Radiation damage models, comparison and perfomance of TCAD simulation

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on behalf of RD50 collaboration

Outline

- Motivation
- Radiation damage
- TCAD simulations
  - Models of bulk damage and their comparison
  - Comparison of Silvaco and Synopsis
  - Initial acceptor removal
  - Models for surface damage
- Signal Simulation Tools (SST)
- Conclusions

Motivation

Why simulations?

Understanding the radiation damage on the level of microscopic defects allows:

- understanding and predicting the operation
- avoiding design mistakes
- radiation hardness optimization of device design and material choice

Roadmap of the radiation hardness simulations:

- Measure macroscopic parameters/properties using test structures - very abundant set already within RD48/50 collaborations.
- Use them to simulate known silicon sensors.
- See if macroscopic properties obtained from simulations agree with measurements on those sensors
- Use simulations to optimize the specific sensor design

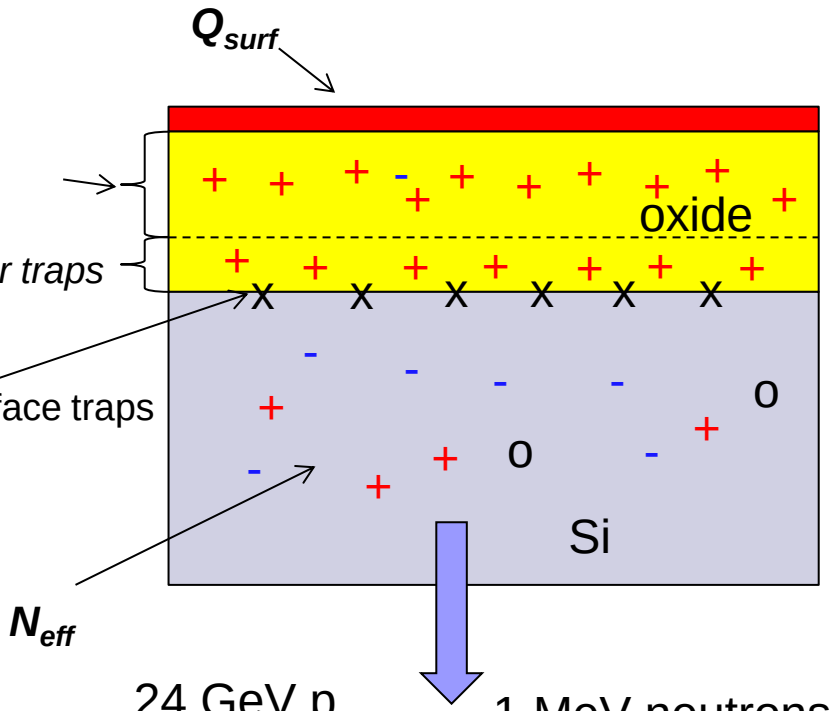
Radiation damage

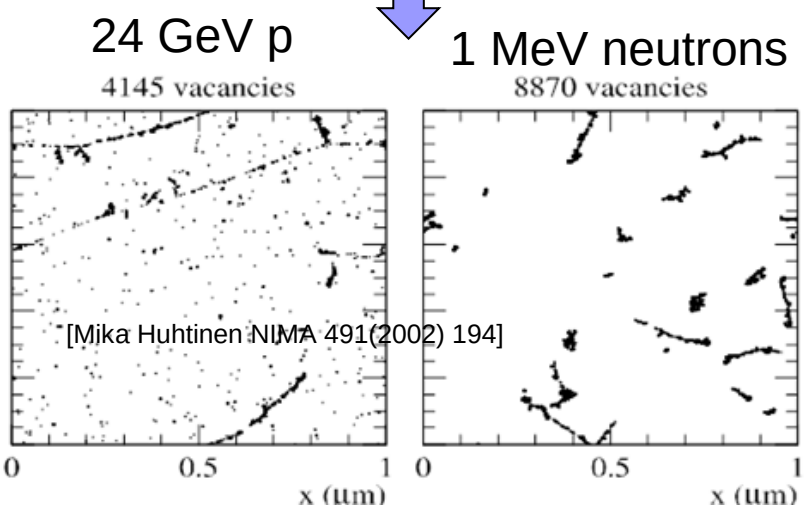
- Surface damage, oxide charge buildup and appearance of interface traps
  - Increase of surface current
  - Modification of electric field underneath the oxide
  - Trapping near the surface

Q-V, I-V, C-V on gate control diodes and MOS capacitors

- Bulk damage (NIEL), creation of silicon lattice defects
  - Increase of leakage current
  - Increase of space charge
  - Trapping of the drifting charge

Q-V, I-V, C-V on pads diodes





[Mika Huhtinen NIMA 491(2002) 194]

Simulations -> device model (TCAD)
bulk radiation damage model
surface damage model
boundary conditions

Simulations

Poisson $\Rightarrow$ $\nabla(\varepsilon_s \nabla U) = -e_0(p - n + \sum P_t N_D - (1 - P_t) N_A)$, $\vec{E} = -\nabla U$

Electron continuity $\Rightarrow$ $\frac{\partial n}{\partial t} = \frac{1}{q}\nabla.\vec{J}_n + (G - R)$ $\qquad \vec{J}_p = q\mu_p \vec{E} - qD_p \nabla p$

Hole continuity $\Rightarrow$ $\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla.\vec{J}_p + (G - R)$ $\qquad \vec{J}_n = q\mu_n \vec{E} + qD_n \nabla n$

$$G - R = (n_i^{\,2} - np)\sum_t \frac{c_n c_p}{c_n n + c_p n_i / \chi_t + c_p p + c_n n_i \chi_t} \quad , \quad \chi_t = \frac{1}{1 + \exp(\frac{E_t - E_i}{k_B T})}$$

- Solution of whole set of equations allows for complete “electric” description of the device, but a complex set of equations **(TCAD):**
  - problems with convergence
  - time consuming - particularly important when simulation is used to extract certain parameter by minimization
- If only e.g. Q-V is of interest, which is determined by electrical field and trapping **(SST)**
  - N_{eff}(x,y,z) parametrization with several free parameters is taken as a model
  - Trapping can be also taken as a free parameter of even fixed

TCAD simulations

More information on TCAD packages
M. Benoit, 11th Trento Workshop, Paris, 2016

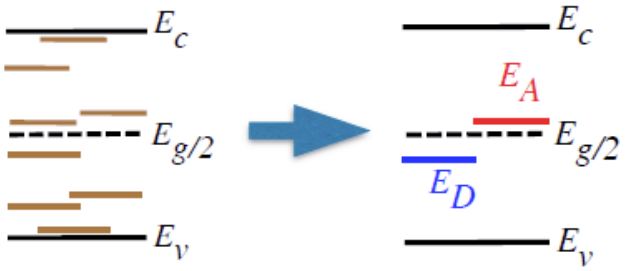
- Simulation steps
  - Device design (different options: hardcoding, GDSII files, GUI designer/editor)
  - **Meshing** (exploit symmetry, reduce complexity, removal of dead area)
  - Differential equations are discretized and solved on discrete mesh (FEM) taking into account different physics processes apart from SRH:
    - Impact ionization
    - Tunnelling (phonon assisted trap-to-band and band-to-band tunnelling)
    - Coupled-Defect-Level models
    - Oxide tunnelling
  - Extraction and calculation of the quantities

- There are two main software suits used: Silvaco and Synopsis , but there is also Cogenda which can become a major player. So far in RD50 the groups used only the first two.

