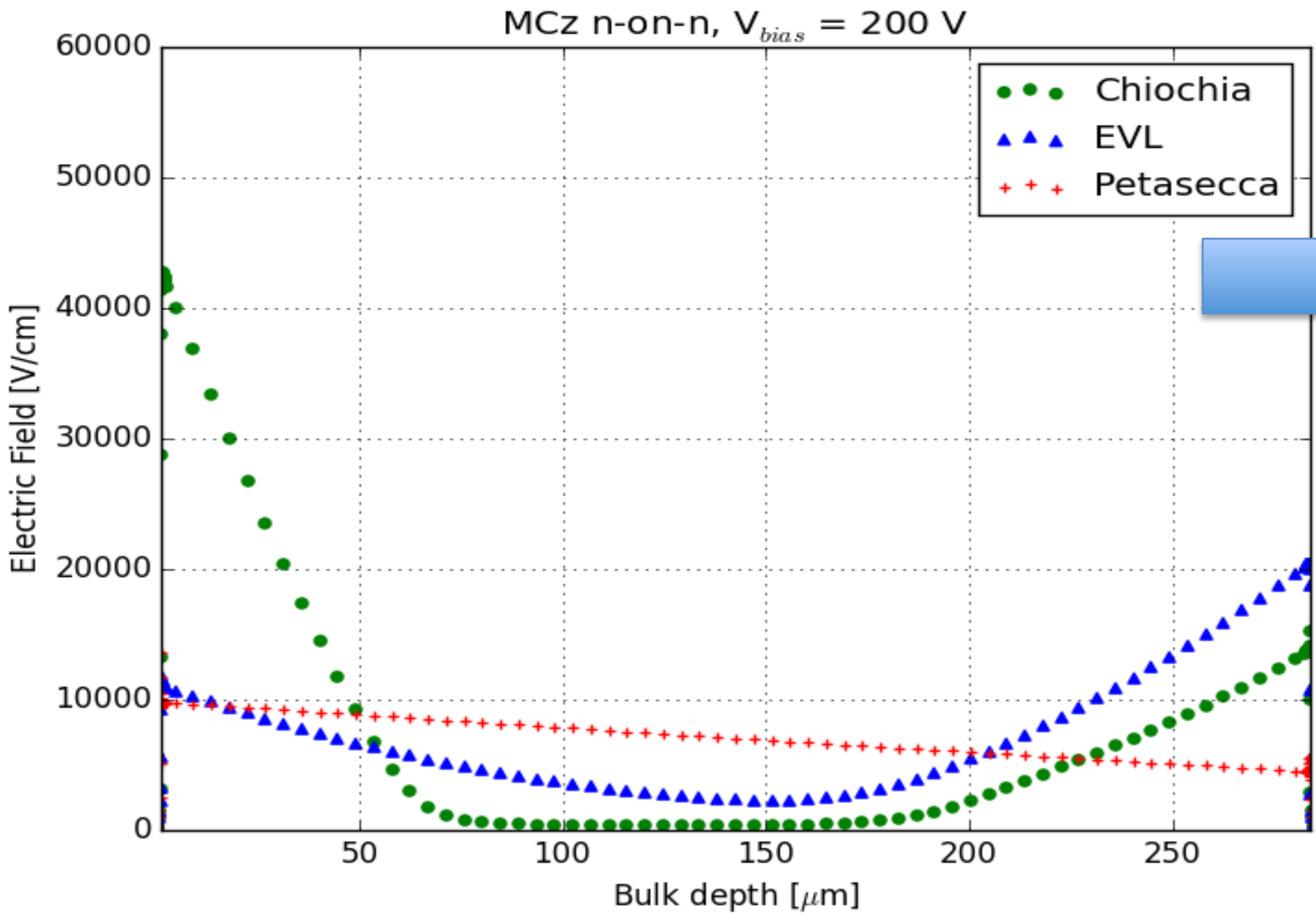


Charge collection profile

We can discriminate them!

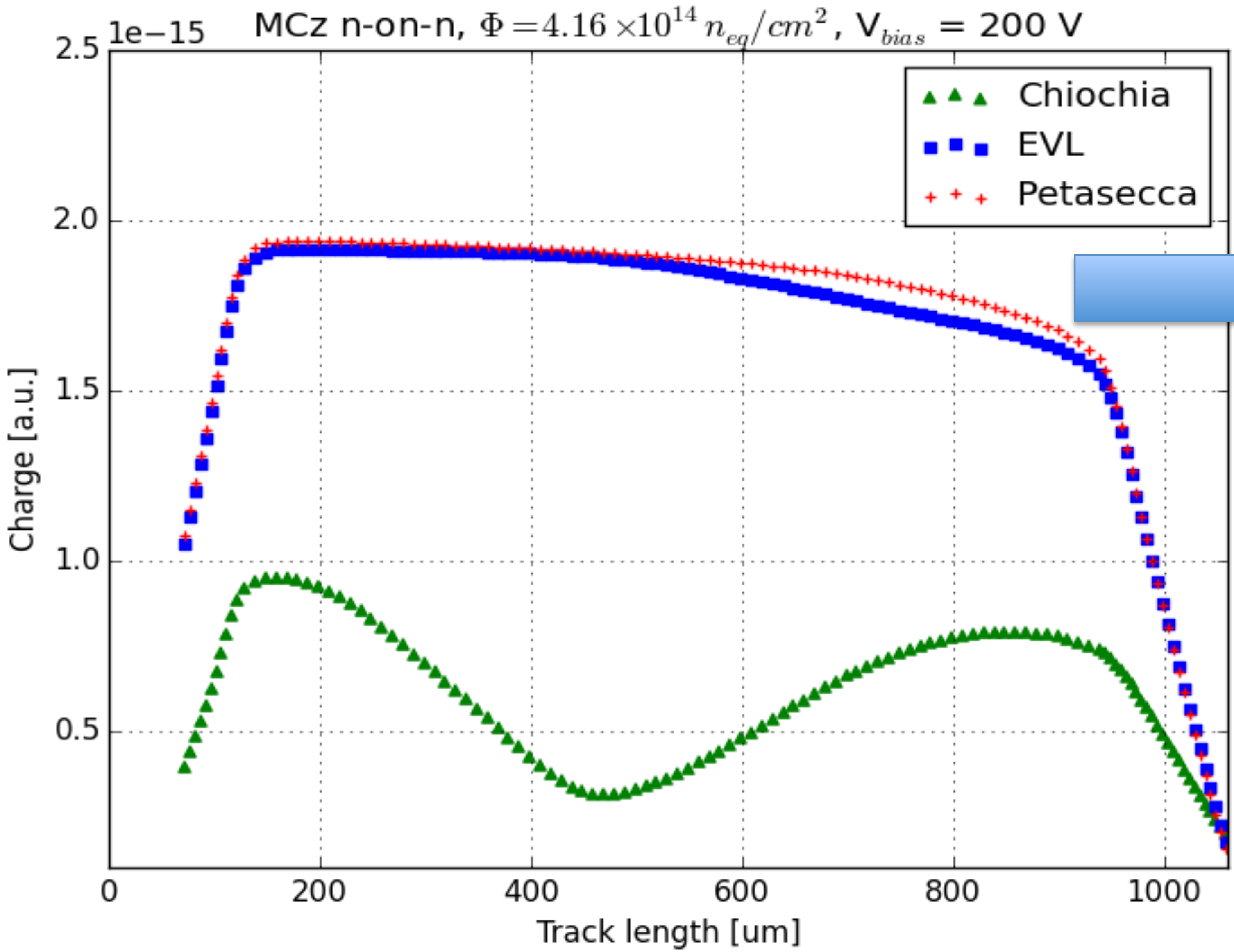


N-on-n pixels – Electric field profile comparison



200 V

N-on-n pixels – Charge profile



200 V

COMMENTS AND CONCLUSIONS

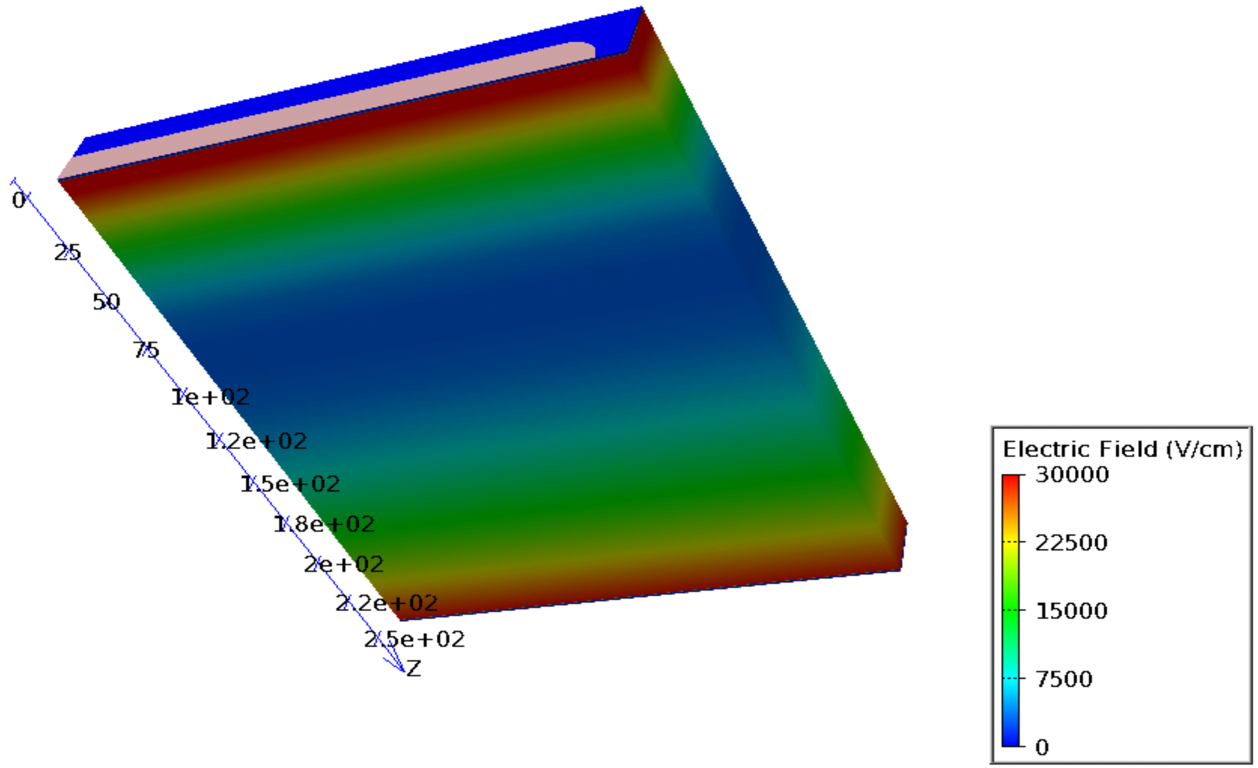
Conclusions

- TCAD is a very powerful tool for HEP silicon sensors
- You can reduce the number of submission, and so cutting time and money to get results
- Combining TCAD simulations and testbeam data can probe fundamental quantities like electric field distribution, trapping, etc.
- A solid knowledge of semiconductor physics,and good data inputs are recommended to fully exploit TCAD simulations

One last remark

- If you are interested in working with TCAD simulations, feel free to contact me: marco.bomben@cern.ch

➢ Thank you!



