13th “Trento” Workshop - MPP, 19-21/2/2018

TCAD Simulations of Silicon Sensors at HL-LHC Conditions

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Outline

- Radiation damage models

- Available software

- 1D vs 2D vs 3D vs 4D simulations

- Conclusions

RADIATION DAMAGE MODELS

Radiation damage models: history

- Modelling all known defects in silicon in TCAD is (still) computationally prohibitive
  - Plus: how to model defects clusters?
- Hence only a certain number of "effective states" are modelled

a. 1 acceptor-like state (q=-/0)
   - e.g. D. Passeri et al., IEEE TNS 45 (1998) 602-608

b. 2 states, 1 acceptor- and 1 donor-like (q=+/0)
   - e.g. V. Eremin et al., NIM A476 (2002) 556-564, aka EVL

c. 3 states, adding 1 acceptor wrt b., very close to mid-gap, to better control type inversion and leakage current increase rate
   - e.g. M. Petasecca et al., IEEE TNS 53 (2006) 2971-2976

d. 4 states, adding 1 acceptor more (rather unique example)
   - e.g. F. Moscatelli et al., NIM B186 (2002) 171

Radiation damage models for HL-LHC

- “Perugia” model: IEEE TNS 64 (2017) 2259-2267
  - Two acceptors and one donor
    - Interface damage modelled too (2 acc. and 1 don. again)
  - Valid up to $2.2\mathrm{x}10^{16}$ n_{eq}/cm^2
- “3D” model: Pennicard et al., NIM A592 (2008) 16-25
  - Two acceptors and one donor as in Perugia model but larger cross sections wrt Petasecca et al. 2006
    - Used recently in M. Baselga et al. “Simulations of 3D-Si sensors for the innermost layer of the ATLAS pixel upgrade” NIM A847 (2017) 67-76
  - Valid up to $1\mathrm{x}10^{16}$ n_{eq}/cm^2
- “LHCb model”: NIM A874 (2017) 94-102
  - Two acceptors and one donor
    - One acceptor and one donor as in EVL plus one acceptor close to the valence band
  - Valid up to $8\mathrm{x}10^{15}$ n_{eq}/cm^2

Radiation damage models for HL-LHC

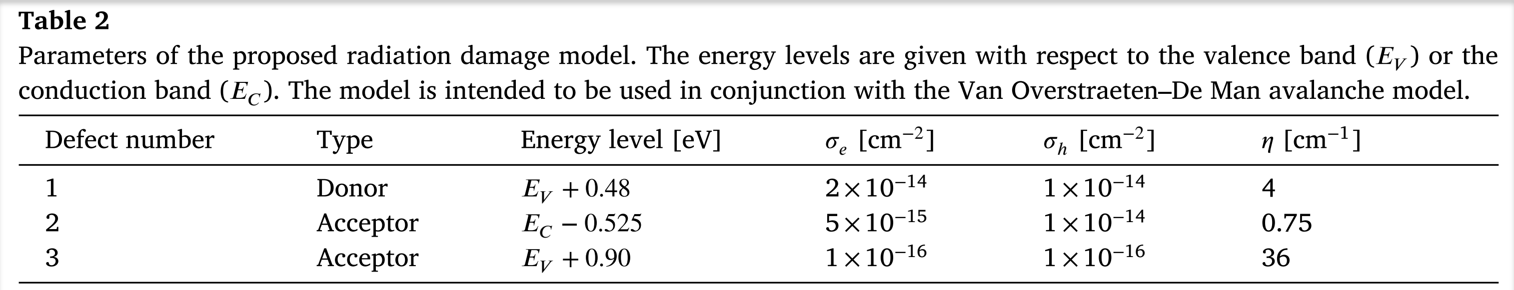


Table 2

Parameters of the proposed radiation damage model. The energy levels are given with respect to the valence band (E_V) or the conduction band (E_C). The model is intended to be used in conjunction with the Van Overstraeten–De Man avalanche model.

Defect number	Type	Energy level [eV]	σ_e [cm^{-2}]	σ_h [cm^{-2}]	η [cm^{-1}]
1	Donor	$E_V + 0.48$	2×10^{-14}	1×10^{-14}	4
2	Acceptor	$E_C - 0.525$	5×10^{-15}	1×10^{-14}	0.75
3	Acceptor	$E_V + 0.90$	1×10^{-16}	1×10^{-16}	36

LHCb

PERUGIA

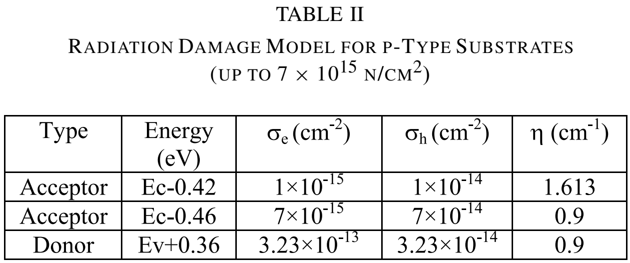


TABLE II

RADIATION DAMAGE MODEL FOR P-TYPE SUBSTRATES (UP TO 7×10^{15} N/CM^2)

Type	Energy (eV)	σ_e (cm^{-2})	σ_h (cm^{-2})	η (cm^{-1})
Acceptor	Ec-0.42	1×10^{-15}	1×10^{-14}	1.613
Acceptor	Ec-0.46	7×10^{-15}	7×10^{-14}	0.9
Donor	Ev+0.36	3.23×10^{-13}	3.23×10^{-14}	0.9

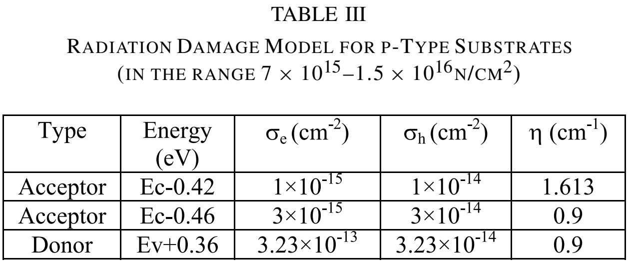


TABLE III

RADIATION DAMAGE MODEL FOR P-TYPE SUBSTRATES (IN THE RANGE 7×10^{15}–1.5×10^{16}N/CM^2)

Type	Energy (eV)	σ_e (cm^{-2})	σ_h (cm^{-2})	η (cm^{-1})
Acceptor	Ec-0.42	1×10^{-15}	1×10^{-14}	1.613
Acceptor	Ec-0.46	3×10^{-15}	3×10^{-14}	0.9
Donor	Ev+0.36	3.23×10^{-13}	3.23×10^{-14}	0.9

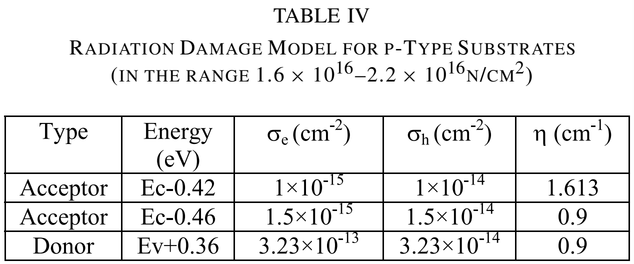


TABLE IV

RADIATION DAMAGE MODEL FOR P-TYPE SUBSTRATES (IN THE RANGE 1.6×10^{16}–2.2×10^{16}N/CM^2)

Type	Energy (eV)	σ_e (cm^{-2})	σ_h (cm^{-2})	η (cm^{-1})
Acceptor	Ec-0.42	1×10^{-15}	1×10^{-14}	1.613
Acceptor	Ec-0.46	1.5×10^{-15}	1.5×10^{-14}	0.9
Donor	Ev+0.36	3.23×10^{-13}	3.23×10^{-14}	0.9

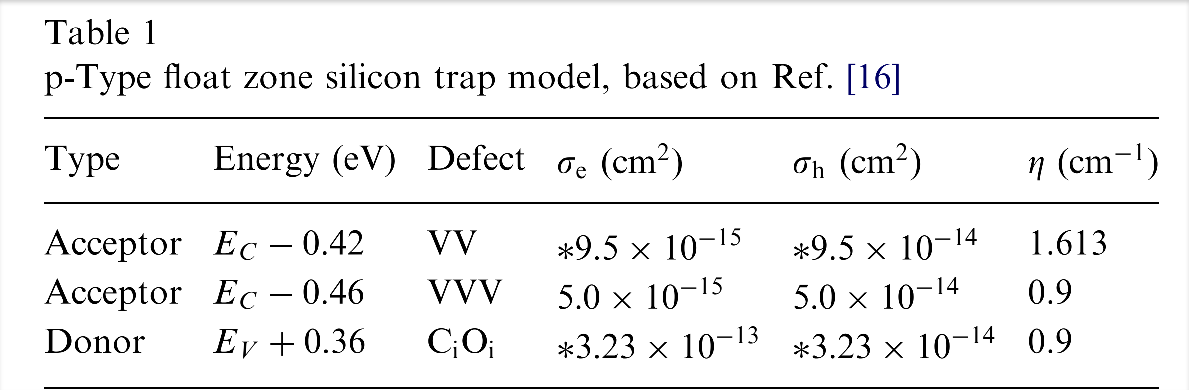


Table 1

p-Type float zone silicon trap model, based on Ref. [16]

Type	Energy (eV)	Defect	σ_e (cm^2)	σ_h (cm^2)	η (cm^{-1})
Acceptor	$E_C - 0.42$	VV	$*9.5 \times 10^{-15}$	$*9.5 \times 10^{-14}$	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	$*3.23 \times 10^{-13}$	$*3.23 \times 10^{-14}$	0.9