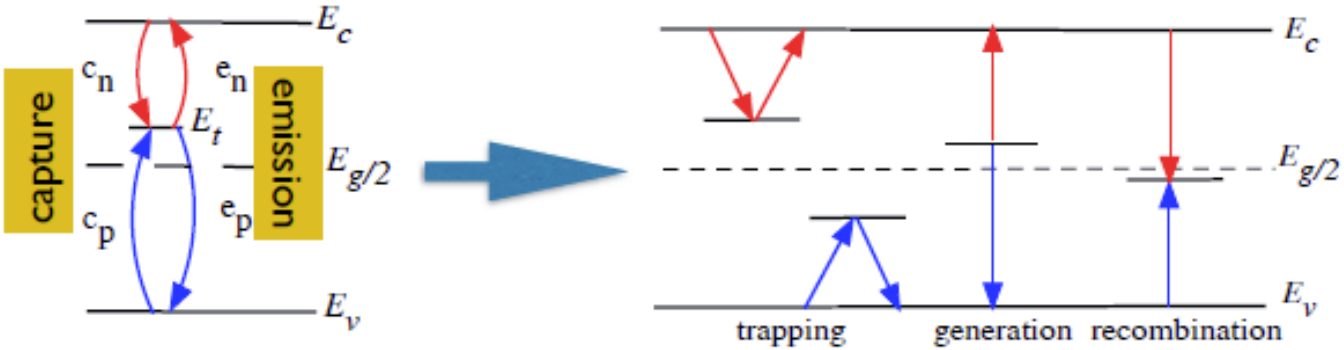
Damage model - bulk

- Damage models
  - fill the simulators with identified levels (convergance problems in simulators)
  - use effective trap levels (2 or 3, not many more)

  to model the large number of traps levels



- Assume the traps obey SRH statistics:



- Any trap level included in simulation requires 4 parameters:
  - defect concentration – function of fluence
  - cross sections for hole and electron capture
  - energy level

Parameters should be precisely known or amount of traps should be small.

Radiation induced bulk defects relevant for detector operation

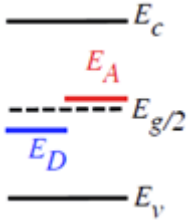
I. Pintilie's list, see talk

Electrical properties

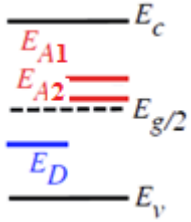
Defects	$\sigma_{n,p}$ [cm^2]	E_A [eV]	Assignment/References	Impact on electrical characteristics at RT
E(30K)	σ_n= 2.3 x 10^{-14}	E_C - 0.1	Electron trap with a donor level in the upper half of the Si bandgap /[Nucl. Instr. and Meth. in Phys. Res. A 611 (2009) 52; J. Appl.Phys. 117 (2015) 164503]	On the N_{eff} by introducing positive space charge *- It makes the difference between proton and neutron irradiations* *- More generated in O rich material*
$BD_A^{0/++}$ $BD_B^{+/++}$	σ_n= 2.3 x 10^{-14} σ_n= 2.7 x 10^{-12}	E_C - 0.225 E_C - 0.15	**Bistable Thermal double donor TDD2** (two configurations A and/or B) - Electron trap with a donor level in the upper half of the Si bandgap/ [Appl. Phys. Lett. 50 (21) (1987) 1500; Nucl. Instr. and Meth. in Phys. Res. A 514 (2003) 18; Nucl. Instr. and Meth. in Phys. Res. A 556 (2006) 197; Nucl. Instr. and Meth. in Phys. Res. A 583 (2007) 58]	On the N_{eff} by introducing positive space charge *- Strongly generated in O rich material*
$I_p^{+/0}$ $I_p^{0/-}$	σ_p= (0.5-9) x10^{-15} σ_n=1.7 x10^{-15} σ_p= 9 x 10^{-14}	E_V + 0.23 E_C - 0.545	Donor level of V_2O or of a still unkown C related defect / [Appl. Phys. Lett. 81 (2002) 165; Appl. Phys. Lett. 83, 3216 (2003); Nucl. Instr. and Meth. in Phys. Res. A 611 (2009) 52] Acceptor level of V_2O or of a still unkown C related defect/[Nucl. Instr. and Meth. in Phys. Res. A 611 (2009) 52, Appl. Phys. Lett. 81 (2002) 165; J. Appl.Phys. 117 (2015) 164503]	On the N_{eff} by introducing negative space charge and on LC *- Strongly generated in O lean material*
E_4 E_5	σ_n=1 x 10^{-15} σ_n=7.8 x 10^{-15}	E_C -0.38 E_C -0.46	**Trivacancy**: Acceptor in the upper part of the gap associated with the double charged and single charged states of V_3, respectively (**$V_3^{=/-}$ and $V_3^{-/0}$**) / [J. Appl. Phys. 111 (2012) 023715.]	On LC
H(116K)	σ_p=4 x 10^{-14}	E_V + 0.33	Hole trap with an acceptor level in the lower part of the Si bandgap - Extended defect (cluster of vacancies and/or interstitials) / [Appl. Phys. Lett. 92 (2008) 024101, Nucl. Instr. and Meth. in Phys. Res. A 611 (2009) 52-68; J. Appl.Phys. 117 (2015) 164503]]	On the N_{eff} by introducing negative space charge
H(140K)	σ_p=2.5 x 10^{-15}	E_V + 0.36	Hole trap with an acceptor level in the lower part of the Si bandgap - Extended defects (clusters of vacancies and/or interstitials)/[Appl. Phys. Lett. 92 (2008) 024101, Nucl. Instr. and Meth. in Phys. Res. A 611 (2009) 52-68; J. Appl.Phys. 117 (2015) 164503]]	On the N_{eff} by introducing negative space charge
H(152K)	σ_p=2.3 x 10^{-14}	E_V + 0.42	Hole trap with an acceptor level in the lower part of the Si bandgap - Extended defects (clusters of vacancies and/or interstitials)/[Appl. Phys. Lett. 92 (2008) 024101, Nucl. Instr. and Meth. in Phys. Res. A 611 (2009) 52-68]; J. Appl.Phys. 117 (2015) 164503]	On the N_{eff} by introducing negative space charge

Models of radiation damage in TCAD

EVL model
A single donor in bottom half of the bandgap and a single acceptor in the upper half of the bandgap



Perugia model
Three levels associated to donor CiOi, 1st acceptor to V_2 and 2nd acceptor to V_3



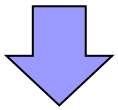
Model	E [eV]	g_{int} [cm^{-1}]	σ_e[cm^2]	σ_h [cm^2]
EVL	Ev+0.48	6	1e-15	1e-15
Neutrons	Ec-0.525	3.7	1e-15	1e-15
Delphi	Ev+0.48	4	2e-15	2.6e-15
23 MeVp	Ec-0.51	3	2e-15	2e-15
KIT (Eber)	Ev+0.48	5.598 (-3.949e14)	2e-15	2.6e-15
23 MeVp	Ec-0.525	1.198 (+6.5434e13)	2e-15	2e-15
HIP	Ev+0.48	5.598 (-3.949e14)	1e-14	1e-14
23 MeVp	Ec-0.525	1.198 (+6.5434e13)	1e-14	1e-14
2 μm from surface only	Ec-0.40	14.417 (+3.168e16)	8e-15	2e-14
Hamburg (new)	Ev+0.48	1.51-2.75	8.37e-15	2.54e-15
	Ec-0.525	0.36-0.93	6.3e-15	8.37e-15

Model	E [eV]	g_{int} [cm^{-1}]	σ_e[cm^2]	σ_h [cm^2]
Perugia	Ev+0.36	0.9	2.5e-13	2.5e-15
p-type	Ec-0.42	1.6	2e-15	2e-14
	Ec-0.46	0.9	5e-15	5e-14
Perugia	Ev+0.36	1.1	2e-18	1.2e-14
n-type	Ec-0.42	13	2.5-15	1.2e-14
	Ec-0.50	0.08	5e-15	3.5e-14
Peniccard	Ev+0.36	0.9	3.23e-13	3.23e-14
	Ec-0.42	1.613	9.5-15	9.5e-14
	Ec-0.46	0.9	5e-15	5e-14
Perugia new	Ev+0.36	0.9	3.23e-13	3.23e-14
(<7e15 cm^{-2})	Ec-0.42	1.6	1e-15	1e-14
	Ec-0.46	0.9	7e-15	7e-14

Models of radiation damage in TCAD

All of the radiation damage models work fine for certain type of sensors and conditions even more so if they were tuned for specific measurements.