BACKUP MATERIAL

Devedit: device structure editor

Deckbuild V3.42.2.R - ledex03.in, dir; /home/mbomben/work/Tcad/tut

File | View | Edit | Find | Main Control | Commands | Tools

```
go devedit
work.area x1=0 y1=-0.1 x2=3.5 y2=10
# devedit 2.8.5.R (Wed Mar  1 14:54:21 PST 2006)
# libMeshBuild 1.24.3 (Wed Mar  1 14:53:36 PST 2006)
# libSVC_Misc 1.28.0 (Tue Jan 31 20:56:53 PST 2006)
# libsflm 7.2.13 (Wed Feb 22 00:28:57 PST
# libSDB 1.8.3 (Tue Feb 21 23:41:46 PST 20
# libSvcFile 1.12.0 (Tue Jan 17 01:48:56 P
# libDW_Version 3.2.0 (Mon Jan 16 23:45:02
region reg=1 mat=GaN color=0xcba2a2 patter
        polygon="1.85,2 1.95,2 3.45,2 3.5,
#
impurity id=1 region.id=1 imp=Donors \
        peak.value=1e+18 ref.value=1000000
#
constr.mesh region=1 default max.height=10

region reg=2 mat=InGaN color=0xfe8282 patt
        polygon="1.85,0.603 0,0.603 0,0.6
#
impurity id=1 region.id=2 imp="Composition
        peak.value=0.2 ref.value=100000000
#
constr.mesh region=2 default

region reg=3 mat=AlGaN color=0xfe8282 patt
        polygon="1.85,0.6 0,0.6 0,0.5 1.85
#
```

Define implants, electrodes, oxidations, ecc using DEVEDIT

Deckbuild V3.42.2.R - munich_diode.de, dir;

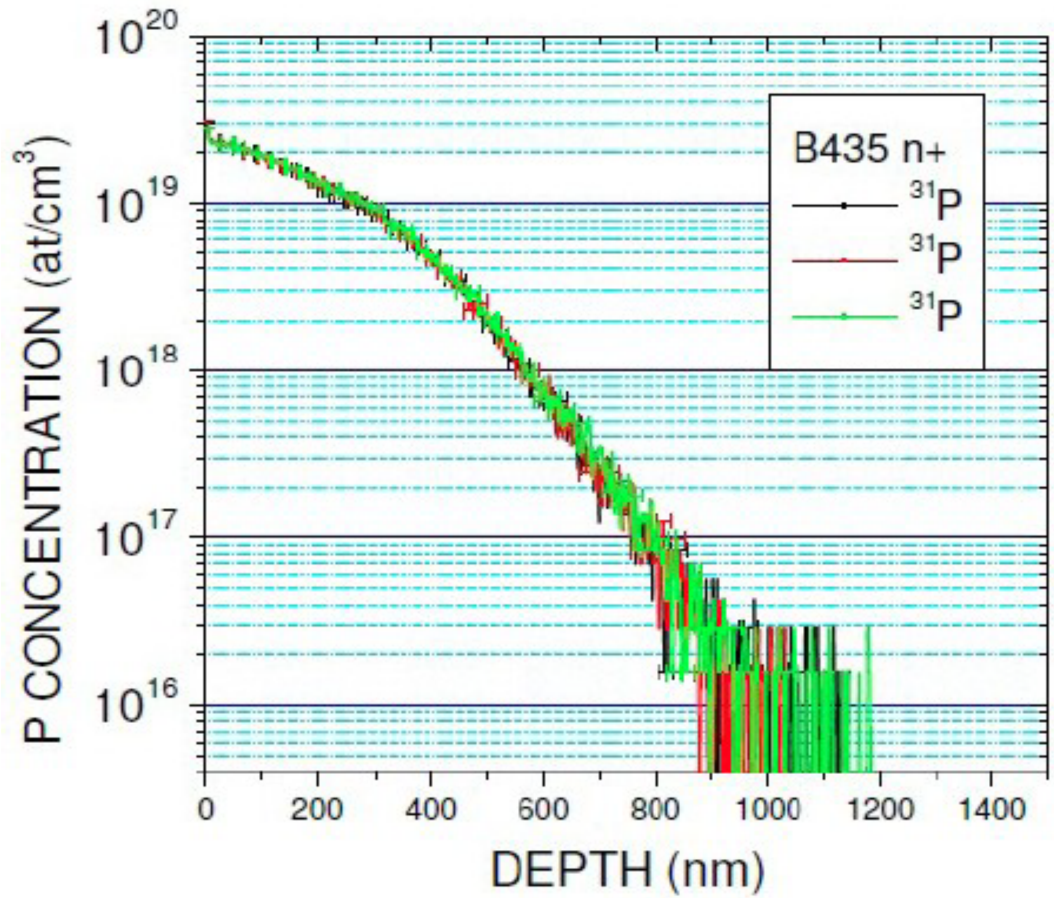
File | View | Edit | Find | Main Control | Commands | Tools

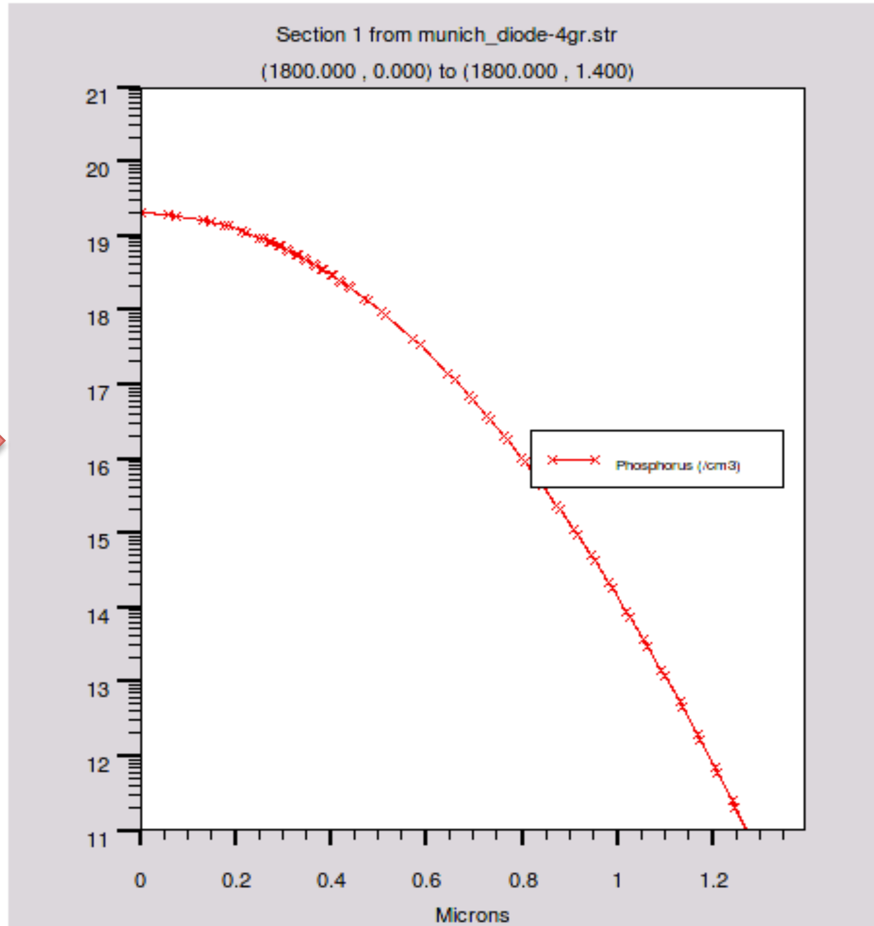
```
  set pixel_rolloff = $nplus_rolloff
else
  set pixel_rolloff = $pplus_rolloff
if.end

set pix_x1=$x_left_implant-($pixel_rolloff*$nsigma_rolloff)
set pix_x2=$x_right_implant+($pixel_rolloff*$nsigma_rolloff)
set pix_y1=0-($pixel_rolloff*2*$nsigma_rolloff)
set pix_y2=0+($pixel_rolloff*2*$nsigma_rolloff)

if cond = ($pix_impurities_conc < 0)
  set pix_imp_c=-$pix_impurities_conc
  impurity id=$id_impur imp=Phosphorus color=0x8c5d00 \
    peak.value=$pix_imp_c ref.value=1e16 \
    comb.func=Multiply \
    y1=0 y2=$pix_depth rolloff.y=high \
    conc.func.y=gauss.dist conc.param.y=$nplus_rolloff \
    x1=$x_left_implant x2=$x_right_implant rolloff.x=both \
    conc.func.x=gauss.dist conc.param.x=$nplus_rolloff
else
  impurity id=$id_impur imp=Boron color=0x8c5d00 \
    peak.value=$pix_impurities_conc ref.value=1e16 \
    comb.func=Multiply \
    y1=0 y2=$pix_depth rolloff.y=high \
    conc.func.y=gauss.dist conc.param.y=$pplus_rolloff \
    x1=$x_left_implant x2=$x_right_implant rolloff.x=both \
    conc.func.x=gauss.dist conc.param.x=$pplus_rolloff
if.end
```

Pixel implant

Intermezzo: TCAD inputs

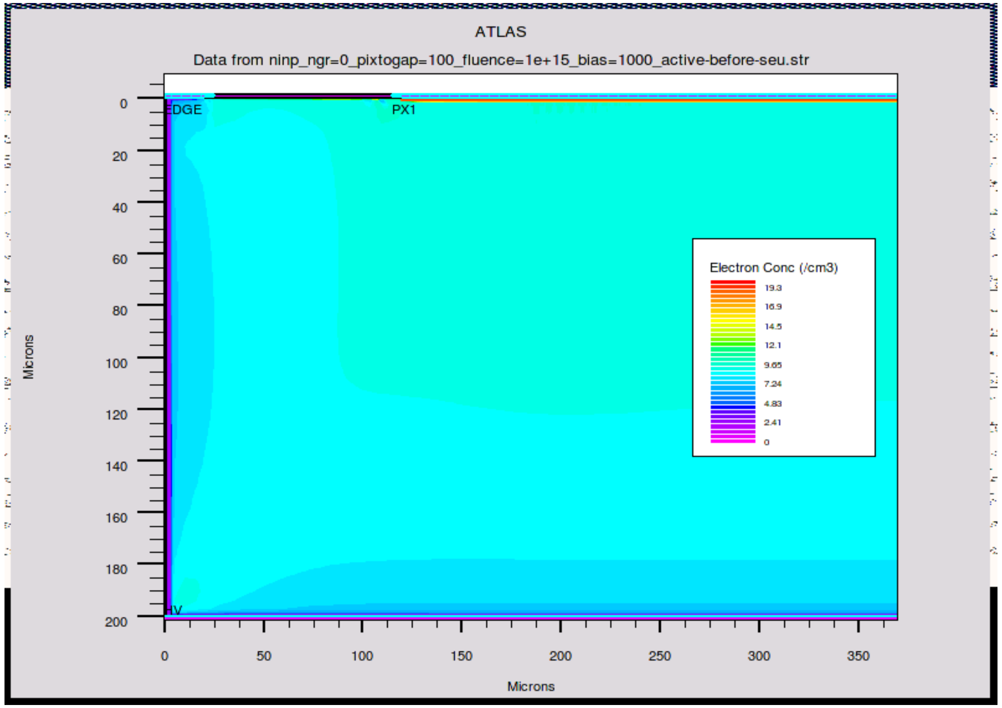
- To get reliable predictions you need precise inputs; *e.g.* doping profiles via SIMS