3D

Comments

- Perugia 2017 and 3D are rather in agreement

- Difference in the capture cross sections
  - Larger for Pennicard for the acceptor states

- LHCb uses EVL levels (1 acc. + 1 don.) and adds a another acceptor level close to the valence band
  - Added to tune the charge collection efficiency without influencing the leakage current level

Other models

- “New Delhi” model: R. Dalal et al., PoS (Vertex2014) 30 (2014), and T.Peltola, PoS (Vertex 2015) 31 (2015) – based on R. Eber PhD th.
  - Based on V. Eremin et al. work
  - Interface damage modelled too
  - Valid up to 1-1.4x10^{15} n_{eq}/cm^2

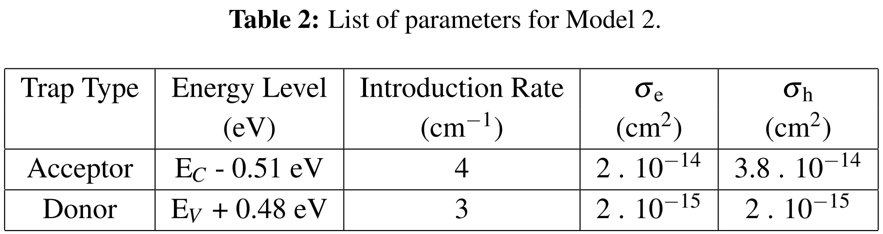
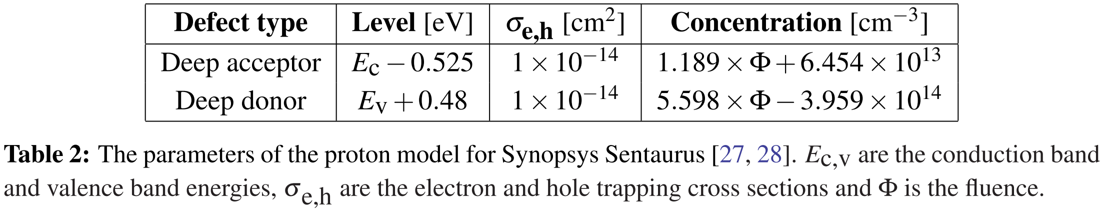


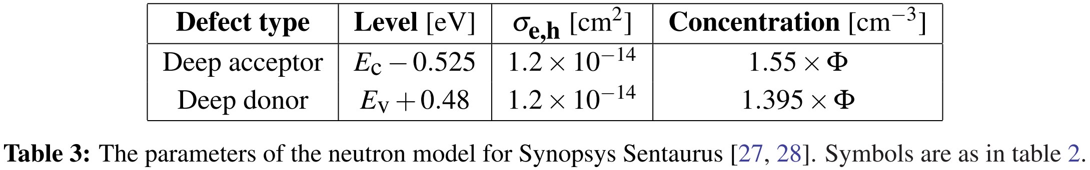
Table 2: List of parameters for Model 2.

Trap Type	Energy Level (eV)	Introduction Rate (cm^{-1})	σ_e (cm^2)	σ_h (cm^2)
Acceptor	E_C - 0.51 eV	4	$2 . 10^{-14}$	$3.8 . 10^{-14}$
Donor	E_V + 0.48 eV	3	$2 . 10^{-15}$	$2 . 10^{-15}$



Defect type	**Level** [eV]	$\sigma_{e,h}$ [cm^2]	**Concentration** [cm^{-3}]
Deep acceptor	$E_C - 0.525$	1×10^{-14}	$1.189 \times \Phi + 6.454 \times 10^{13}$
Deep donor	$E_V + 0.48$	1×10^{-14}	$5.598 \times \Phi - 3.959 \times 10^{14}$

Table 2: The parameters of the proton model for Synopsys Sentaurus [27, 28]. $E_{C,V}$ are the conduction band and valence band energies, $\sigma_{e,h}$ are the electron and hole trapping cross sections and Φ is the fluence.



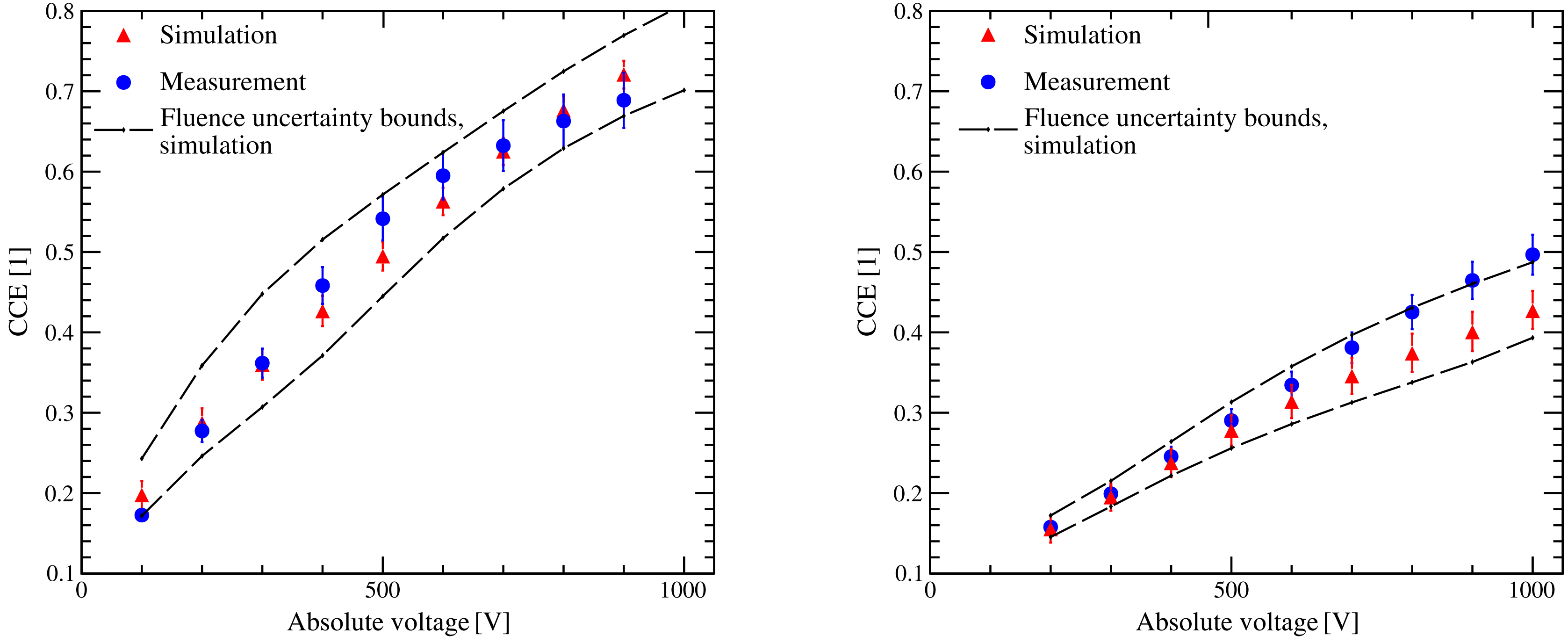
Defect type	**Level** [eV]	$\sigma_{e,h}$ [cm^2]	**Concentration** [cm^{-3}]
Deep acceptor	$E_C - 0.525$	1.2×10^{-14}	$1.55 \times \Phi$
Deep donor	$E_V + 0.48$	1.2×10^{-14}	$1.395 \times \Phi$

Table 3: The parameters of the neutron model for Synopsys Sentaurus [27, 28]. Symbols are as in table 2.

Predictions from TCAD models - LHCb

$4\text{x}10^{15}\ n_{eq}/cm^2$

$8\text{x}10^{15}\ n_{eq}/cm^2$



(a) 4×10^{15} 1 MeV n_{eq}/cm^2.

(b) 8×10^{15} 1 MeV n_{eq}/cm^2.

- In the conclusions authors mention that the model has been tested for temperatures between −38°C and −31°C on a range of sensors with different irradiation types and profiles.
- Predictions on IVs too

Predictions from TCAD models - Perugia

CCE

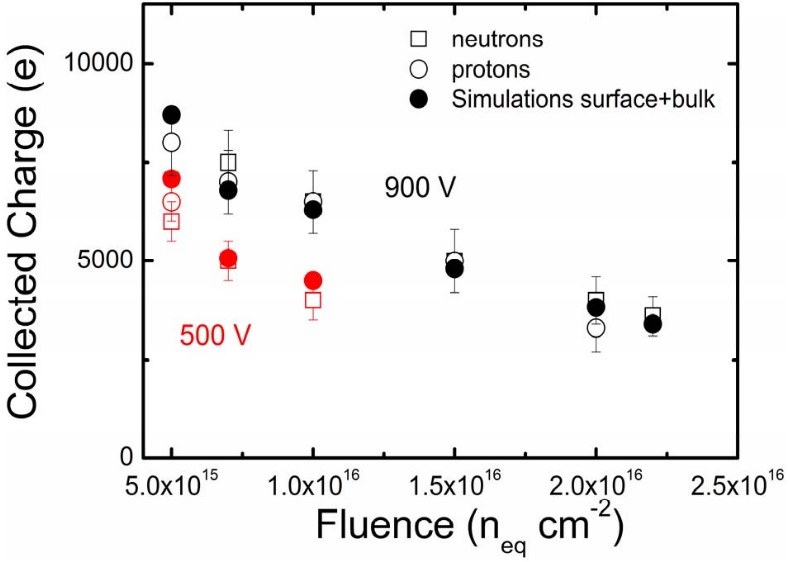


Fig. 17. Comparison between simulated and experimental charge collection [36] in n-on-p strip detectors at 248 K and 500 V (red symbols) and 900 V (black symbols) bias.