- We don't have a unique set of parameters that completely describes the performance irradiated detectors at different irradiation levels of different particles.
- In n-trap model there are 5·n independent parameters, which could all be in principle time dependent (annealing) and irradiation particle dependent – huge parameter space.
- For very high fluences some of the physics processes in TCAD, not directly linked to properties of traps are not adequate:
  - Mobility decreases with irradiation – recent findings of RD50 (*M. Mikuž 28th RD 50 workshop*)
  - Intrinsic resistivity changes
  - Impact ionization may decrease with irradiation

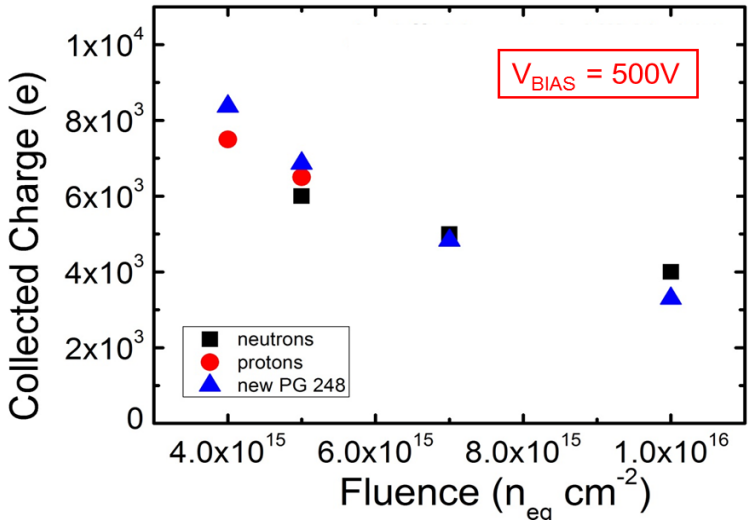


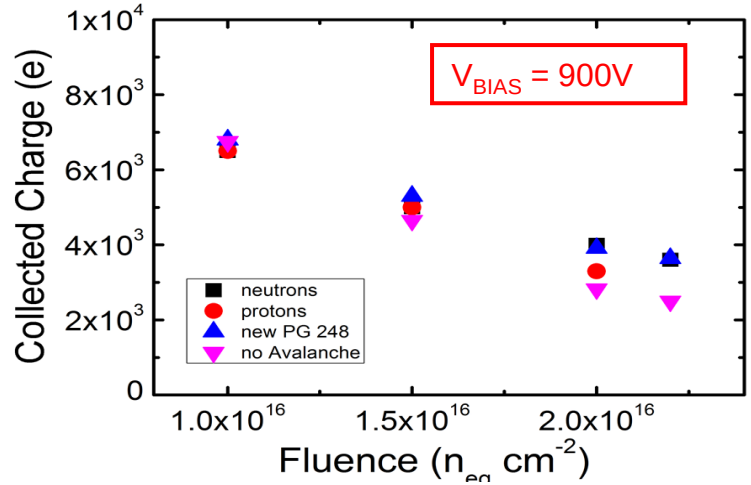
Is it possible at all to get the "best" model – the one that approximately agrees with different set of detectors and irradiations?

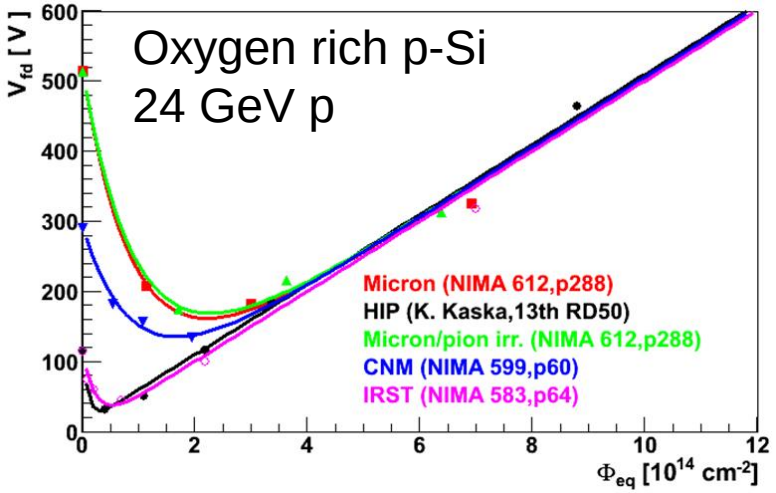
Examples of simulations

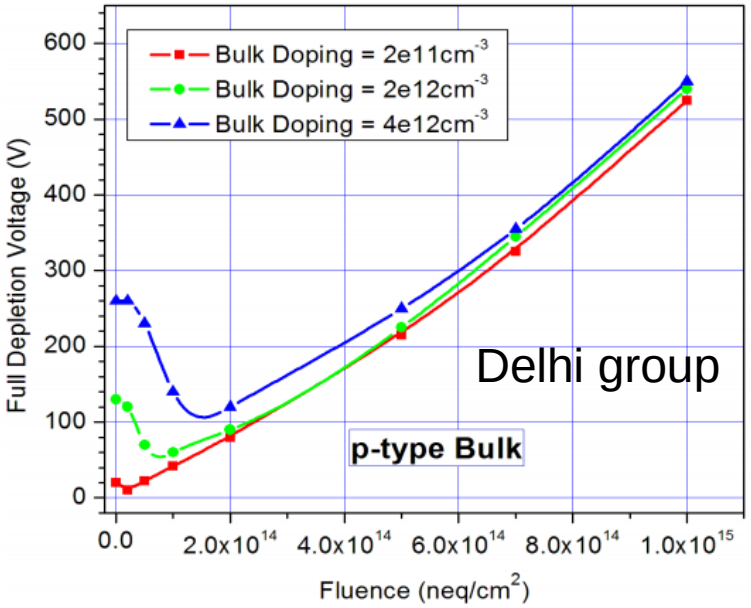
data Affolder et al., NIM A, Vol. 623 (2010), pp. 177-179.

Moscatteli et. al., 10th TRENTO workshop









Simulations of CCE and electric field that explain the measured data well.

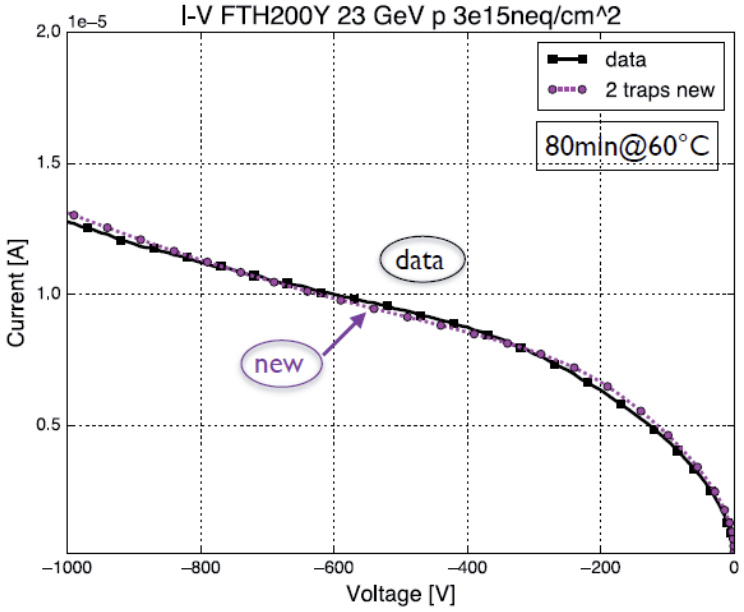
How to get the best effective model?

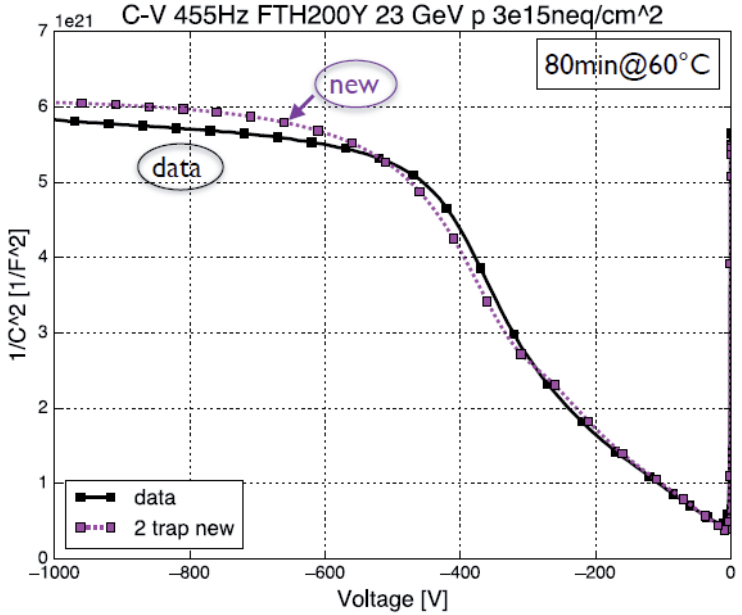
- A set of parameters can be obtained from minimizing the difference between measurement and simulation – not an easy task in TCAD (from minutes to hours for single property calculation) when trying to minimize multi parameter function *F*

$$F = \sum_n w_n \int_{V_{min}}^{V_{max}} \left(1 - \frac{M_n}{S_n}\right)^2 dV$$