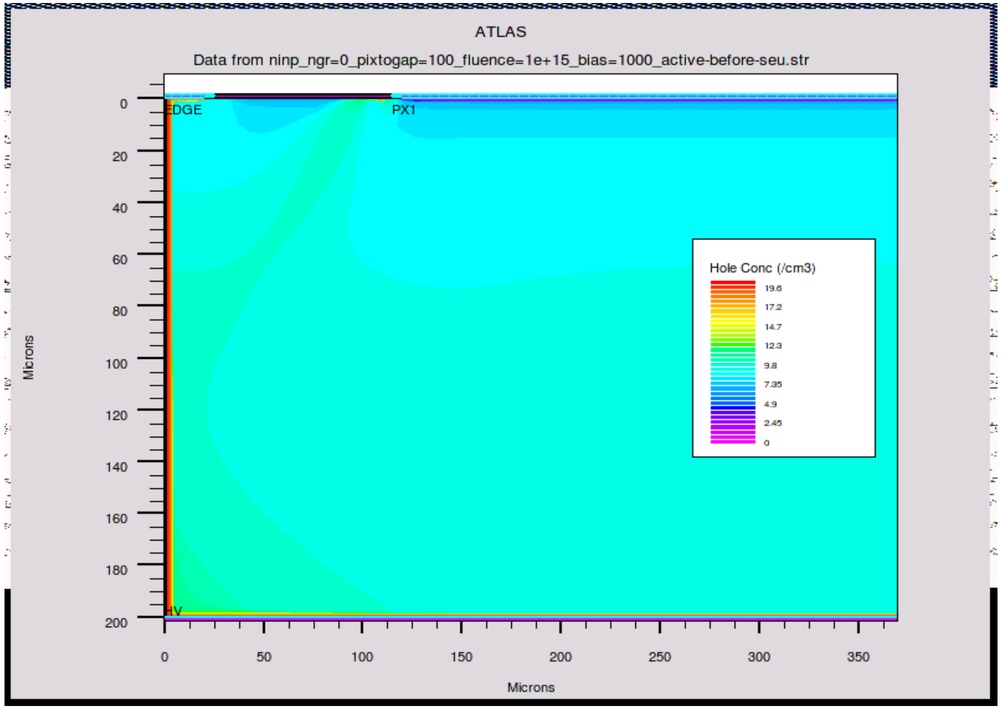


Before strike

Electrons

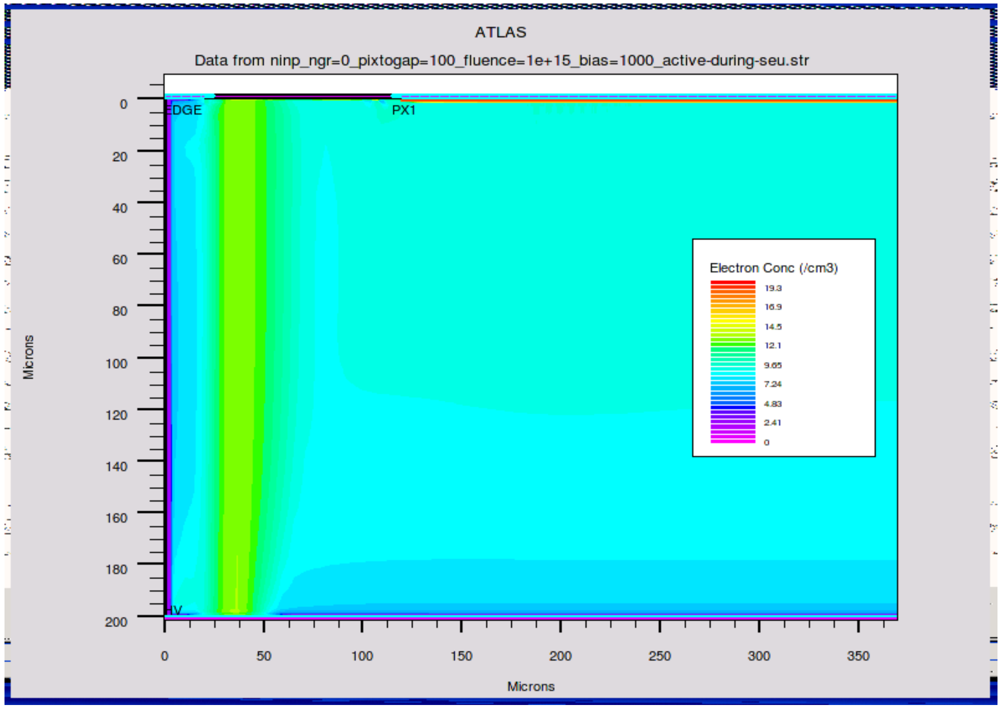


Holes

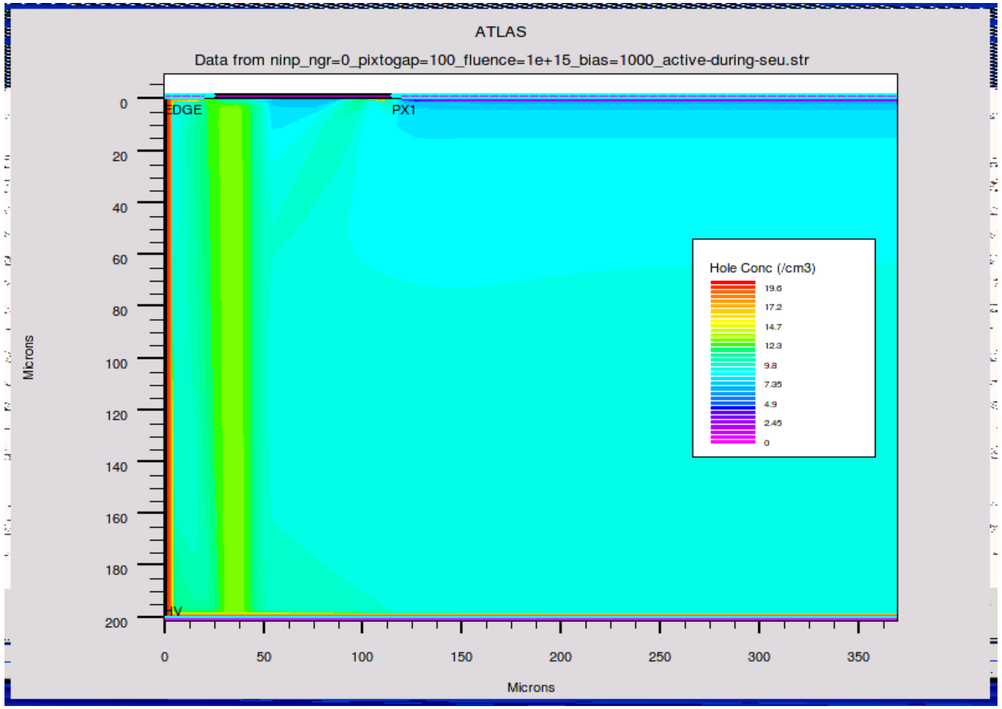


30 ps after particle hit

Electrons

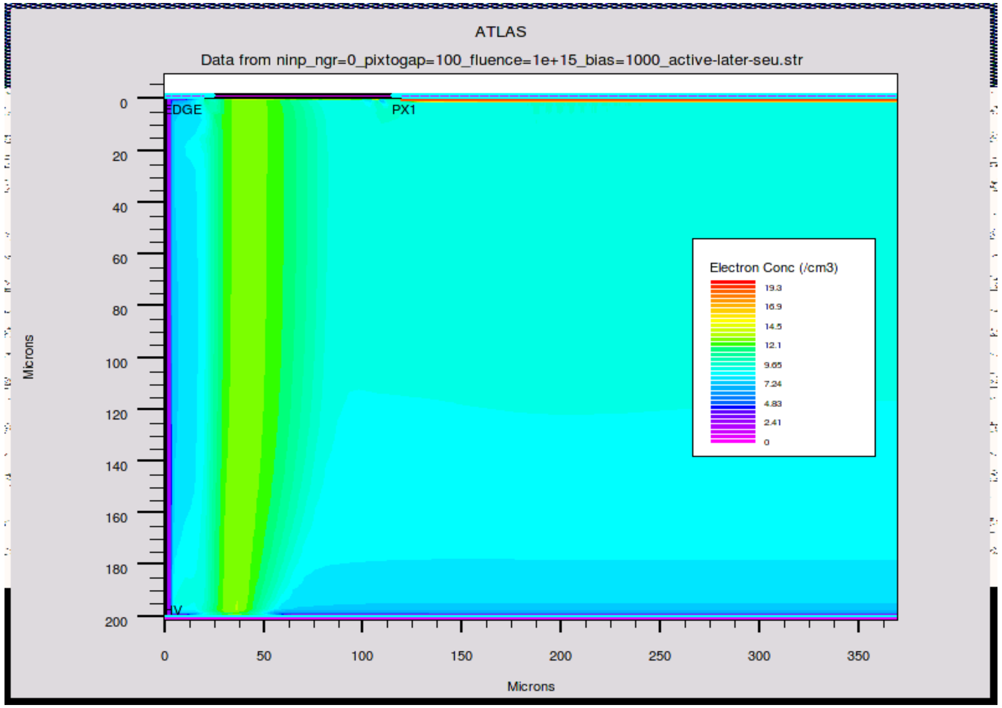


Holes

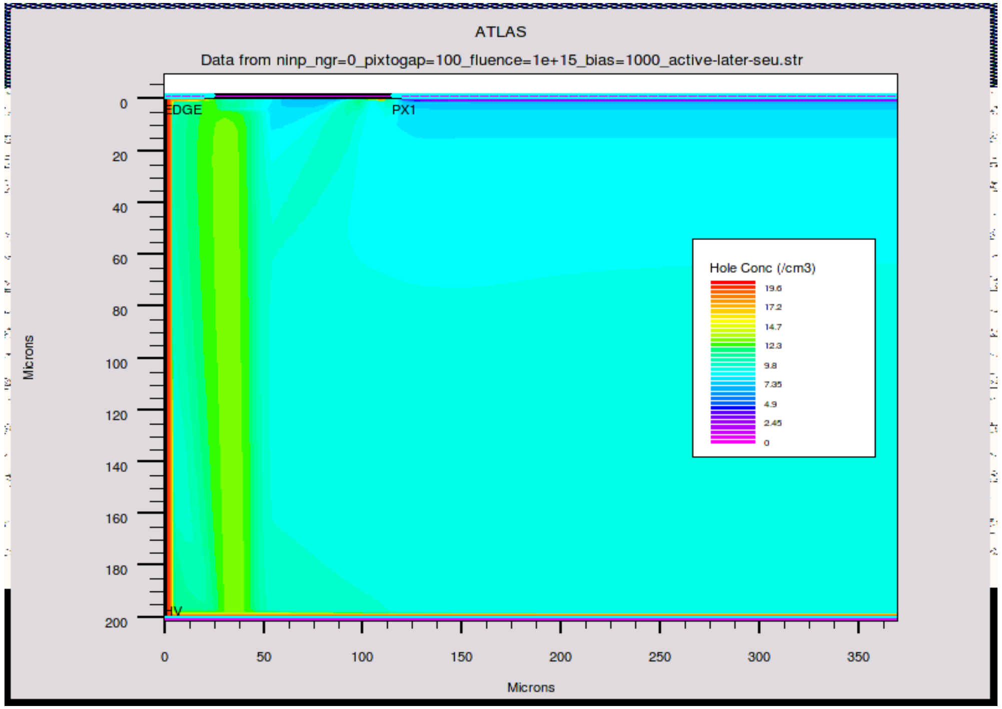


80 ps after particle hit

Electrons