R_{INT}

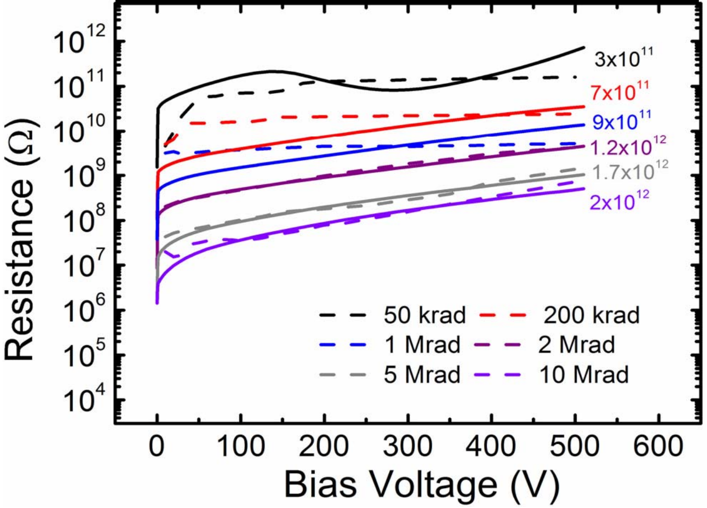


Fig. 15. Measured (dashed lines) and simulated (solid lines) interstrip resistance as a function of the V_{BIAS} at different X-ray doses. Simulations are obtained considering two acceptor interface traps with Gaussian distributions with peak energy at $E_T = E_C - 0.4$ eV and at $E_T = E_C - 0.6$ eV and one donor interface trap with Gaussian distribution with peak energy at $E_V + 0.7$ eV. $\sigma = 0.07$ eV for all traps. In this case, $N_{\mathrm{IT}} = 0.85 \times N_{\mathrm{OX}}$.

- In the conclusions authors mention that aspects not fully addressed are temperature variation and annealing conditions
  - *Nota bene: this is true also for the other models*

Predictions from TCAD models – 3D

V_{depl} (on pad diodes)

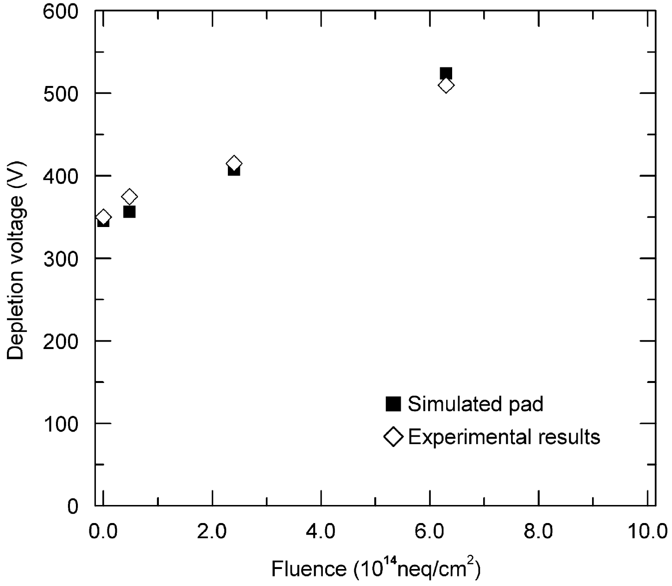


Fig. 1. Comparison between simulated and experimental depletion voltages in n-in-p pad detectors. Experimental results are taken from Ref. [20].

CCE (3D det.)

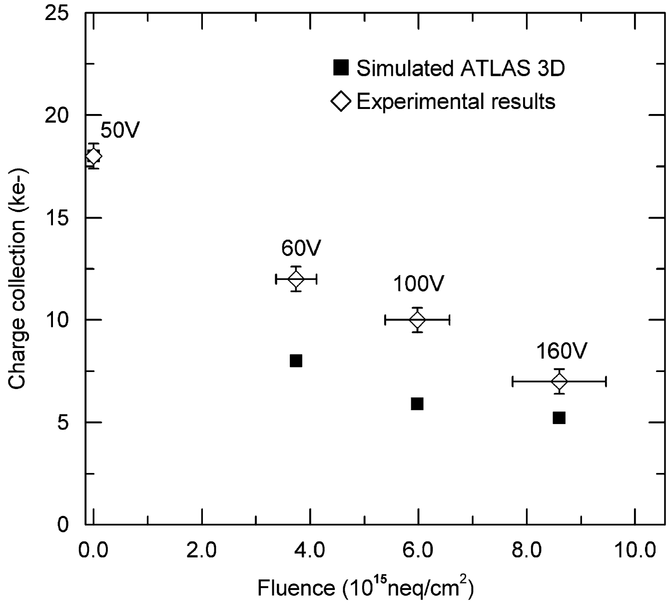


Fig. 5. Comparison between simulated and experimental charge collection in a “3-column” ATLAS pixel detector. Experimental results are taken from Ref. [24]. The labels indicate the bias used in both the experiments and the simulations.

- *Nota bene: depletion voltage can be measured (and simulated!)*
- *This is generally true for 3-levelsmodels à la Perugia*

Electric field – 2 states models

LHCb

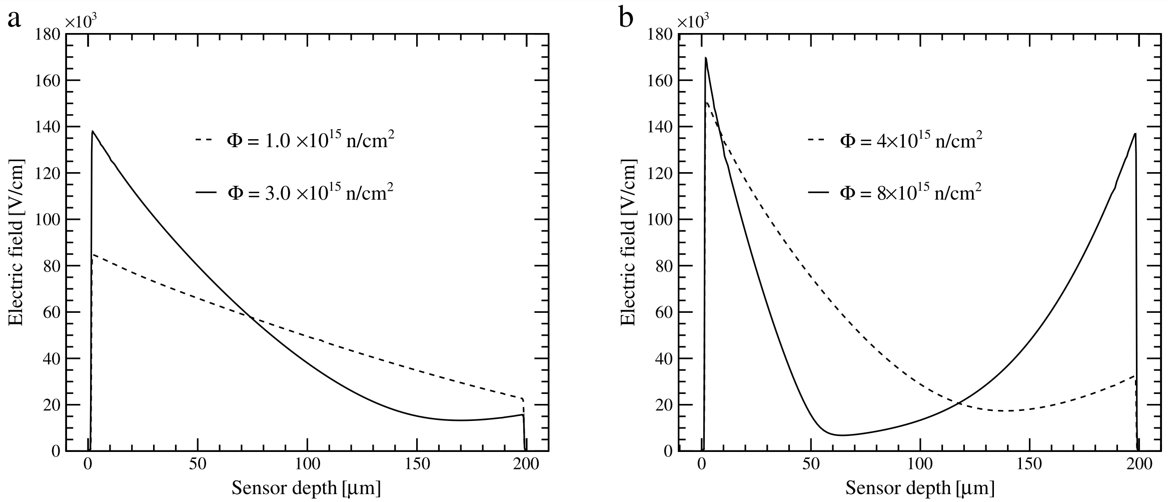


Fig. 15. Electric field (simulated using a 2D mesh) in the centre of a pixel as a function of distance from the pixel side, at a bias voltage of 1000 V, for different fluence levels.

The “third” level is very close to the valence band that it doesn’t affect too much the electric field distribution