J. Schwandt, 11th Trento Workshop

- *S, M* are simulated and measured properties: I_{rev}, I_{for}, *C*, CCE
- V_{min} , V_{max} min. and max of voltage range, w_n – the weight in minimization of property



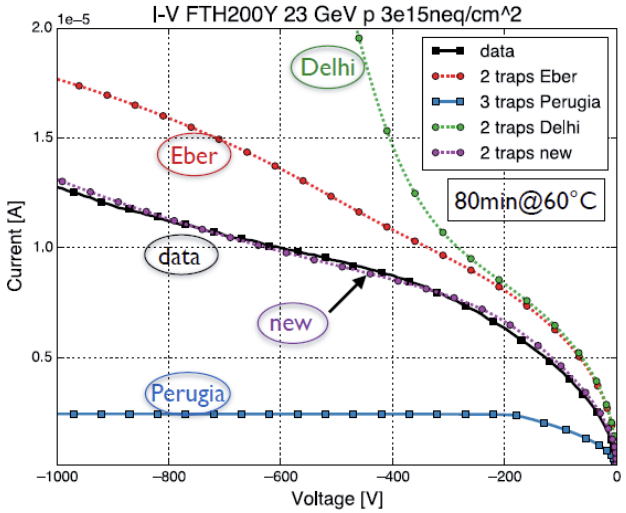


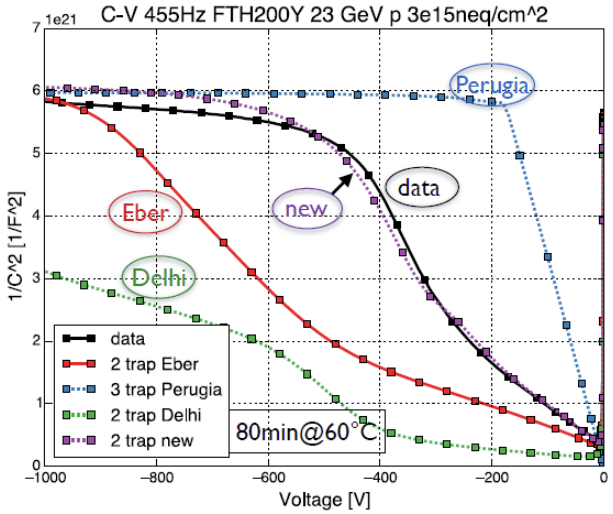
EVL model energy levels with other 6 parameters left for minimization for I_{ref} and *C*.

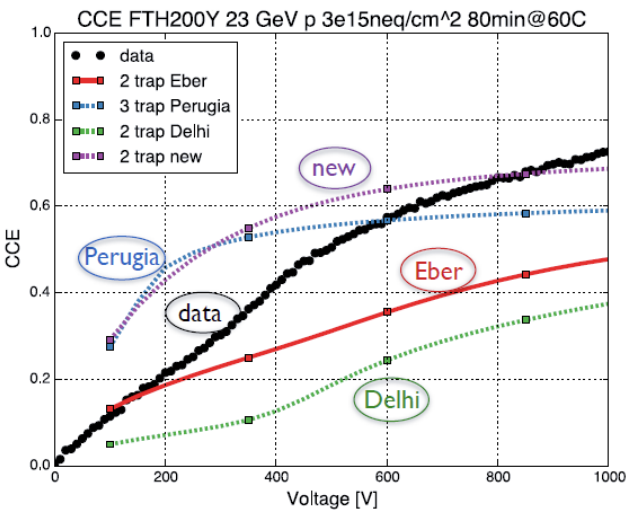
Comparison of models (synopsis)

200 μm thick p-type pad detector Φ_{eq}(23 GeV p)=3e15 cm^{-2}, annealed 80min@60ºC, T=-20ºC

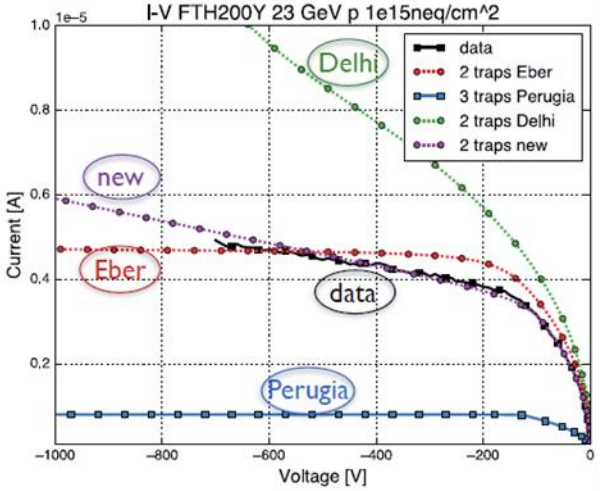
Simulation same device with different models – **a clear disagreement between different models**