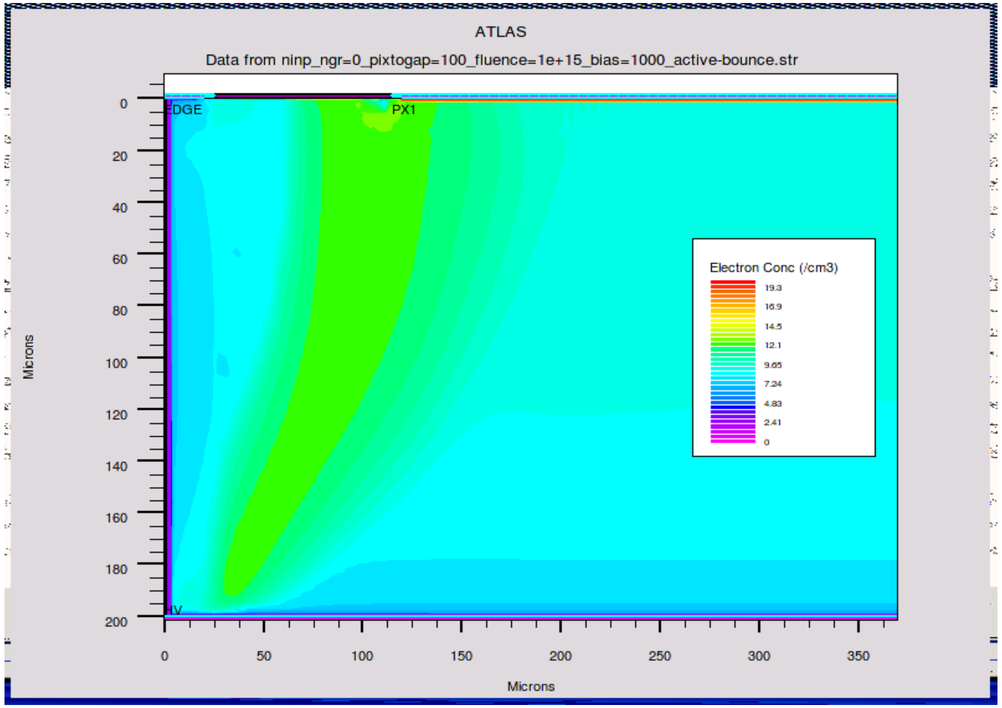


Holes

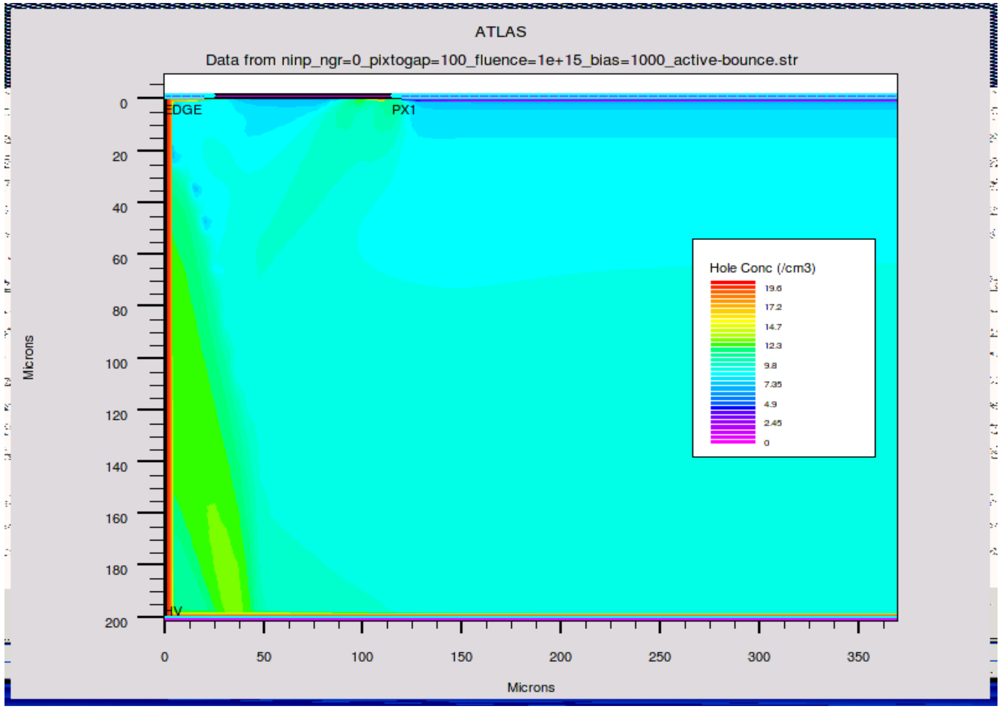


780 ps after particle hit

Electrons



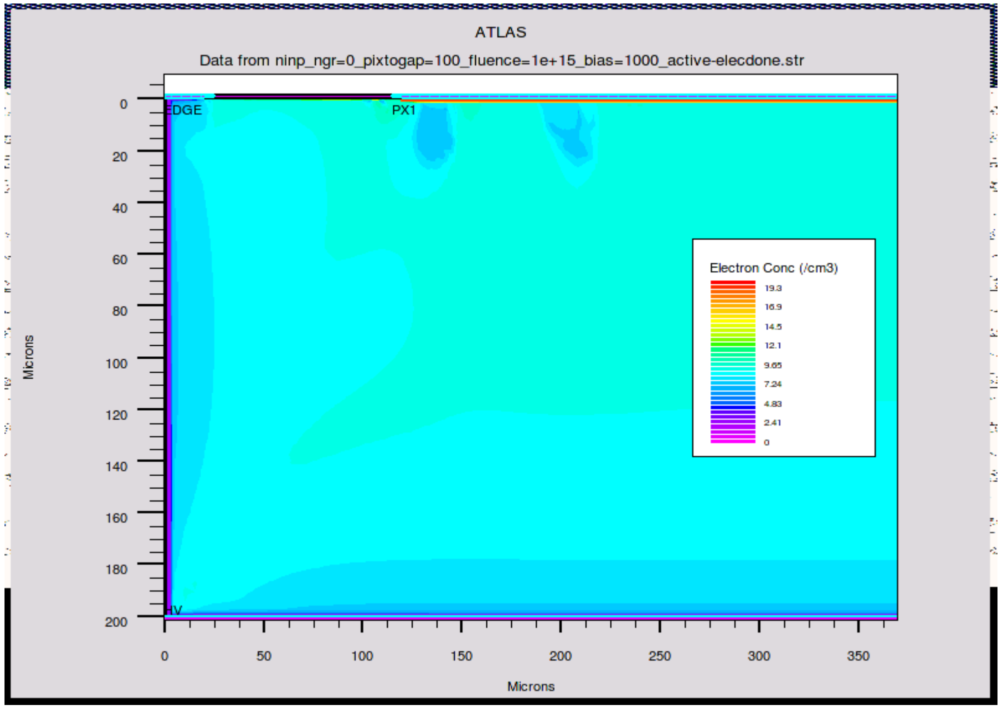
Holes

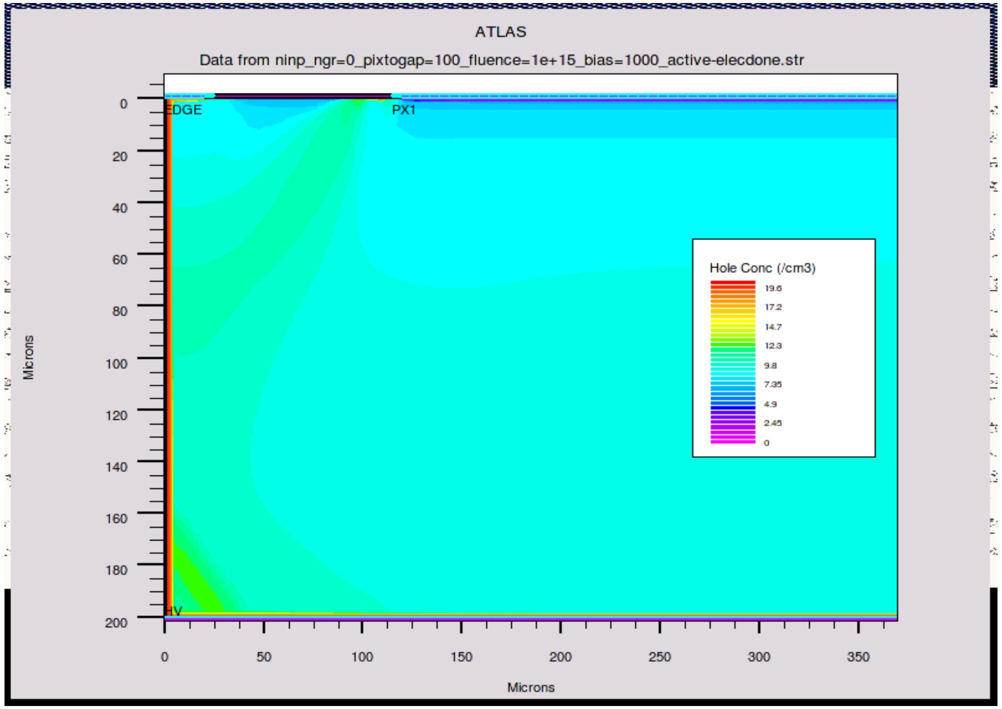


4 ns after particle hit

Electrons

Holes

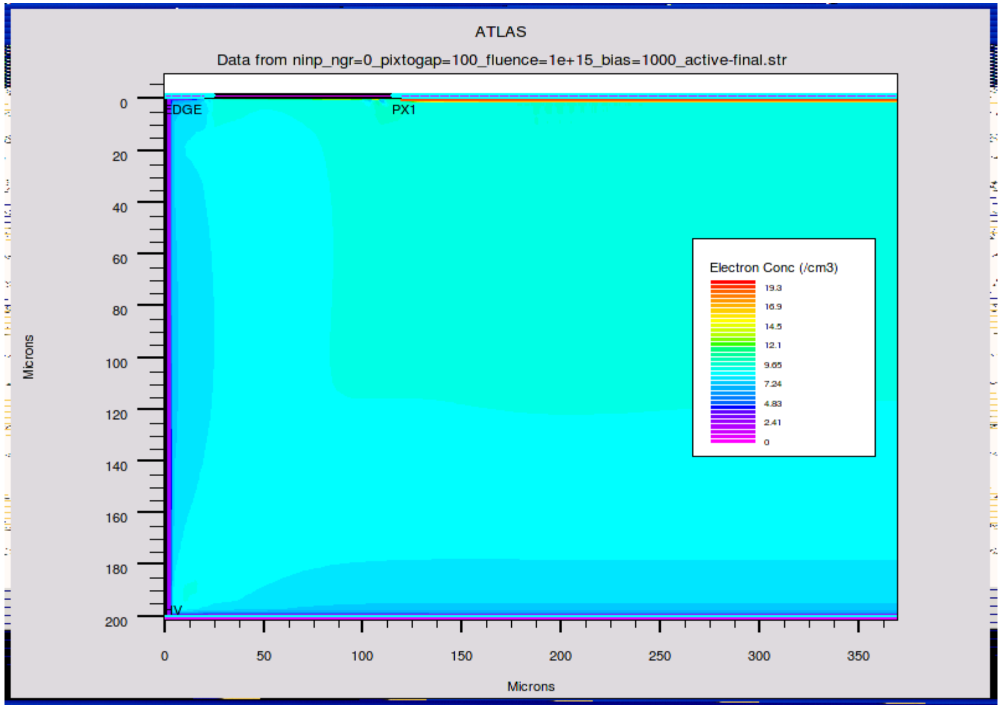