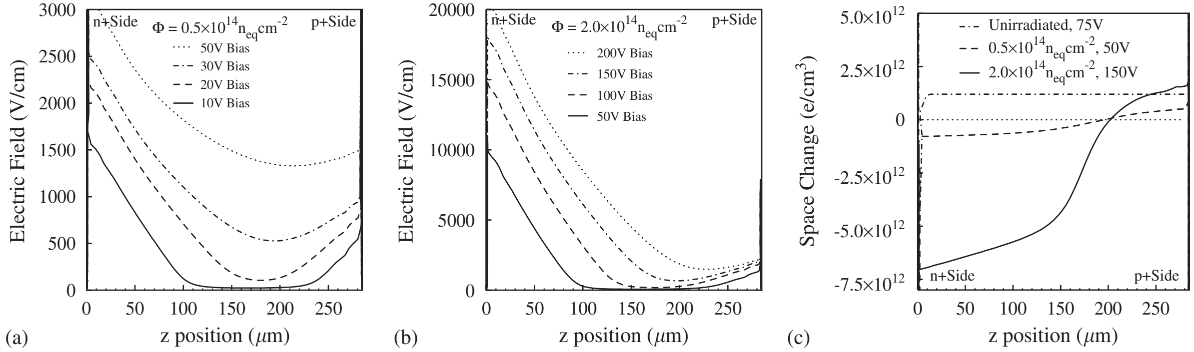


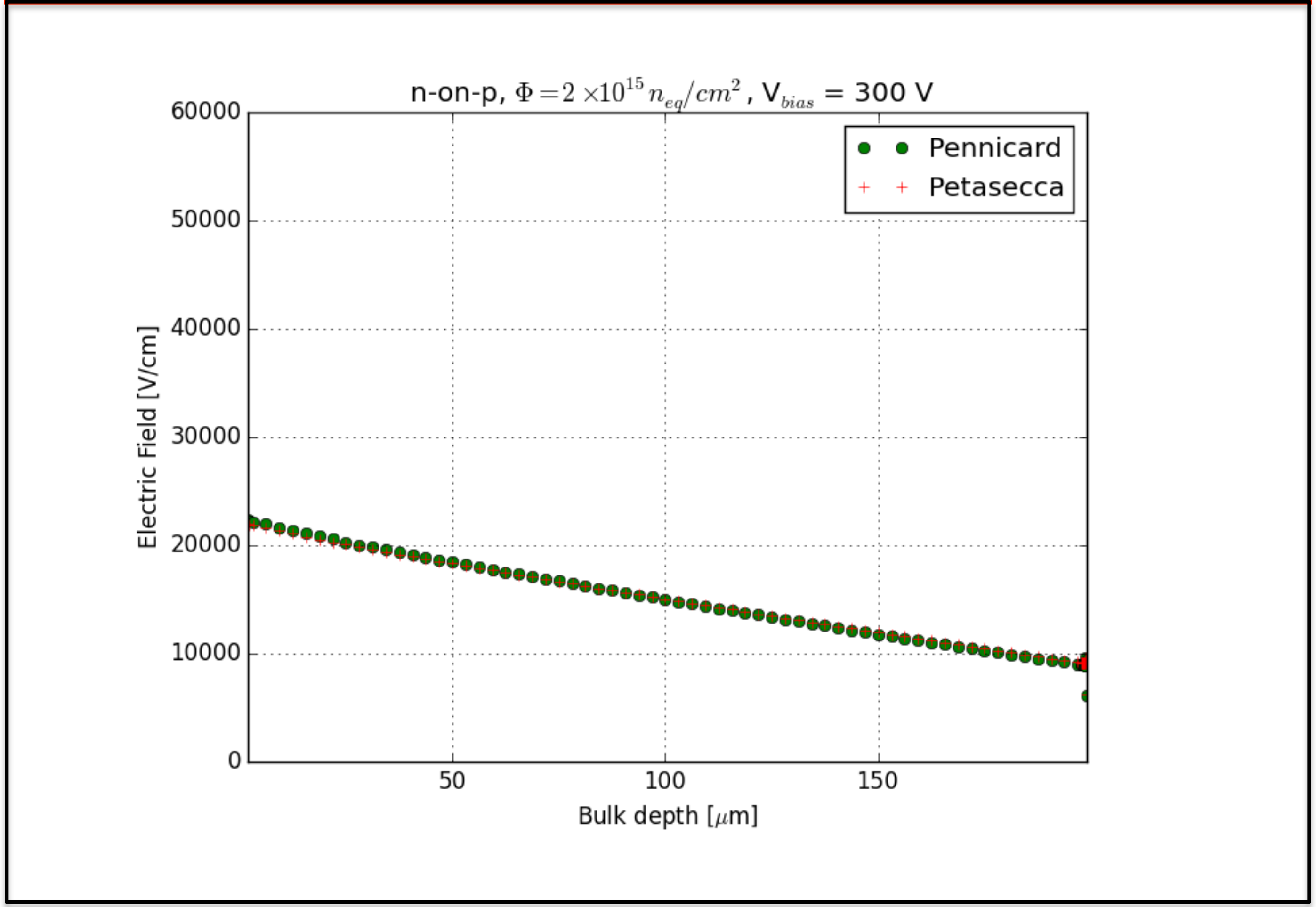
Fig. 4. The z-component of the simulated electric field resulting from the model best fit is shown as a function of z for a sensor irradiated to a fluence of $\Phi = 0.5 \times 10^{14}$ n$_{eq}$/cm^2 (a) and $\Phi = 2 \times 10^{14}$ n$_{eq}$/cm^2 (b). (c) Space charge density as a function of the z coordinate for different fluences and bias voltages.

Cfr. Chiochia et al. NIM A568 (2006) 51–55

The model is based on EVL levels only

Electric field – 3 states models

Perugia & 3D



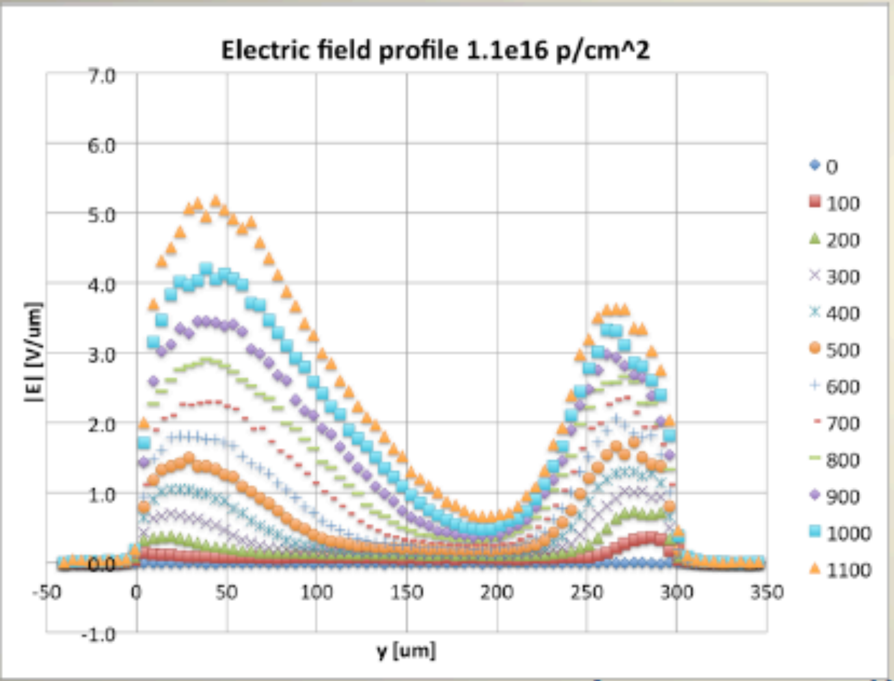
- Why they differ with respect to EVL/Chiochia/LHCb?
- Just a combination of thickness/fluence/particle energy?

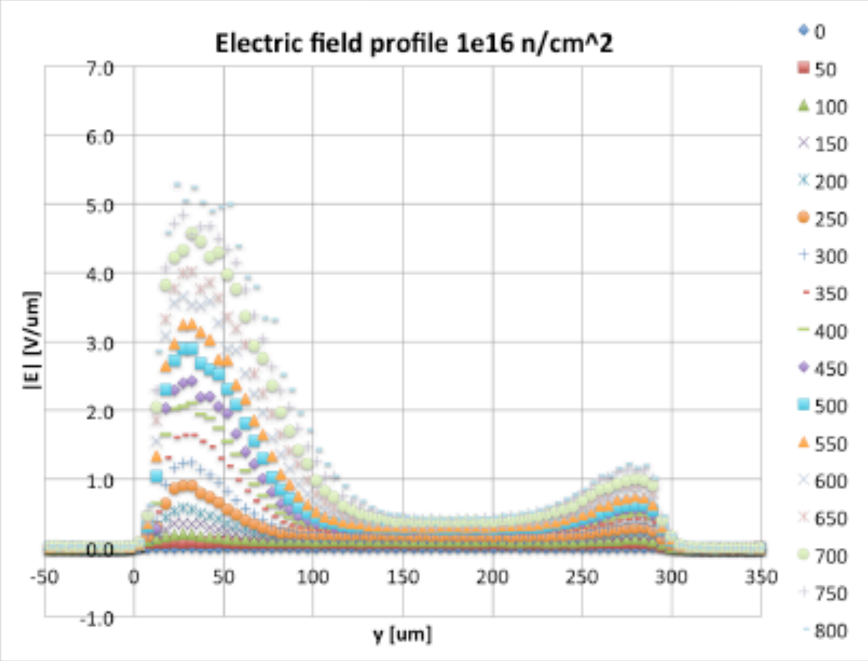
Comments

- In 2-states models energies are closer to the intrinsic level than in 3-states models
- Yet they both reproduce correctly the level of leakage current
- And the CCE
- Why then do they differ in the predicted electric field?

Protons <-> Neutrons ~10^{16}

- Field profiles compared

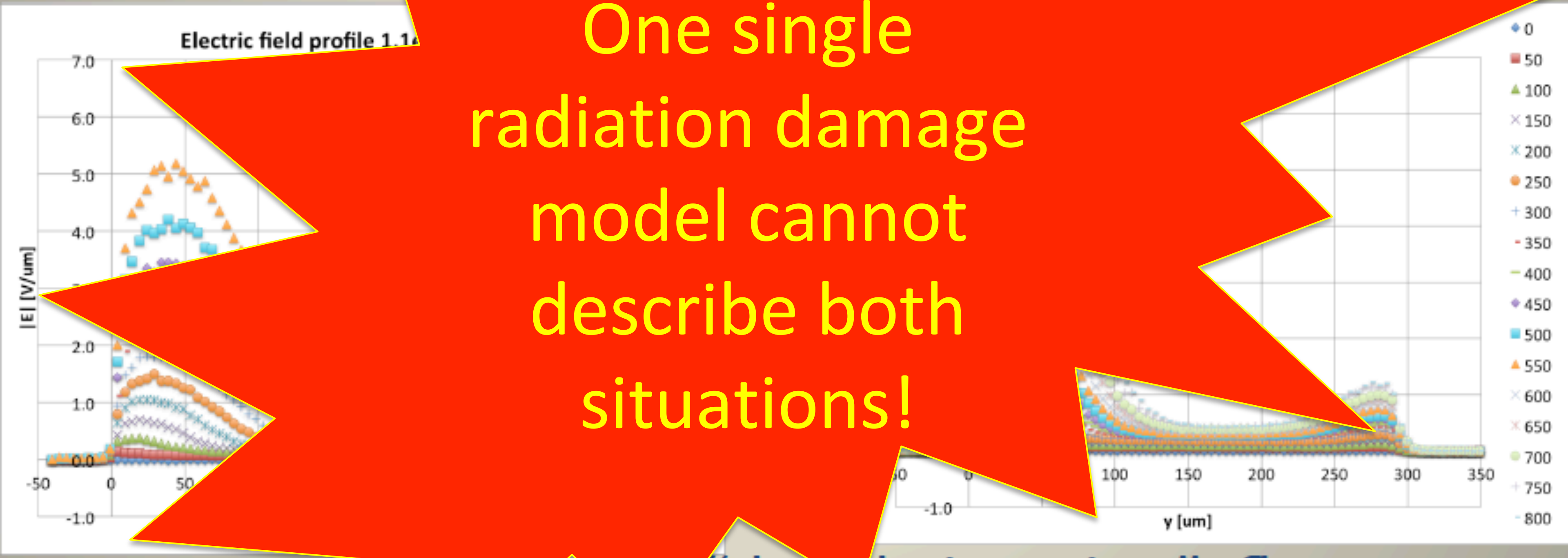




- Protons with more “double junction”, flatter field, less peaked at junction

Protons <-> Neutro ~10^{16}

- Field pro om



One single radiation damage model cannot describe both situations!