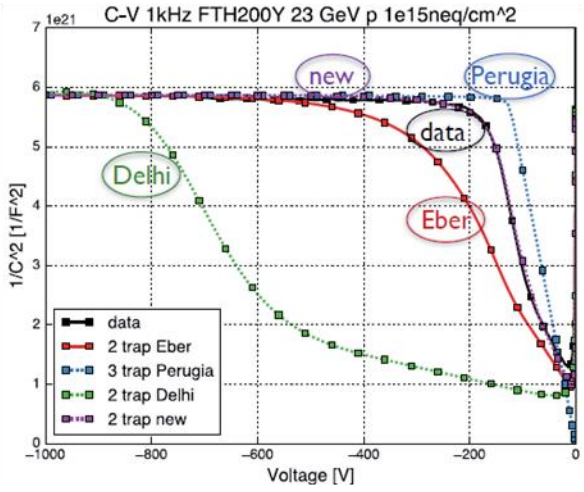


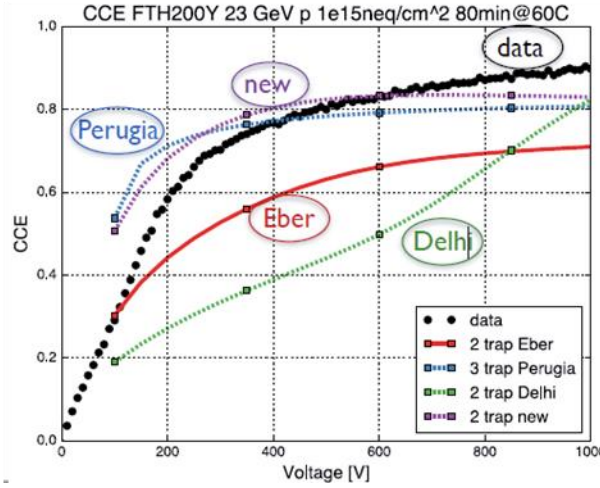




Somewhat better agreement for lower fluences Φ_{eq}(23 GeV p)=1e15 cm^{-2}





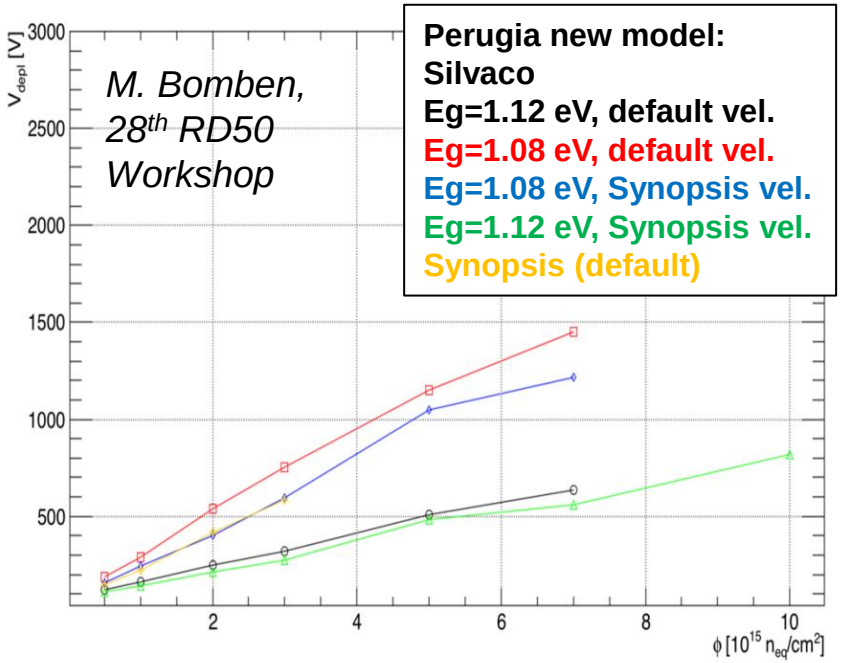


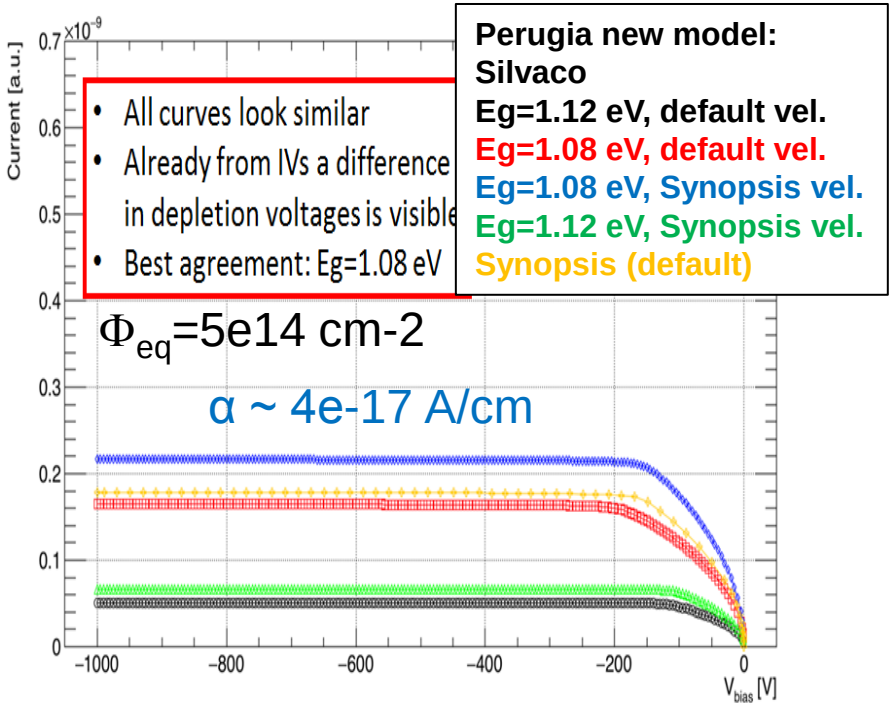
Comparison of the simulators (I)

Already in simulators there are differences in underlying physics – beware of "time saving black box approach":

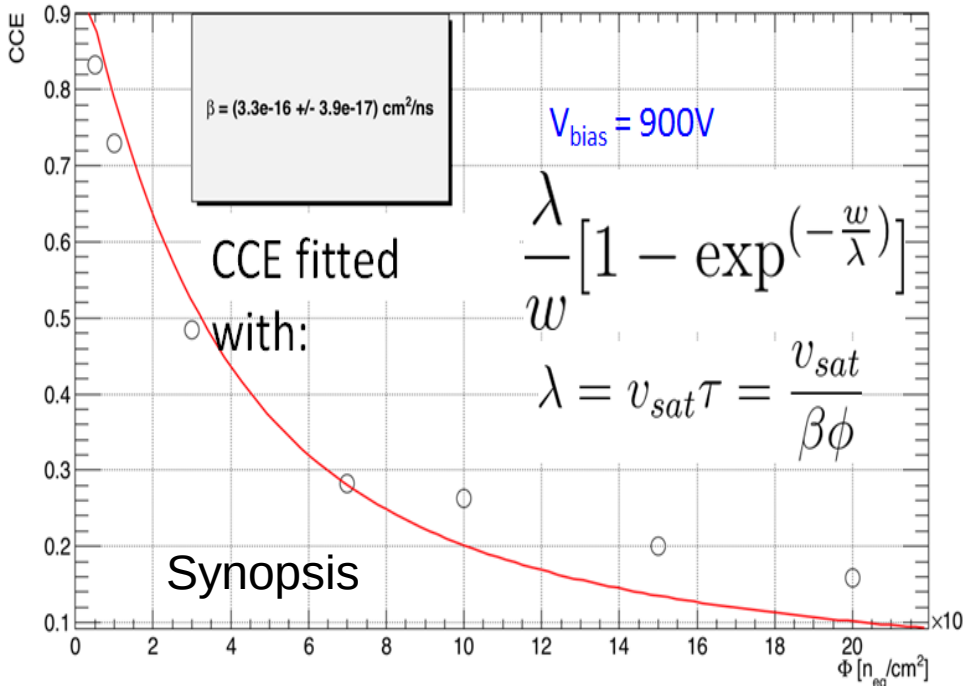
- Sysnopsis and Silvaco have a very large difference in "default" thermal velocities v_n =2.02e+07 cm/s , v_p=1.54e+07 cm/s and v_n=9.97e+06 cm/s, v_p=1.21e+07 cm/s
- Default band gap in Silvaco at 300 K is E_g=1.08 eV, however the simulation results are comparable with Synopsis which uses E_g=1.12 eV.

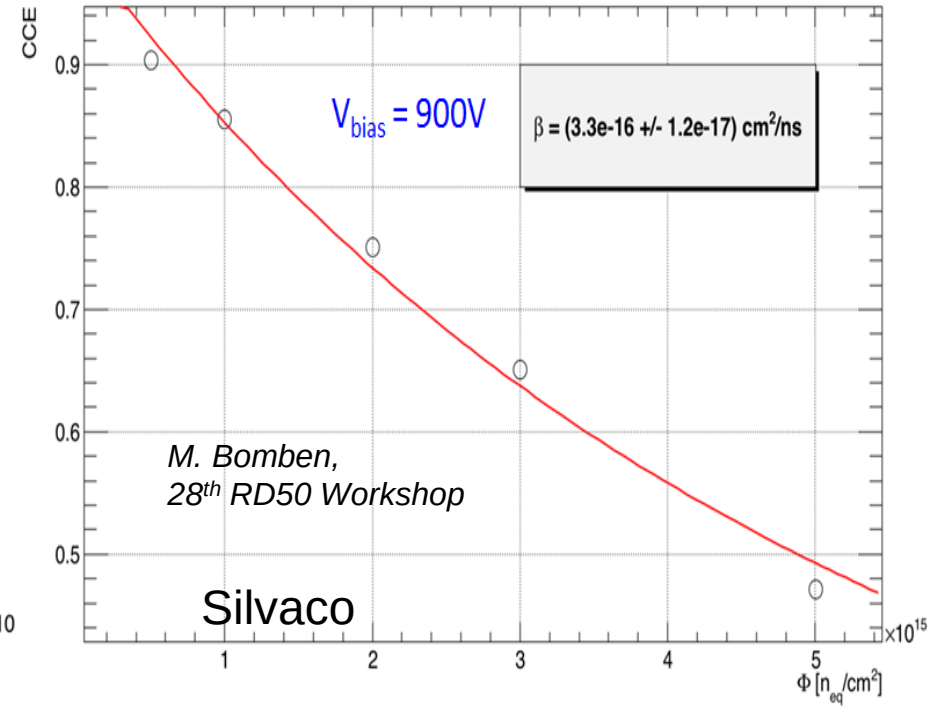
200 μm thick n-p pad diode (50 μm wide), N_{eff}=3e12 cm^{-3}, T=20°C





Comparison of the simulators (II)





data Affolder et al., NIM A, Vol. 623 (2010), pp. 177-179.