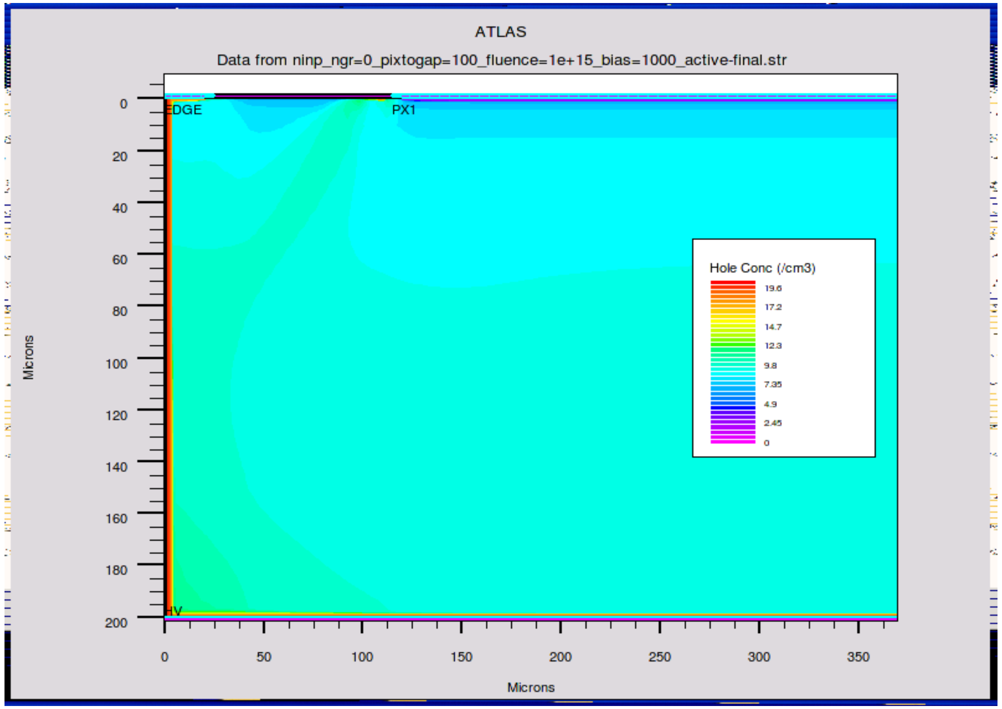


100 ns after particle hit

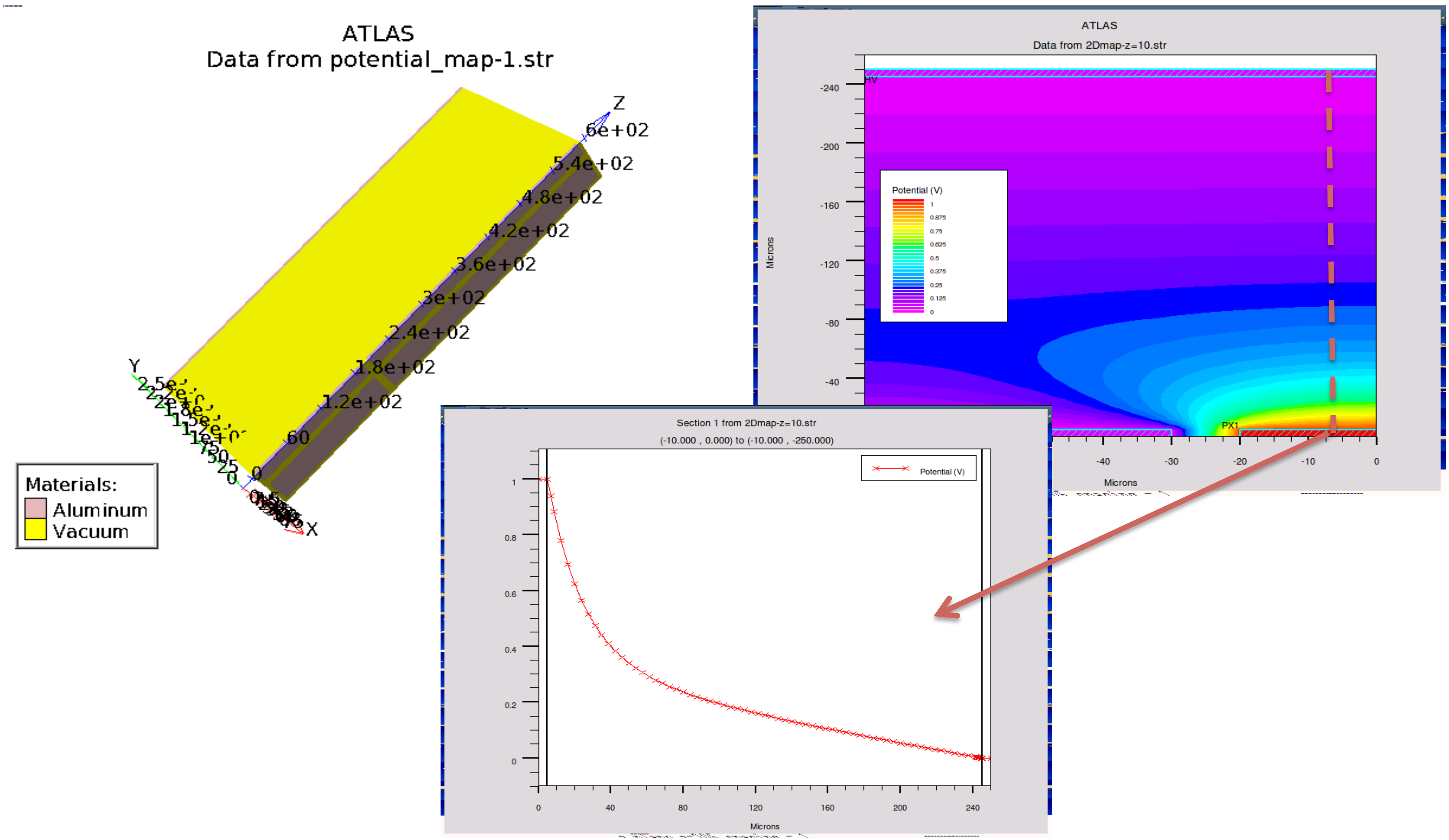
Electrons

Holes

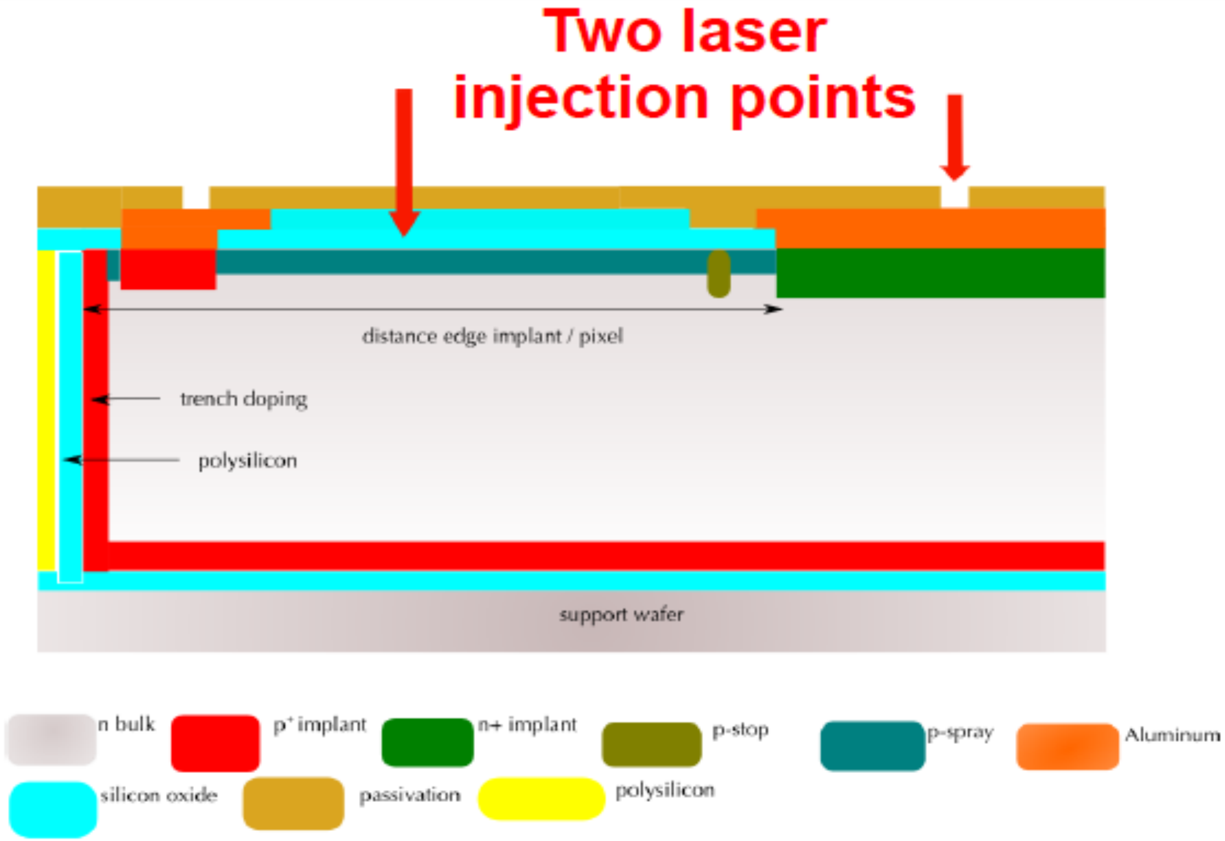




Digitizer inputs from TCAD: ramo potential



Simulation of CCE studies with laser

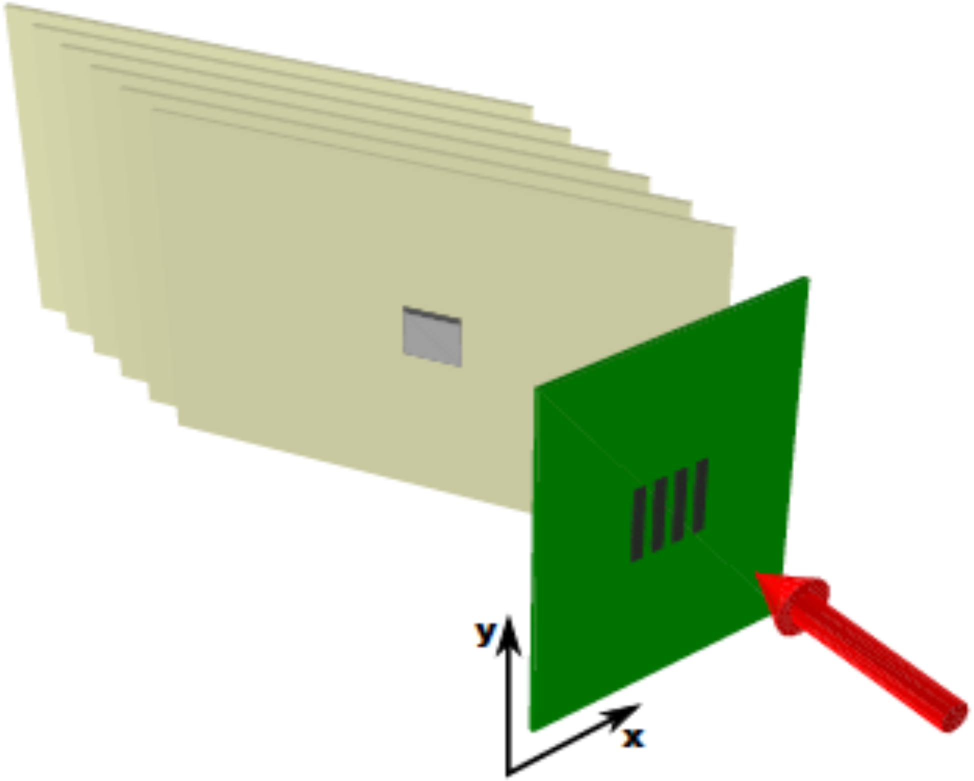


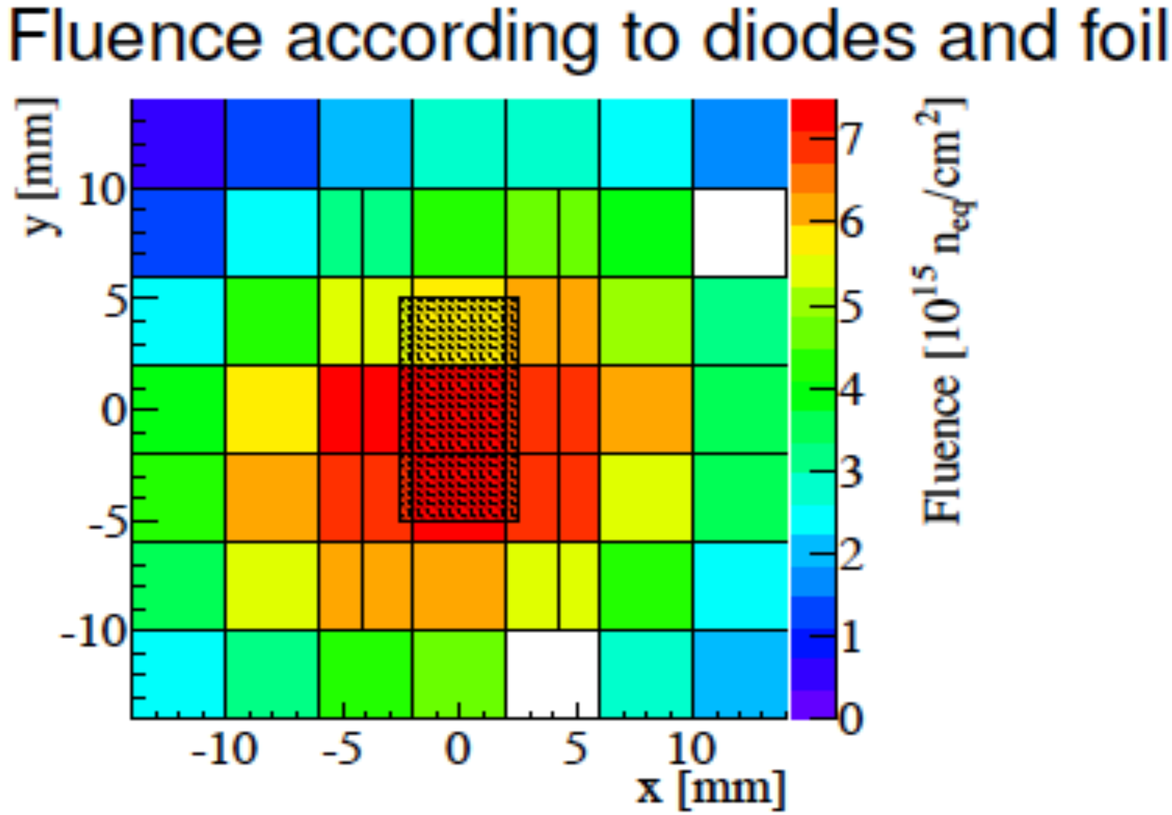

```