- Protons mo “dou ble junction”, flatter field, les peaked at junction

Comments

- In 2-states models energies are closer to the intrinsic level than in 3-states models
- Yet they both reproduce correctly the level of leakage current
- And the CCE
- Why then do they differ in the predicted electric field?

➢ Use grazing angle technique, edge-TCT and TPA to study “your” field

AVAILABLE SOFTWARE

Available software

- By now you should know that the most used TCAD tools in HEP are:
  - Silvaco ATLAS
  - Synospys SENTAURUS
- And that the two do not agree on some fundamental aspects ☺
  - AIDA 2020 WP7 meeting (Paris, 2/2016): https://indico.cern.ch/event/477003/contributions/1155199/attachments/1234150/1811069/bomben_comparison_160225.pdf
  - 28th RD50 WS (Torino, 6/2016): https://agenda.infn.it/getFile.py/access?contribId=3&sessionId=1&resId=0&materialId=slides&confId=11109
  - 31st RD50 WS (Geneva, 11/2017): https://indico.cern.ch/event/663851/contributions/2788159/attachments/1562199/2460062/bomben_silvaco_simulations.pdf

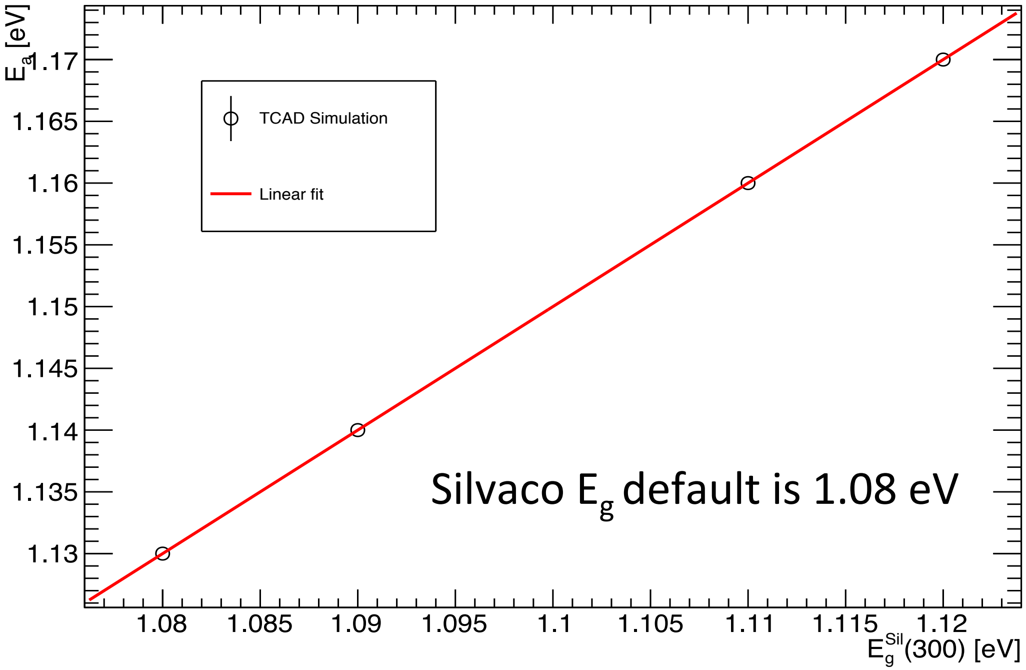
So....

- If you use Synopsys you are not alone (Hamburg, LHCb, Perugia, MPP, ...)
- If you use Silvaco... let me know ☺

$$I = I_{ref}\left(\frac{T}{T_{ref}}\right)^{n} exp\left[-\frac{E_a}{2k_B}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right)\right]$$

Thermal carrier velocities to be tuned too

Activation energy vs bandgap energy in Silvaco



Silvaco E_g default is 1.08 eV

1D VS 2D VS 3D VS 4D SIMULATIONS

1D vs 2D simulations

1D simulations are OK for:

- Leakage current density
- Electrode to backside capacitance
- Charge collection efficiency
  - For pads
  - For strip detectors at low fluences

2D simulations are OK for:

- Interstrips capacitance
- Charge collection efficiency
  - For strip detectors
  - For pixels detectors at low fluences

2D vs 3D simulations

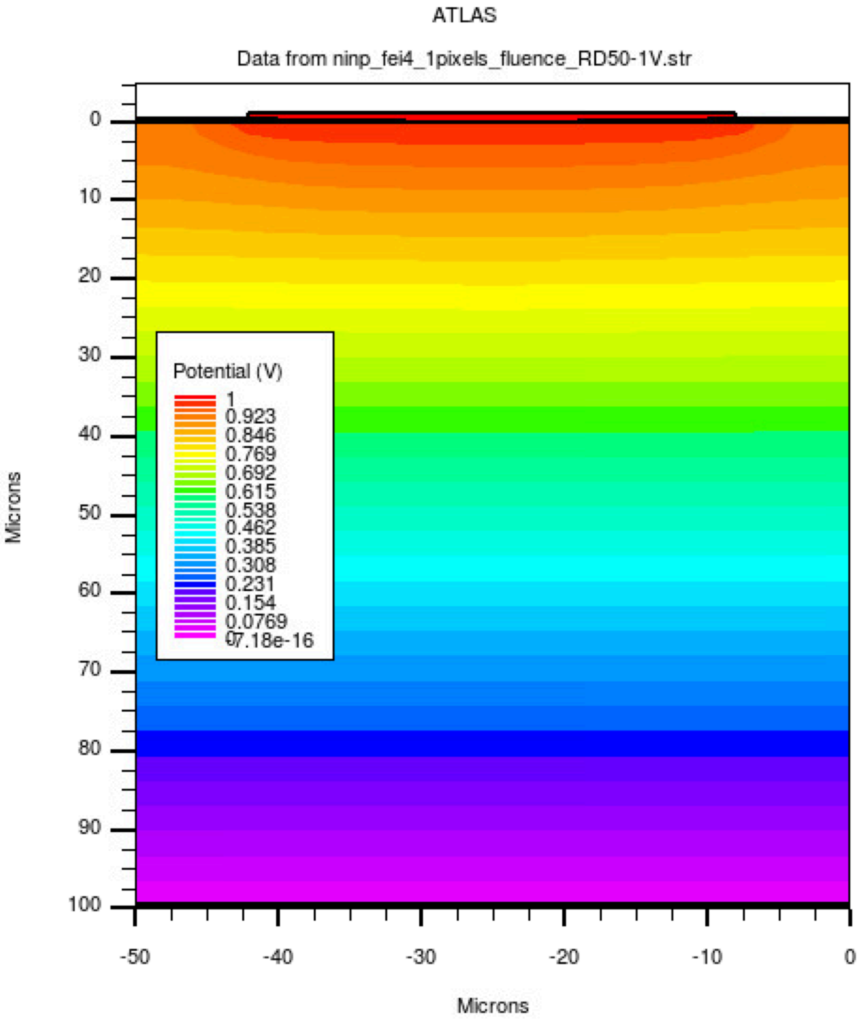
2D simulations are OK for:

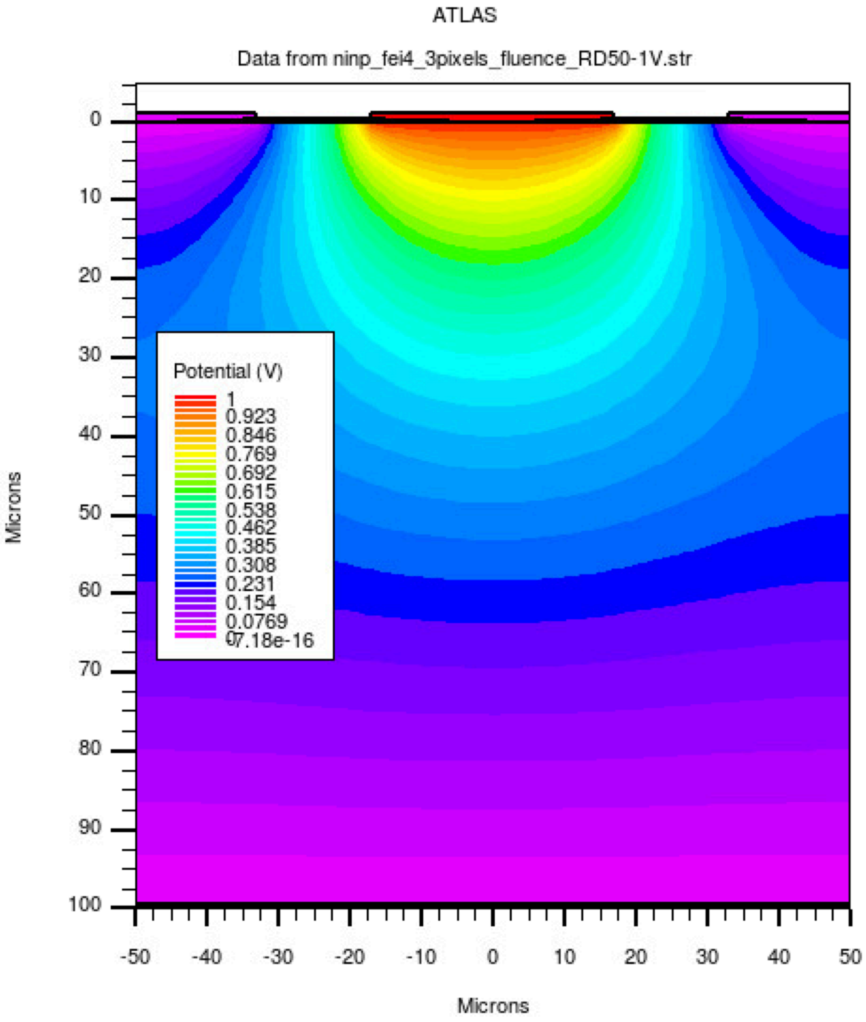
- Interstrips capacitance
- Charge collection efficiency
  - For strip detectors
  - For pixels detectors at low fluences

3D simulations are perfect for:

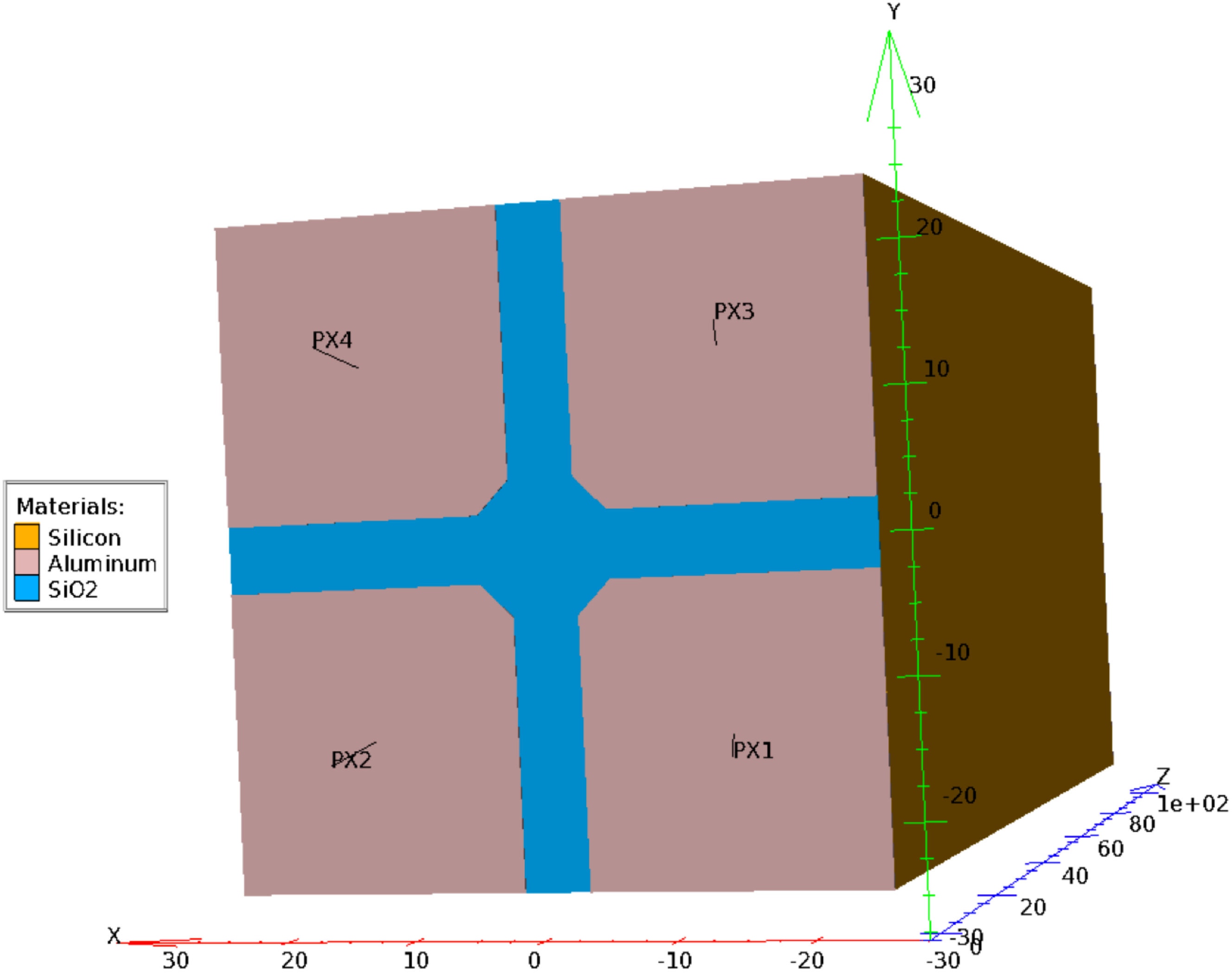
- Interpixels capacitance
- Charge collection efficiency
  - For pixel detectors