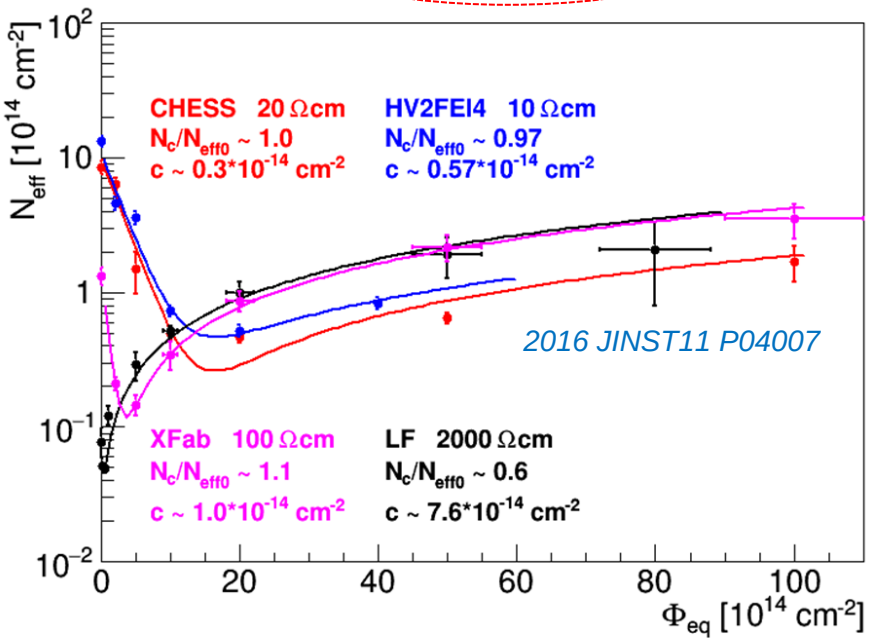
- Both give the same CCE and also same trapping damage constant.

  v_{th} that comes into calculation of trapping times : $1/\tau=\beta\,\Phi_{eq}=v_{th}\,\sigma\,N\,P$ is compensated by lower trap occupancy P
- Make sure that you take into account also (data from strip and simulation from pads)

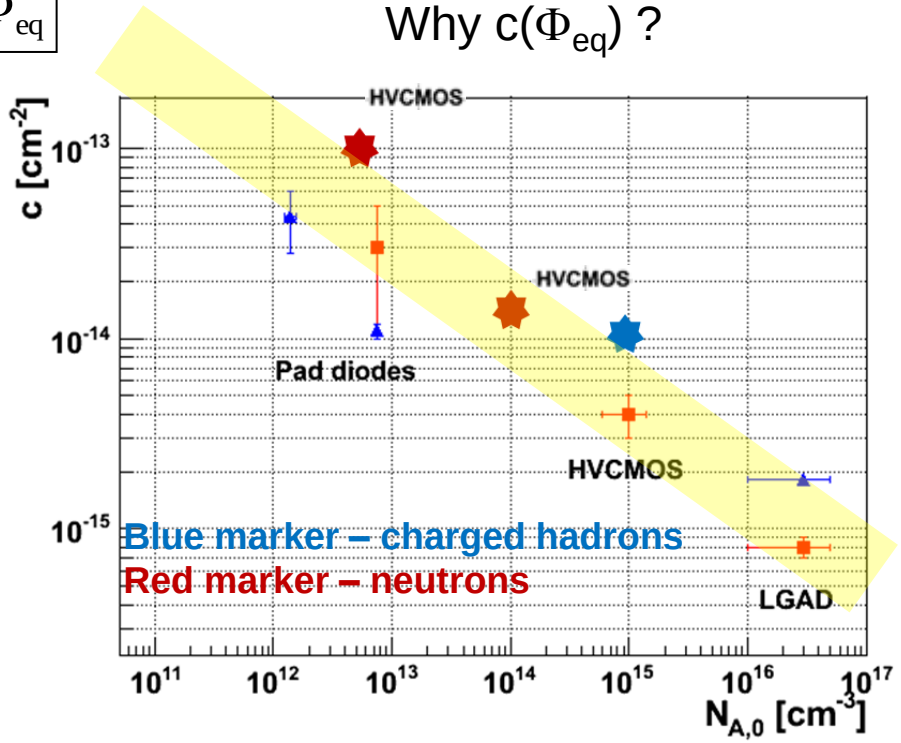
Initial dopant removal in TCAD simulations

- A lot of studies of donor removal for low initial donor concentrations during RD48 times - part of “New Perugia model”.
- Understanding the effective acceptor removal seen in LGAD (with TCT) and HVCMOS (with Edge-TCT) detectors

$$N_{\text{eff}} = N_{\text{eff0}} - N_c \cdot (1 - \exp(-c \cdot \Phi_{\text{eq}})) + g_c \cdot \Phi_{\text{eq}}$$



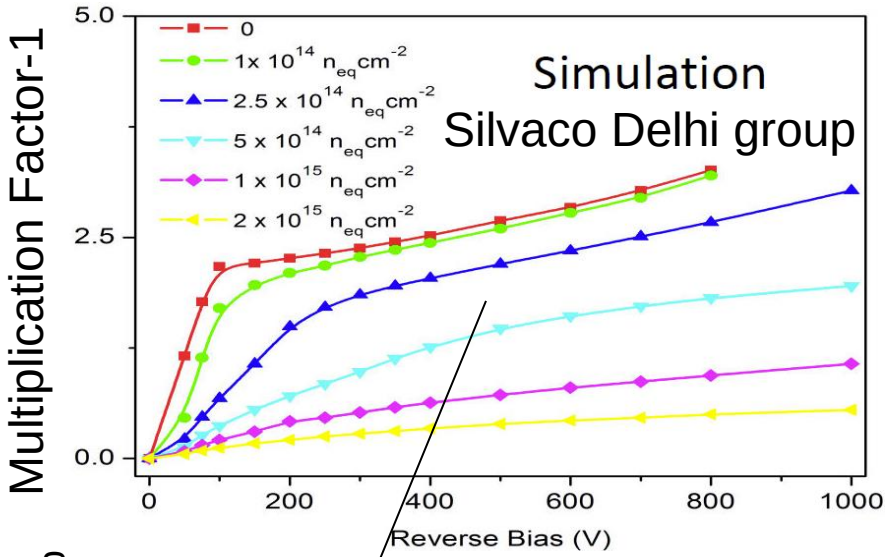
Why c(Φ_{eq}) ?

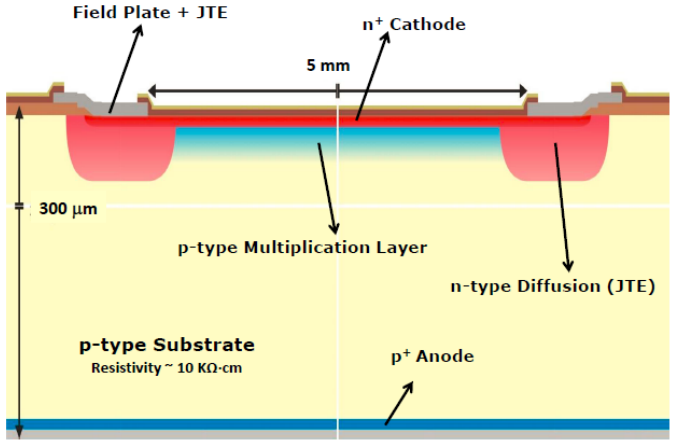


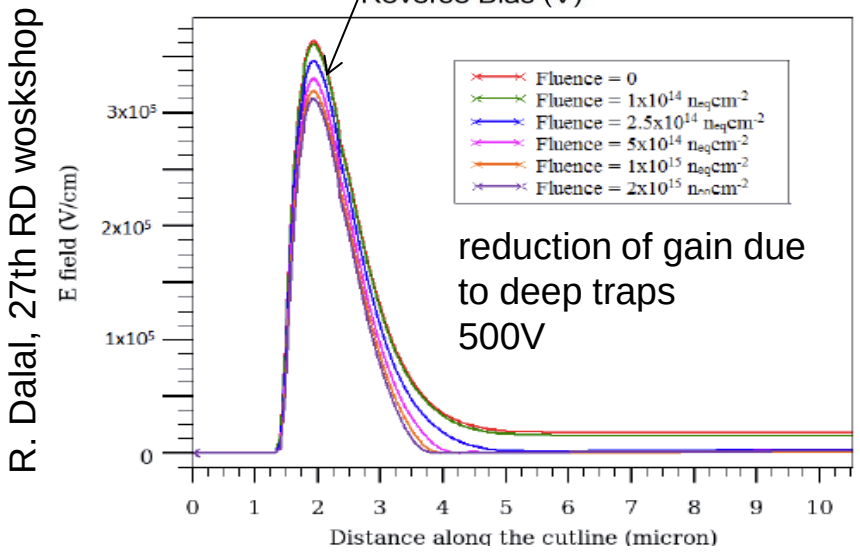
The measurements point to same effective acceptor removal in LGAD and HVCMOS detectors.