ATLAS> # BEAM DEFINITION
ATLAS> beam num=1 x.origin=200 y.origin=-2.0 angle=90 wavelength=1.06 rays=101 gaussian
 mean=0 xsigma=5
```

```
ATLAS> solve     b1=18 ramp.lit ramptime=1e-9 tstop=10e-9 tstep=2e-10
```

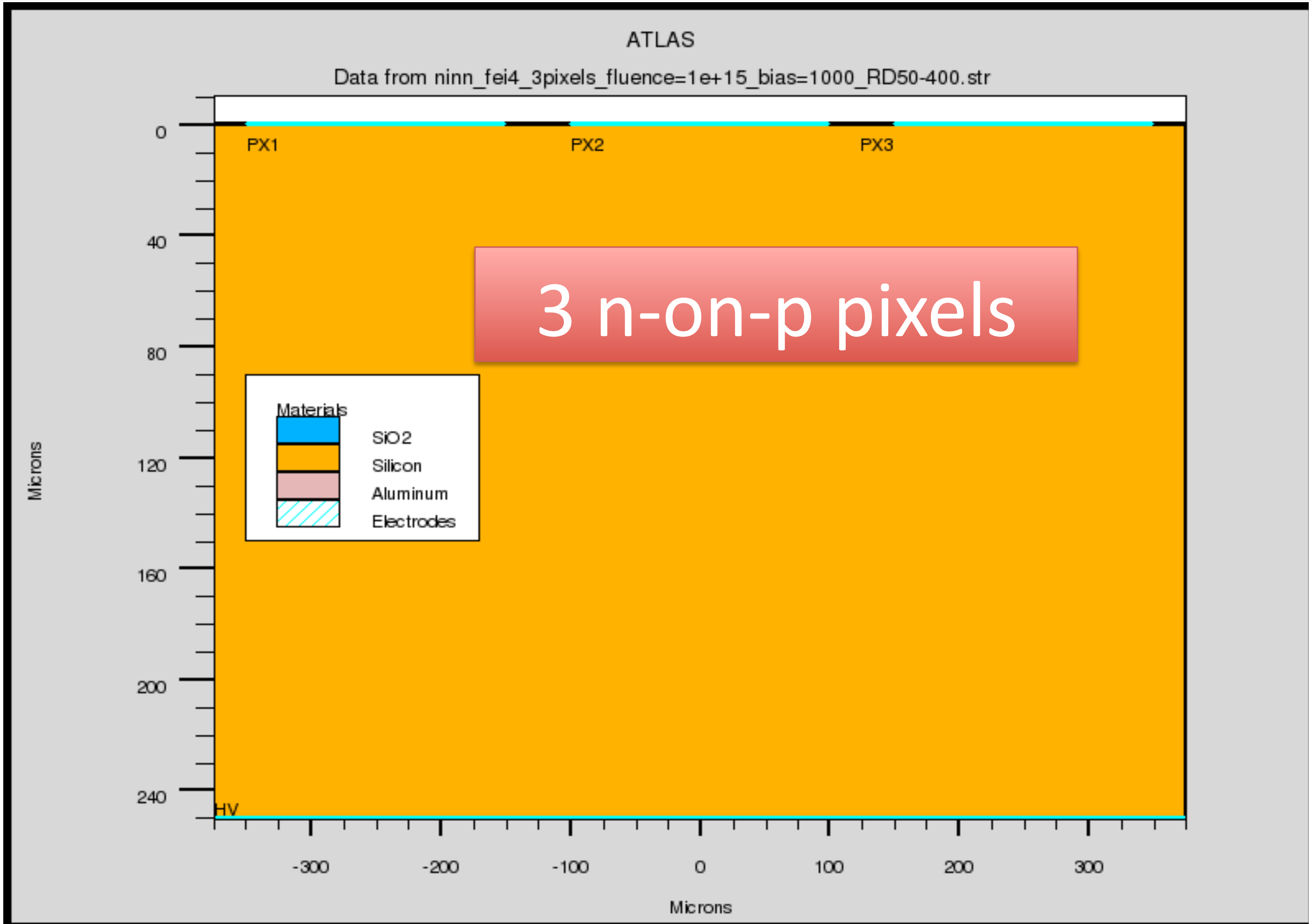
```
ATLAS> solve     b1=0 ramp.lit ramptime=1e-9 tstop=50e-9 tstep=5e-10
```