Ramo Potential: 1D vs 2D

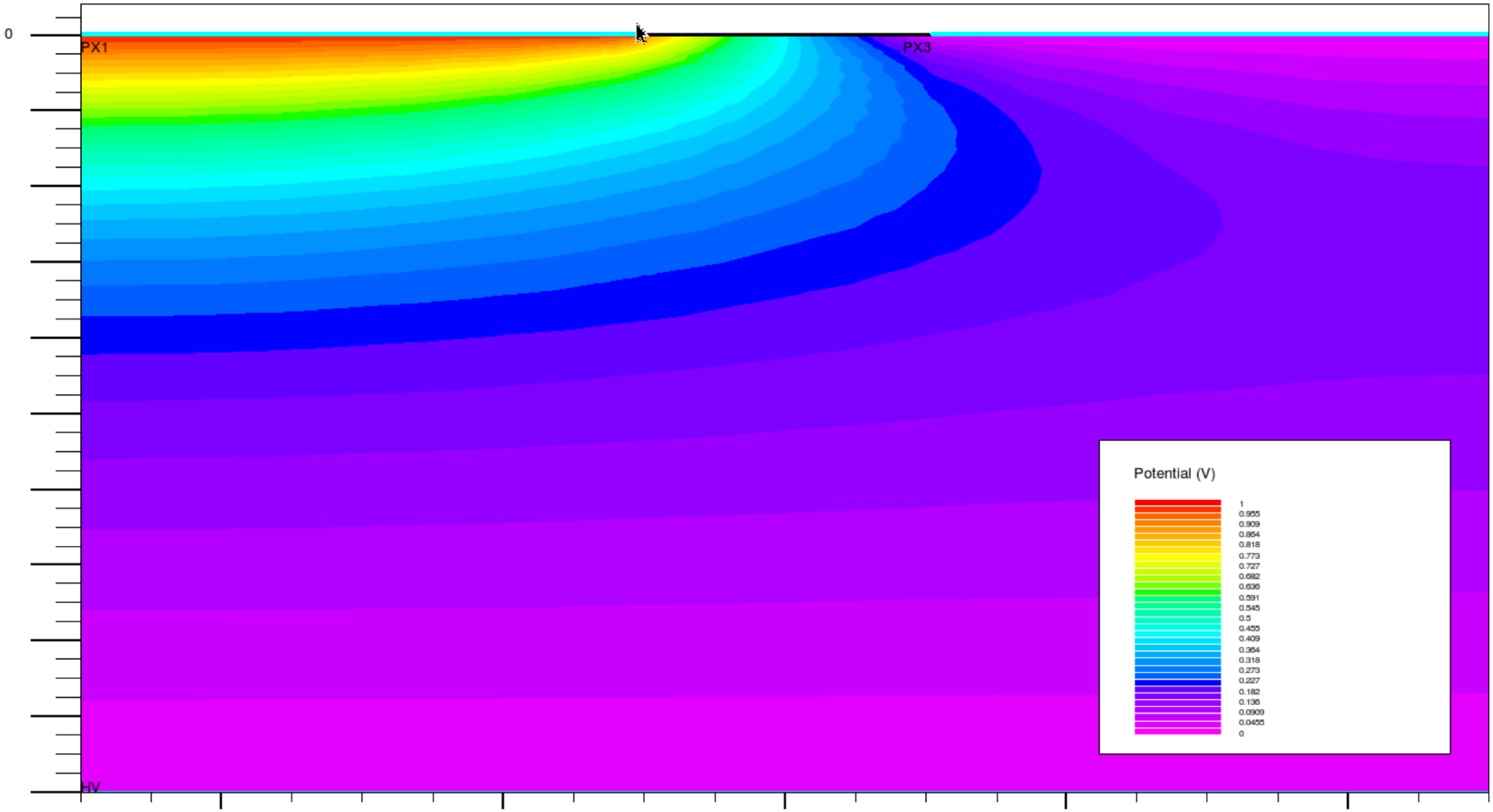




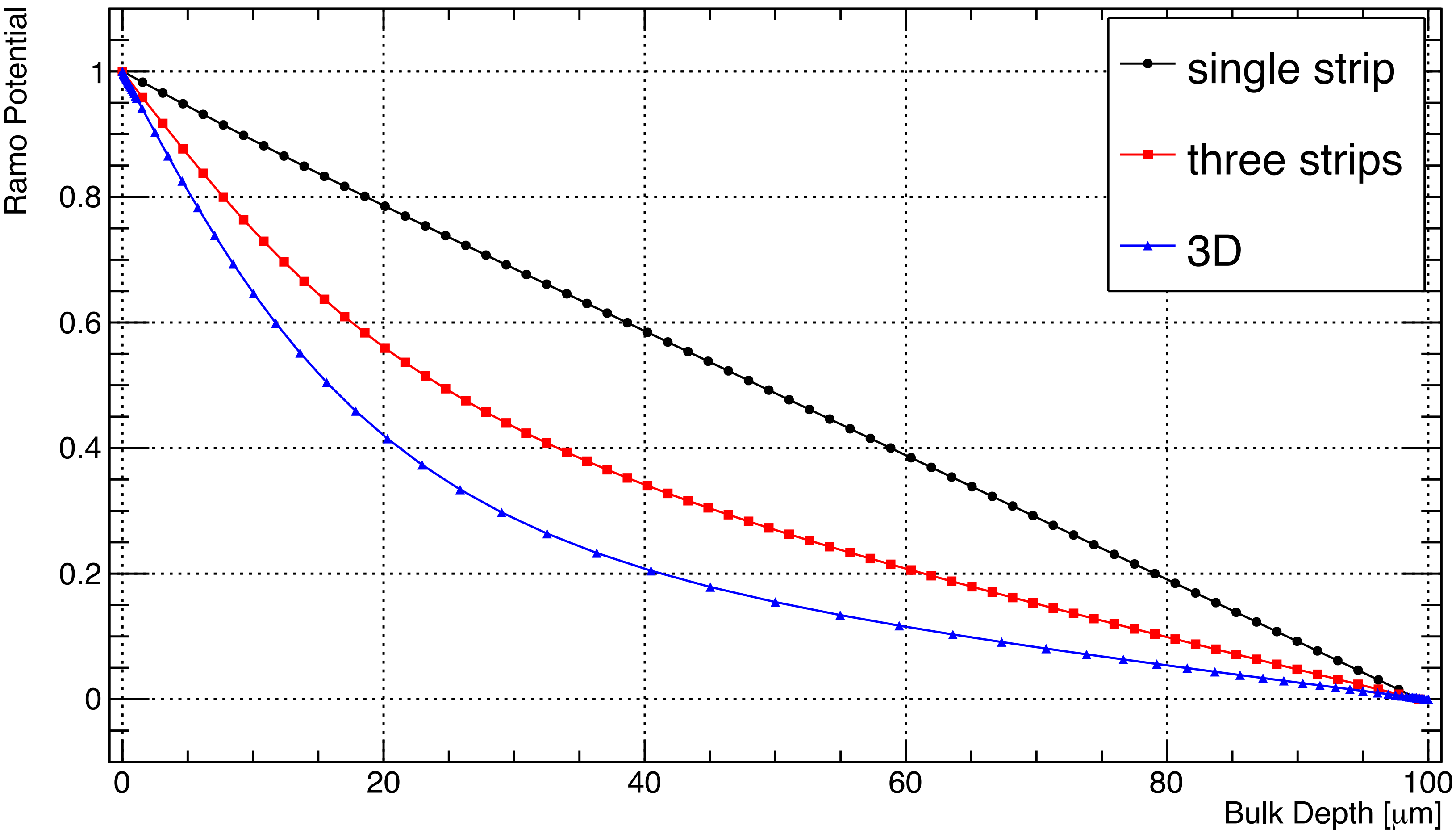
3D 50x50 μm^2 structure



Ramo Potential: 3D

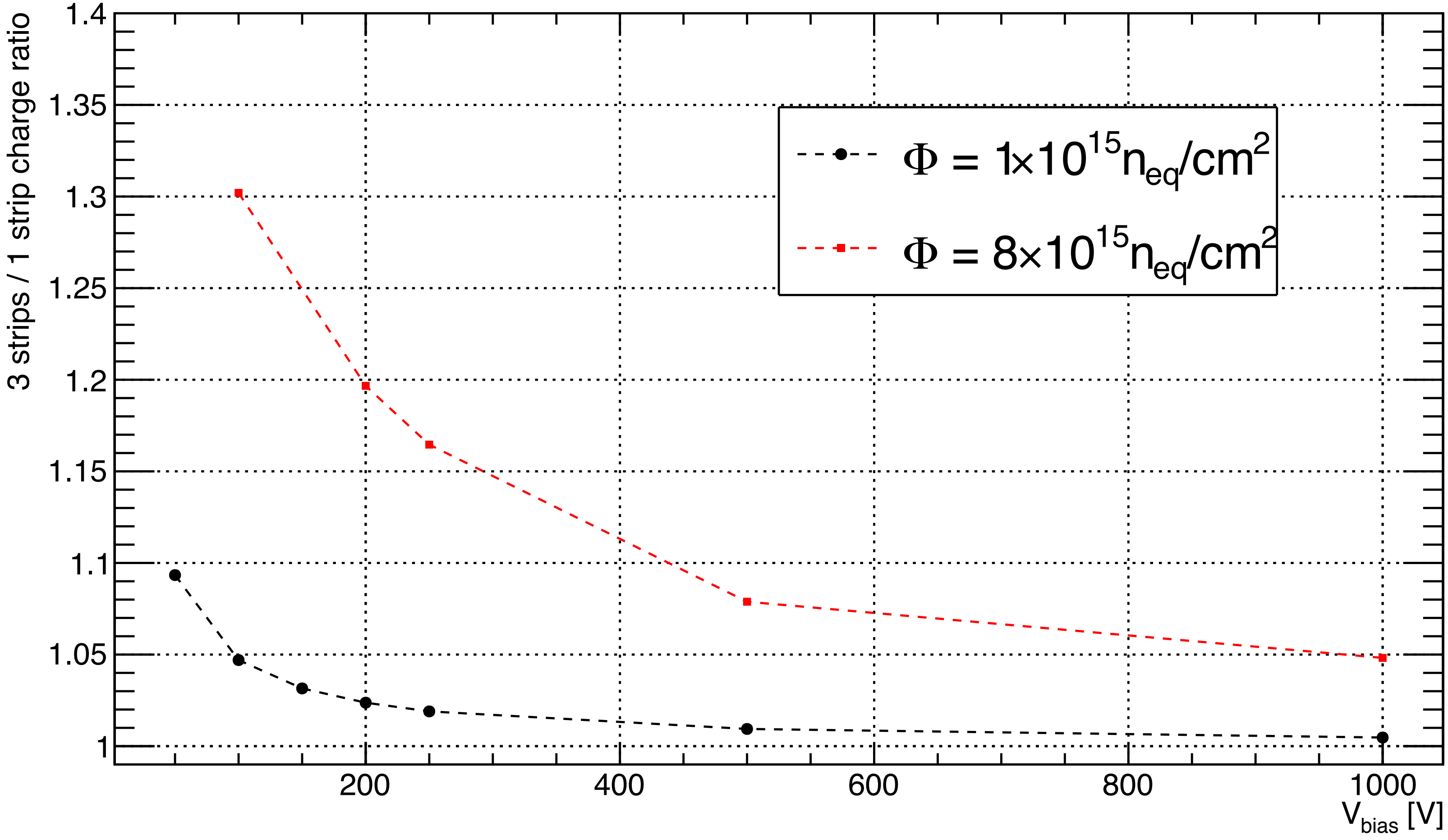


Ramo potential: comparison



Charge Collection Efficiency: comparison

Perugia model, Q(3 strips sim.)/Q(single strip)



4D simulations?

- Time dependent simulations of segmented LGADs...