Is initial B removal needed?– TCAD of LGAD

However TCAD simulations (2 and 3 levels) show that the decrease of charge can be described by adding deep traps only – **the field in multiplication layer is reduced by double junction only**

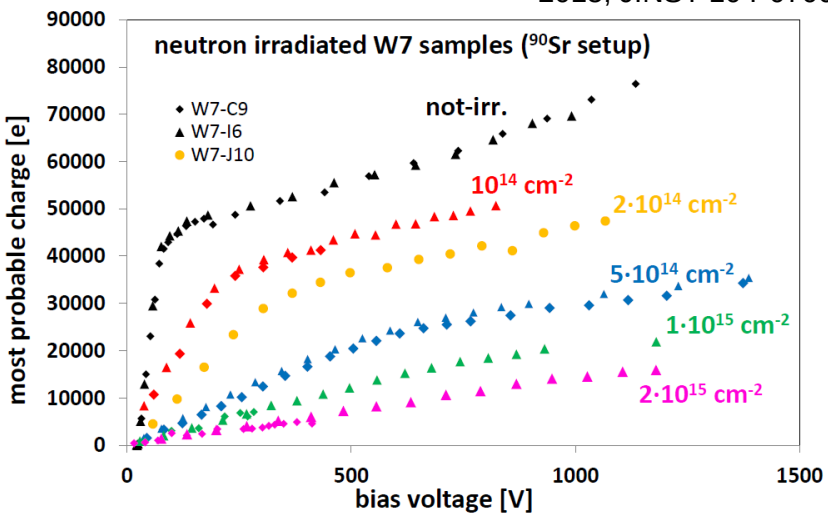






Qualitative agreement

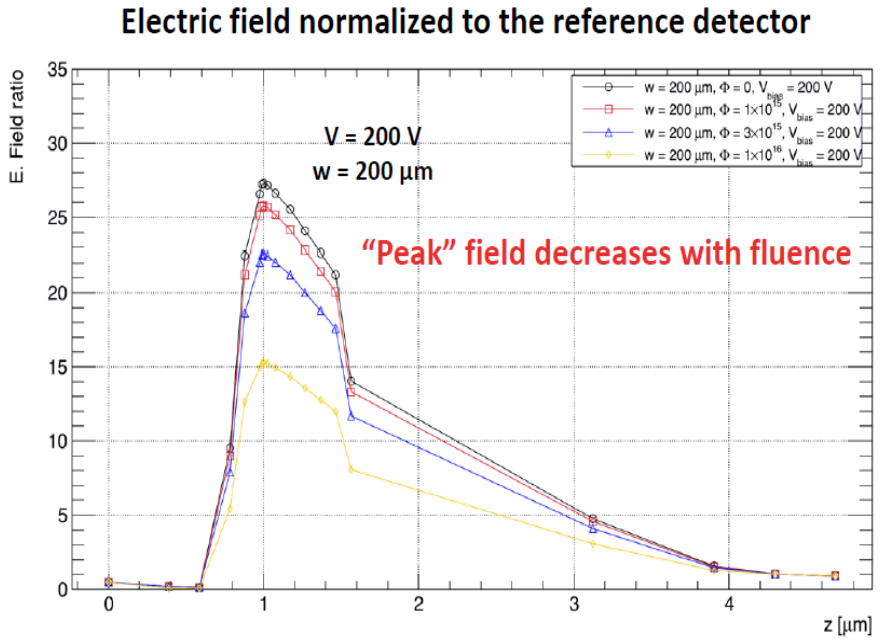
2015, JINST 10 P07006



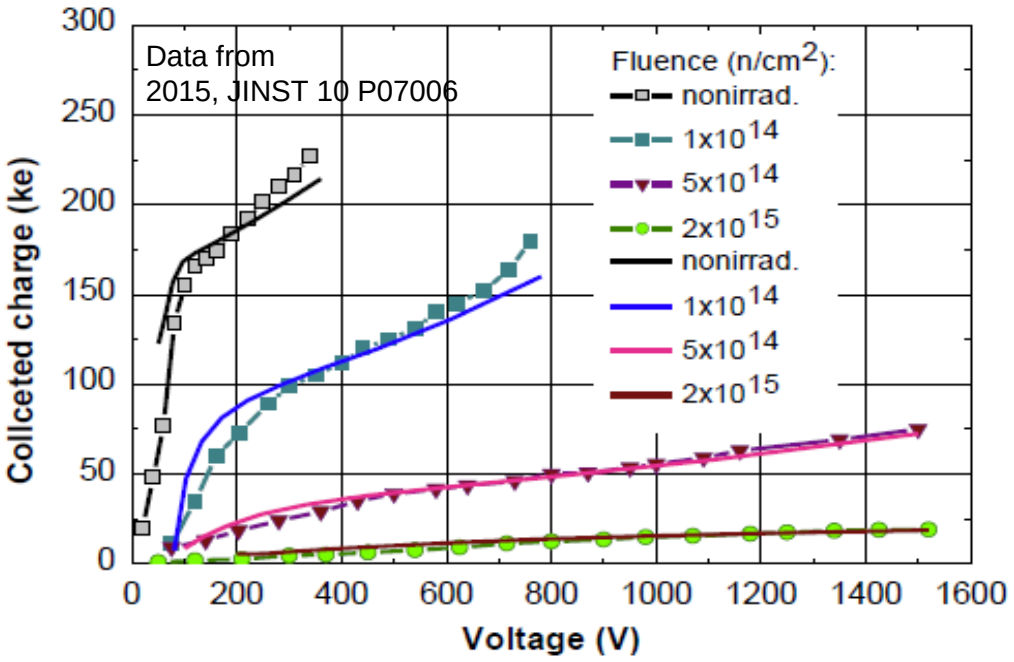
Is initial B removal needed?– TCAD of LGAD

However TCAD simulations (2 and 3 levels) show that the decrease of charge can be described by adding deep traps only – **the field in multiplication layer is reduced by double junction only**

LPNHE group



Ioffe group - custom 1D simulator



However, preliminary measurements of detector operation with enhanced free carrier concentration (DC illumination with red light) show that deep traps alone can not explain the loss of gain!