Non uniform irradiation at LANSCE



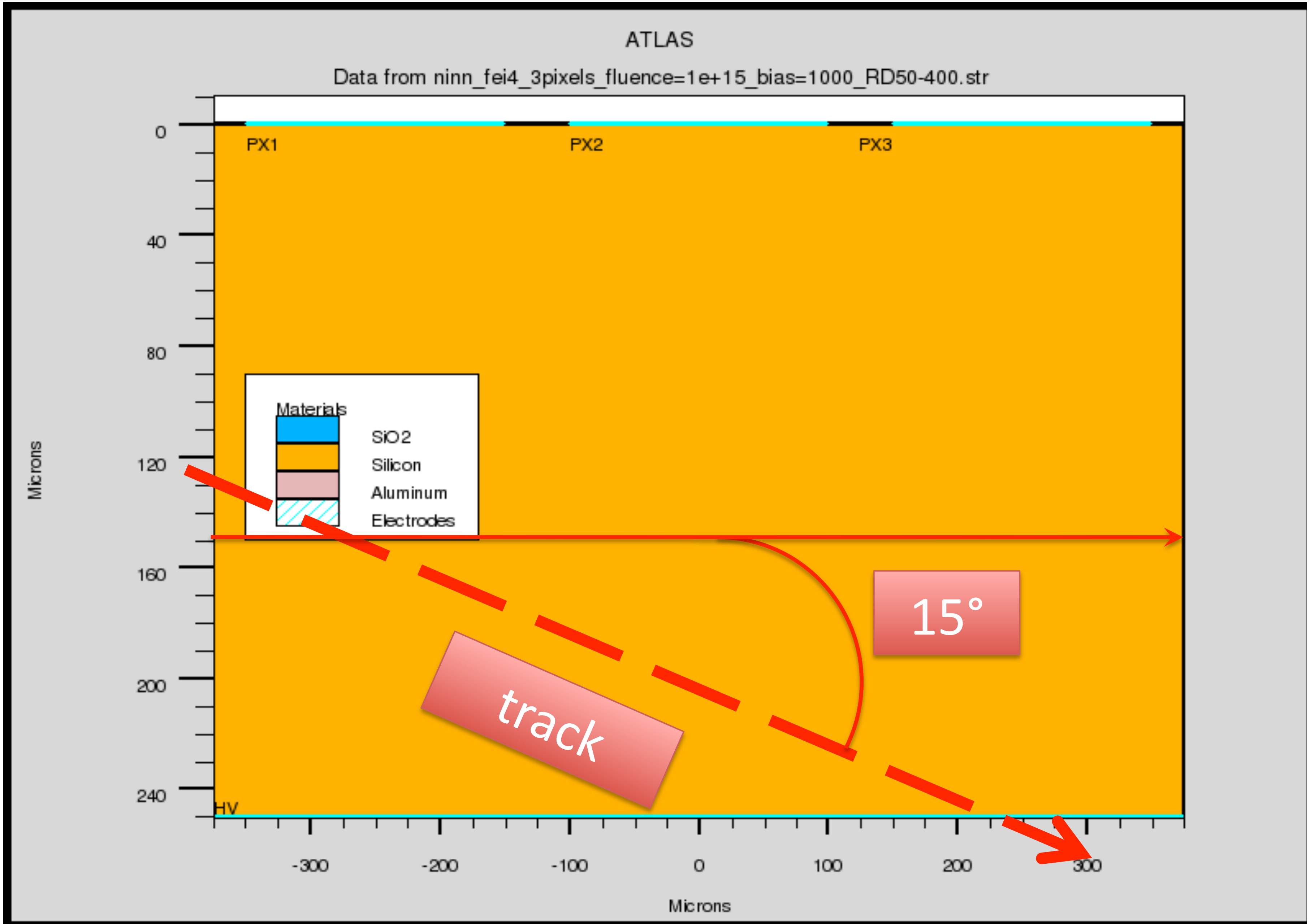


Simulated structure

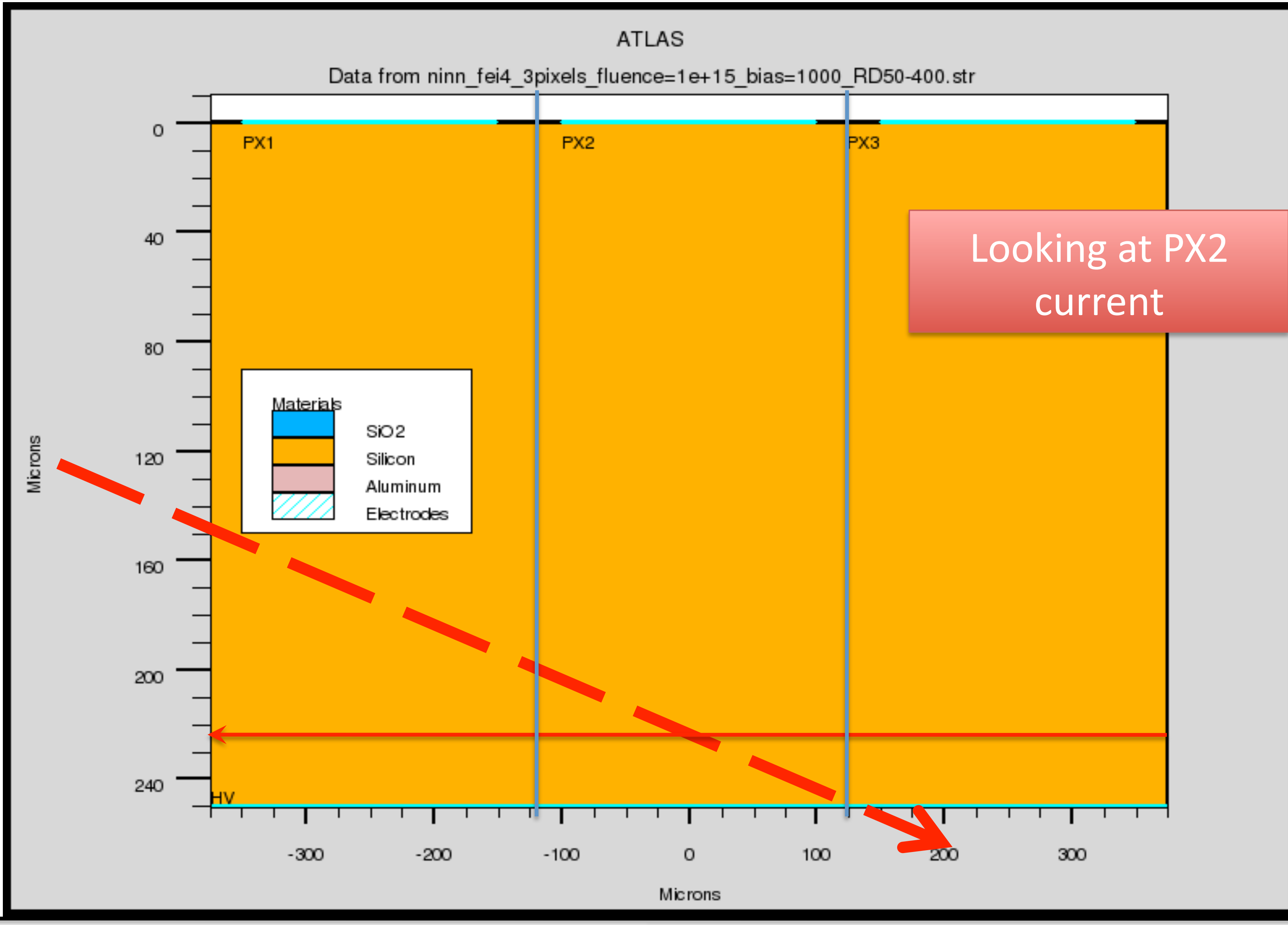


3 n-on-p pixels

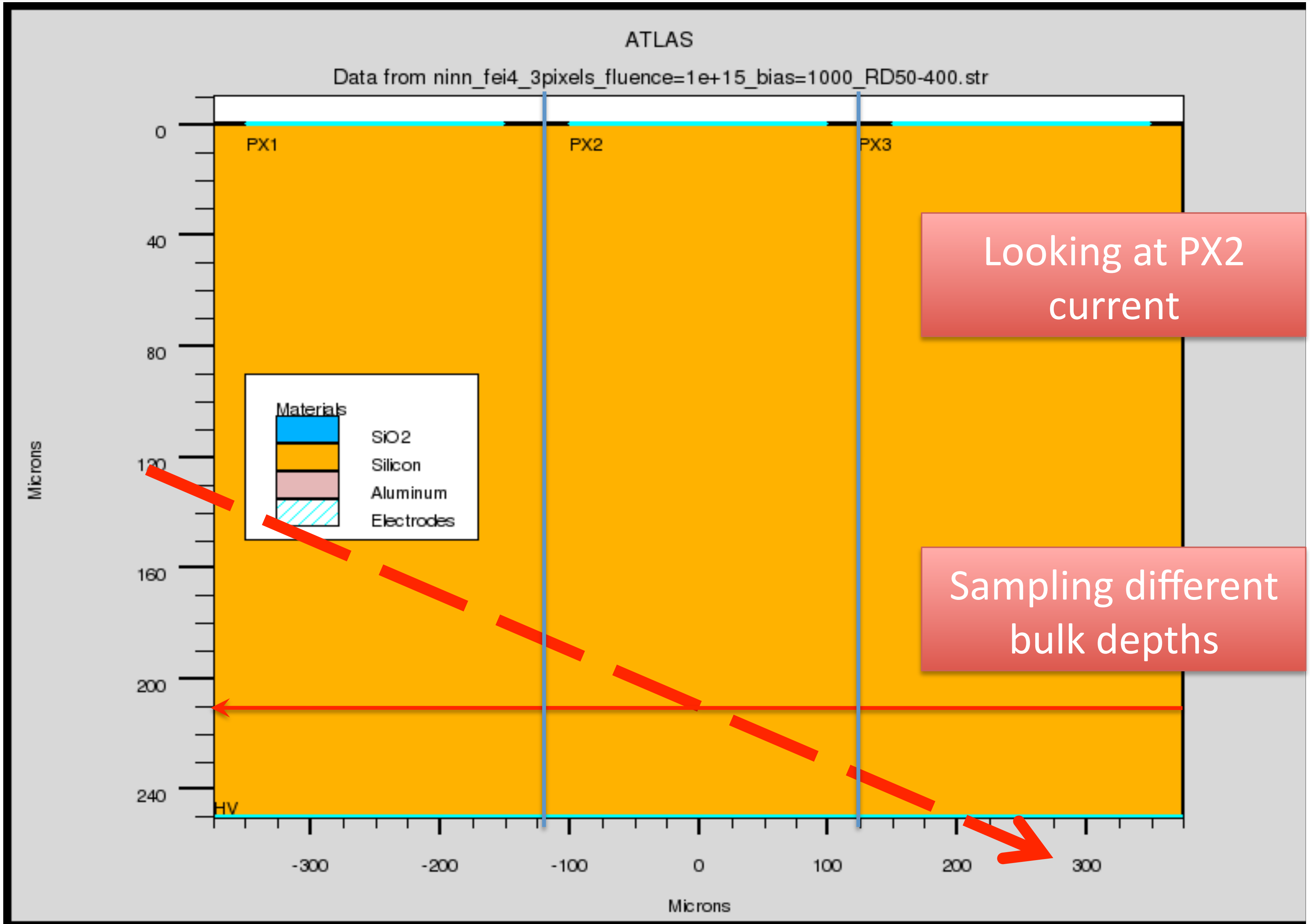
Collected charge vs track entry point



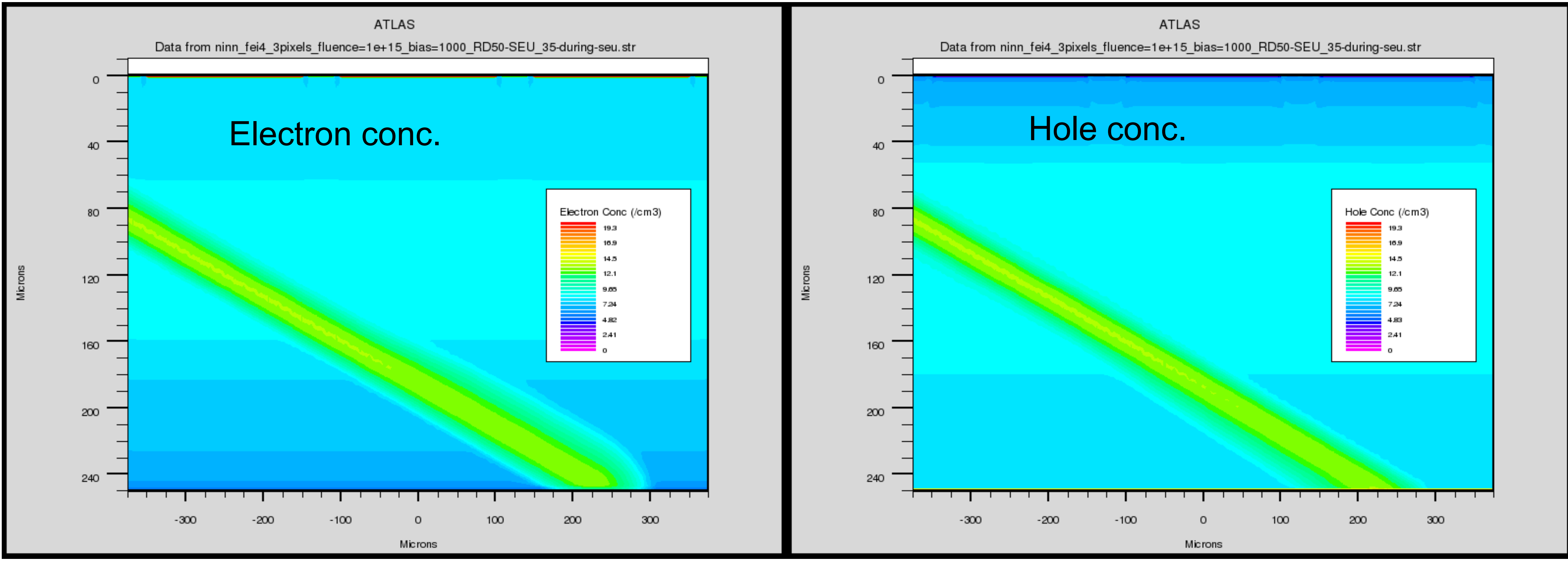
Scanning the bulk depth



Scanning the bulk depth

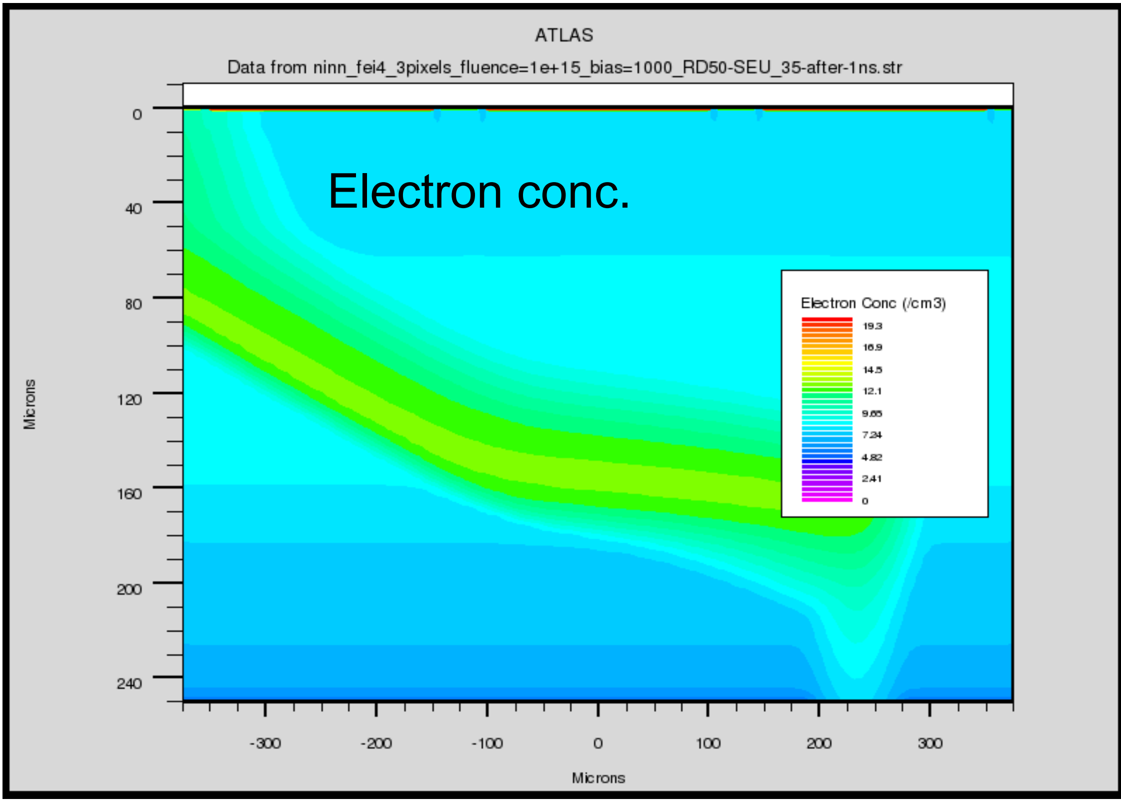


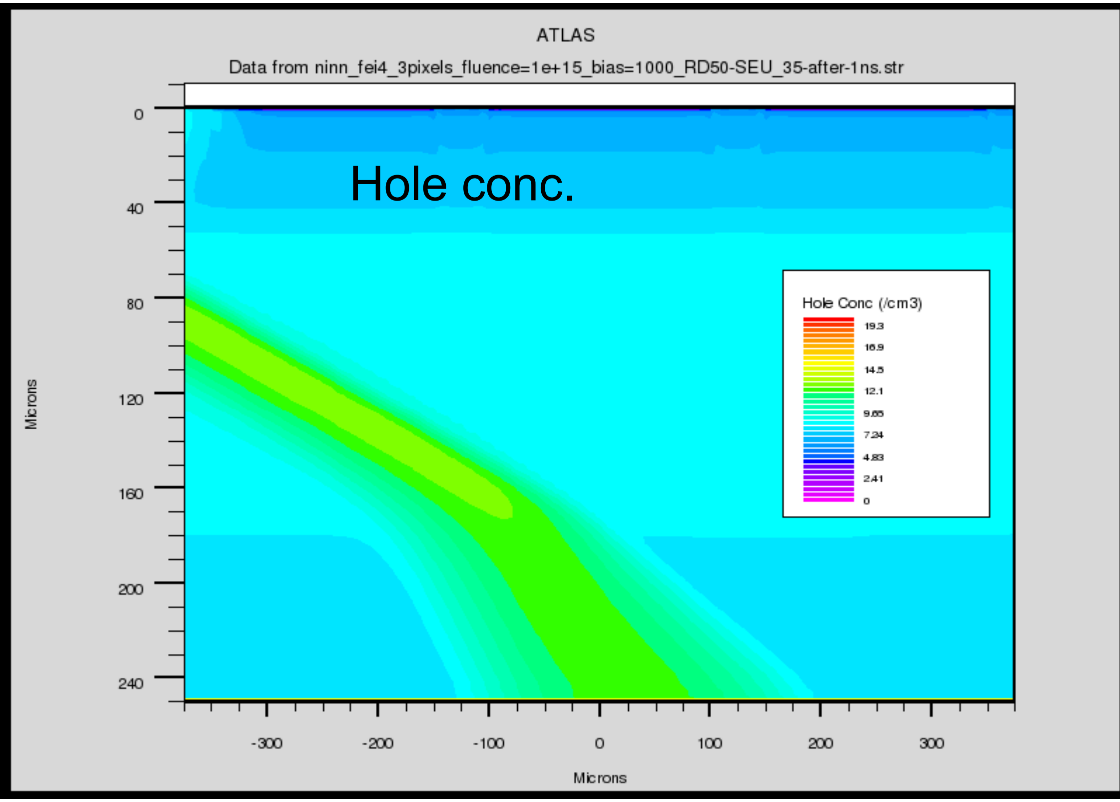
Ionizing particles and carrier distributions



- Carrier distribution during the particle strike

Ionizing particles and carrier distributions





- Carrier distribution 1 s after the particle strike

TCAD simulations: time needed

- The CPU time increases with number of meshing points
- Some analysis are not parallelized (*e.g.* AC)
- E.g. : 1 minute per bias point for ~ 100k nodes mesh on a 8 core 3GHz machine
- For irradiated sensors this translates into ~ 1 week to get full depletion
- Another example: time-domain solution. For the same structure above you need to solve for ~ 10 ns in time steps of ps, with ~ 1 minute per point → 1 week needed

Reminder: N-bulk irradiation models