- Computational complexity might be prohibitive, though

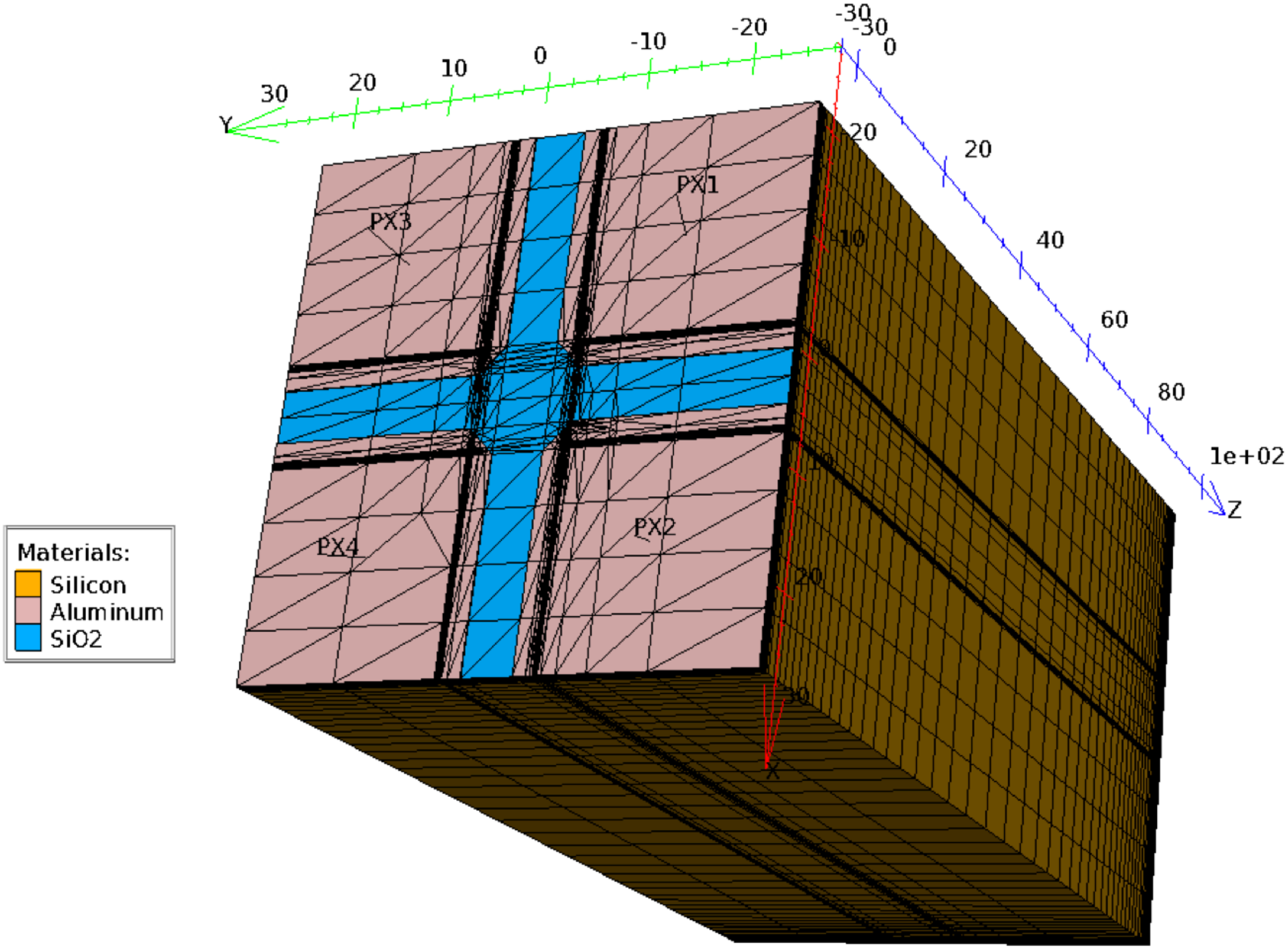
CONCLUSIONS

Conclusions and Outlook

- TCAD simulations help in optimizing new detector design and they offer insight in observables otherwise difficult to access
  - e.g. electric field, ramo potential
- It is important to correctly model the detector geometry to get the correct answer, even if in some cases simple approaches are possible
- The challenge of HL-LHC for silicon detectors is signal loss
- For this challenge TCAD simulations have to be validated on testbeam data to assess their predictive power
- Correct temperature dependence and annealing are not yet correctly modelled in actual radiation damage models
- Future: at the moment a combination of Geant4 and TCAD looks like the best way to make solid predictions
  - Allpix & allpix-sqaured; application: see also the talk by Lorenzo Rossini on new ATLAS pixel digitizer

Backup

3D mesh


Y
30
20
10
0
-10
-20
-30
-30
0
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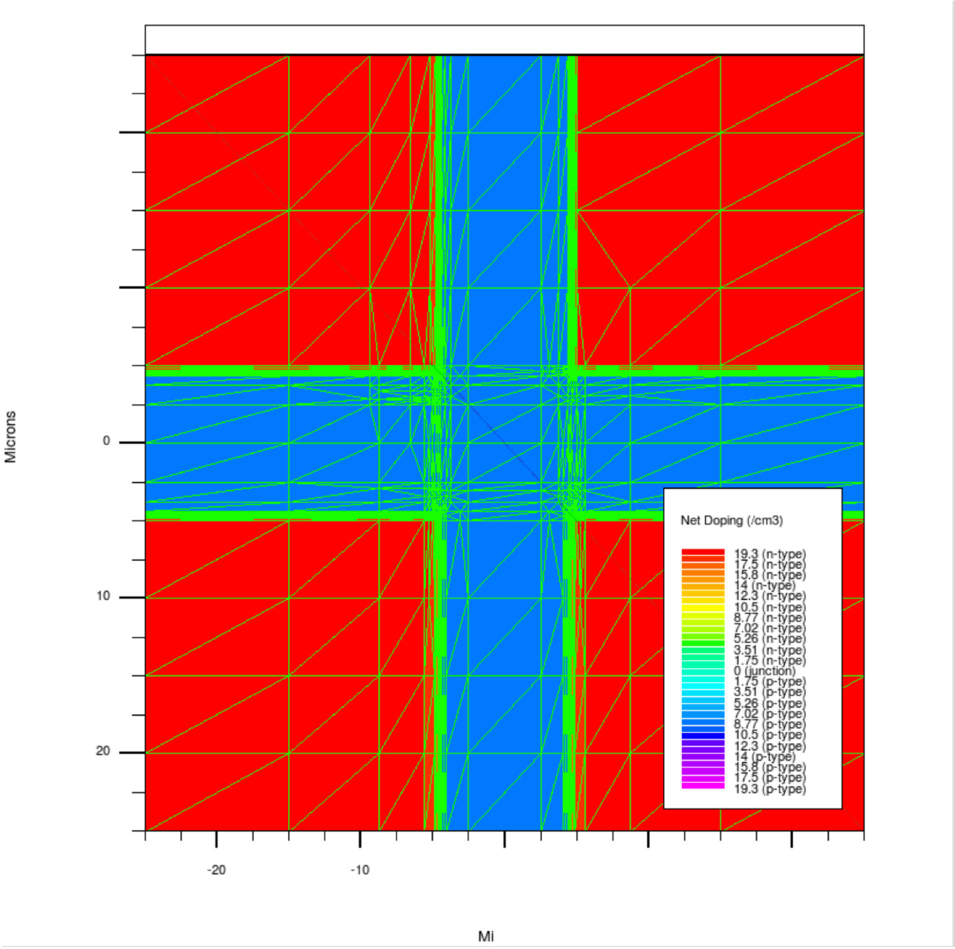
40
60
80
1e+02
Z
X
PX1
PX2
PX3
PX4
Materials:
Silicon
Aluminum
SiO2

Doping


Microns
0
10
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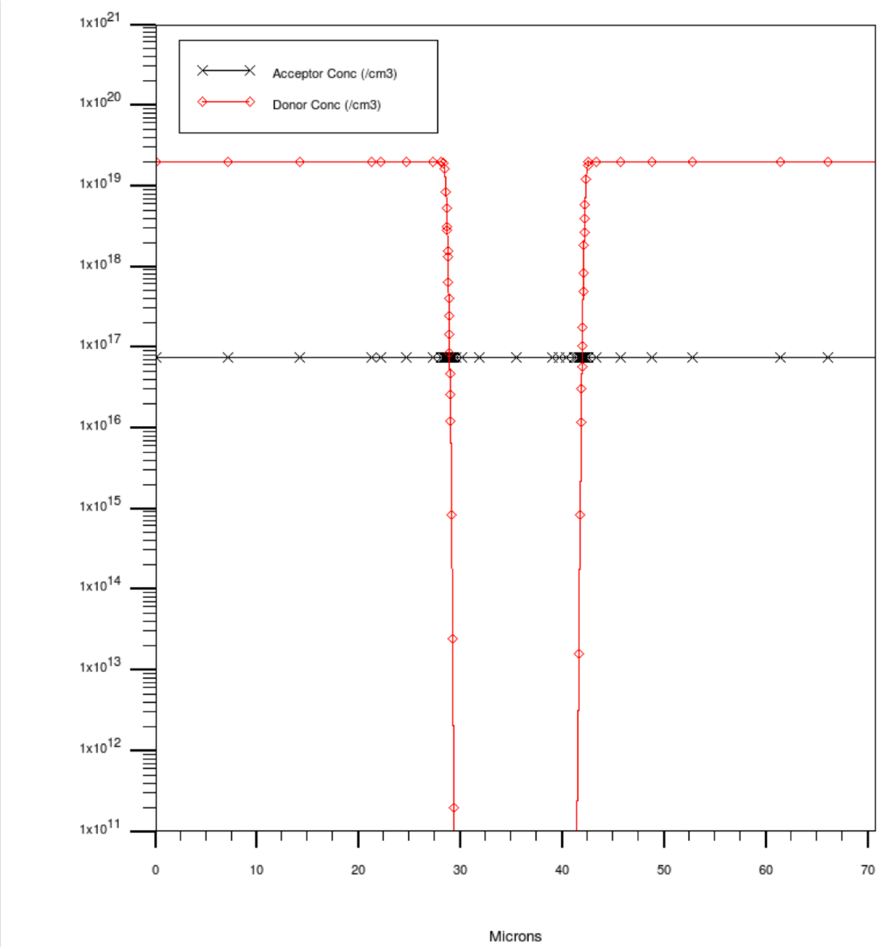
-20
-10
Mi
Net Doping (/cm3)
19.3 (n-type)
17.5 (n-type)
15.8 (n-type)
14 (n-type)
12.3 (n-type)
10.5 (n-type)
8.77 (n-type)
7.02 (n-type)
5.26 (n-type)
3.51 (n-type)
1.75 (n-type)
0 (junction)
1.75 (p-type)
3.51 (p-type)
5.26 (p-type)
7.02 (p-type)
8.77 (p-type)
10.5 (p-type)
12.3 (p-type)
14 (p-type)
15.8 (p-type)
17.5 (p-type)
19.3 (p-type)


Acceptor Conc (/cm3)
Donor Conc (/cm3)
1x10^21
1x10^20
1x10^19
1x10^18
1x10^17
1x10^16
1x10^15
1x10^14
1x10^13
1x10^12
1x10^11
0
10
20
30
40
50
60
70
Microns