V. Eremin, E. Verbitskaya, and Z. Li, **"The origin of double peak electric field distribution in heavily irradiated silicon detectors," Nucl. Instrum.** Methods Phys. Res. A, vol. A476, pp. 556**–564, 2002.**

Petasecca model for N-type

Level	Ass.	$\sigma_{n,p}$ (cm^2) Exp.[2,9]	σ_n (cm^2)	σ_p (cm^2)	η (cm^{-1})
Ec-0.42eV	$VV^{(-/0)}$	$2\text{x}10^{-15}$	$2\text{x}10^{-15}$	$1.2\text{x}10^{-14}$	13
Ec-0.50eV	VVO(?)	$5\text{x}10^{-15}$	$5\text{x}10^{-15}$	$3.5\text{x}10^{-14}$	0.08
Ev+0.36eV	C_iO_i	$2.5\text{x}10^{-15}$	$2\text{x}10^{-18}$	$2.5\text{x}10^{-15}$	1.1

EVL model for N-type

Plus: fluence dependent carrier lifetime

Trap	E (eV)	g_{int} (cm^{-1})	σ_e (cm^2)	σ_h (cm^2)
Donor	$E_V + 0.48$	6	1×10^{-15}	1×10^{-15}
Acceptor	$E_C - 0.525$	3.7	1×10^{-15}	1×10^{-15}

Chiochia model for N-type

Same levels as EVL model

Φ (n$_{eq}$/cm^2) ($\times 10^{14}$)	N_A(cm^{-3}) ($\times 10^{15}$)	N_D(cm^{-3}) ($\times 10^{15}$)	$\sigma_e^{A/D}$(cm^2) ($\times 10^{-15}$)	σ_h^A(cm^2) ($\times 10^{-15}$)	(cm^2) σ_h^D ($\times 10^{-15}$)
0.5	0.19	0.25	6.60	1.65	6.60
2	0.68	1.0	6.60	1.65	6.60
5.9	1.60	4.0	6.60	1.65	1.65