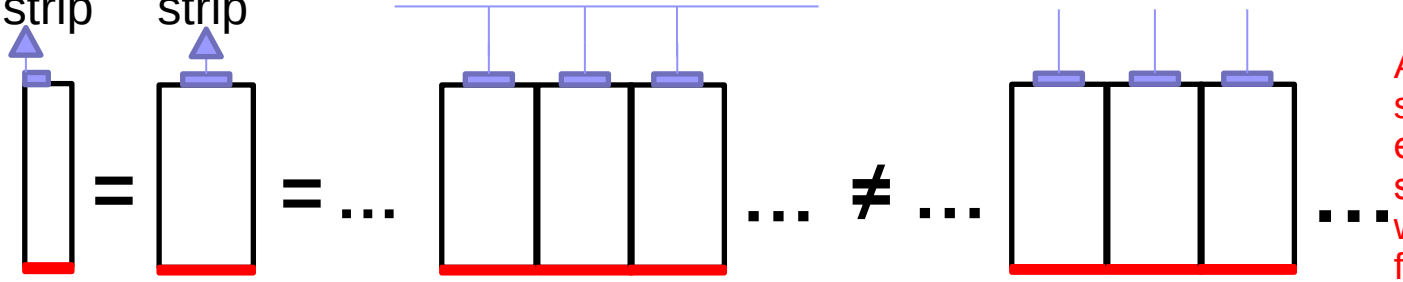
Choice of boundary conditions

Half strip

Full strip

DETECTOR WITH ALL ELECTRODES SHORTENED

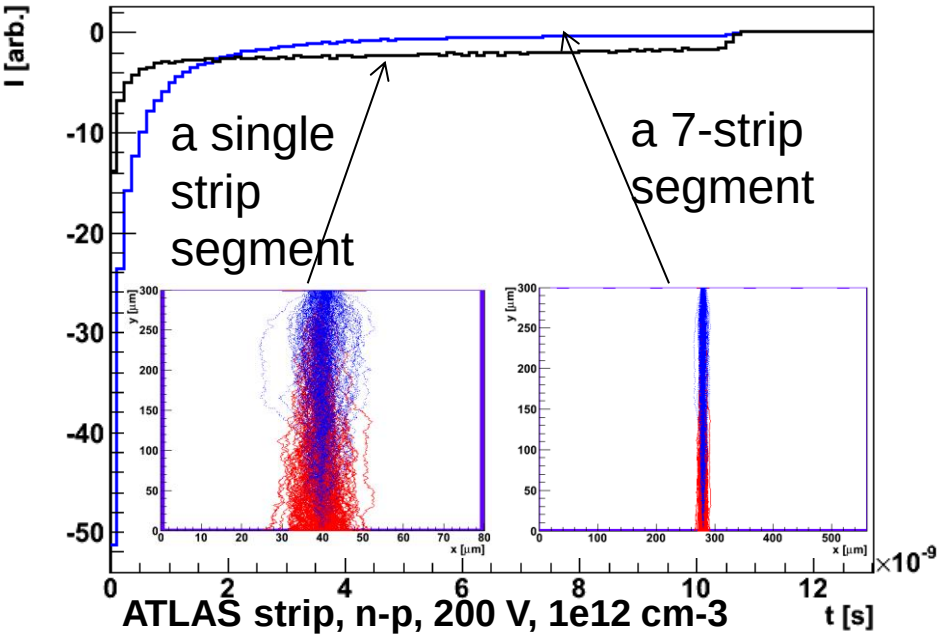
REAL SEGEMENTED DETECTOR



A lot of effects in irradiated silicon detectors – such as e.g. “trapping induced charge sharing” can not be simulated without proper weighting field.

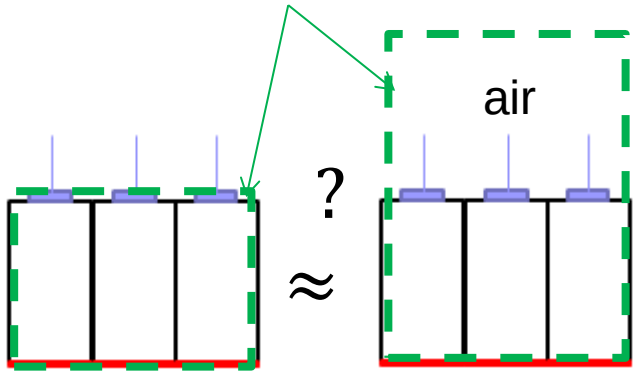
All electrodes with U_w=1 –> all strips shortened

All neighboring electrodes at U_w=0 –> individual channels



Also pay attention to simulated volume

Simulated volume



Effects of the surface

Main effects why these are studied

- Breakdown performance
- Strip isolation (interstrip resistivity, capacitance)
- Charge collection for particles of short penetration depth (XFEL)
- Time dependence of charge collection due to outer surface charge redistribution/also break down perfomance

Models:

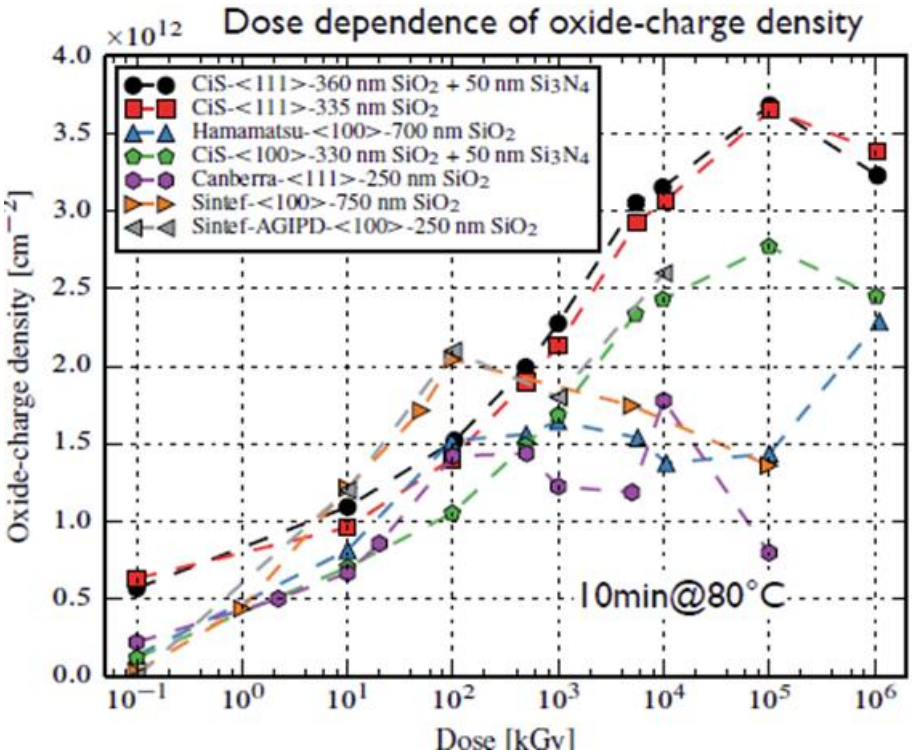
- Oxide charges (MOS-C)

N_{OX} = 1.8x10^{12} cm^{-2} for fluences > 2x10^{14} n_{eq}/cm^2

- Interface traps (TDRC and CGD)
  - 2 acceptors

  (Ec-0.6 eV, Ec-0.39 eV σ_e=σ_h=1e-15 cm^2)
  - 2 acceptors+donor (Perugia)

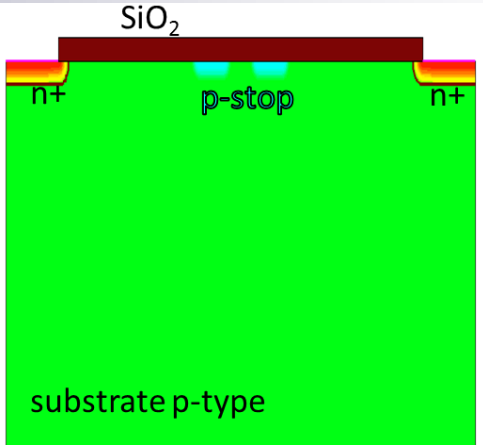
Type	Energy (eV)	Concentration (cm^{-2}) N_{it}=0.8·N_{ox}
Acceptor	E_C - 0.40	40% of acceptors N_{it}
Acceptor	E_C - 0.60	60% of acceptor N_{it}
Donor	E_V + 0.60	100% of donor N_{it}

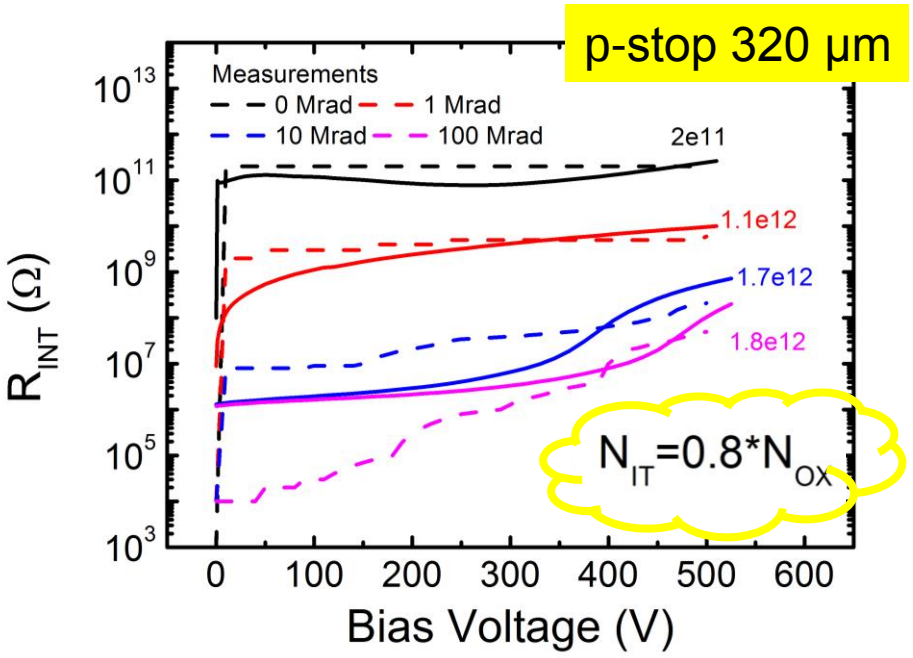


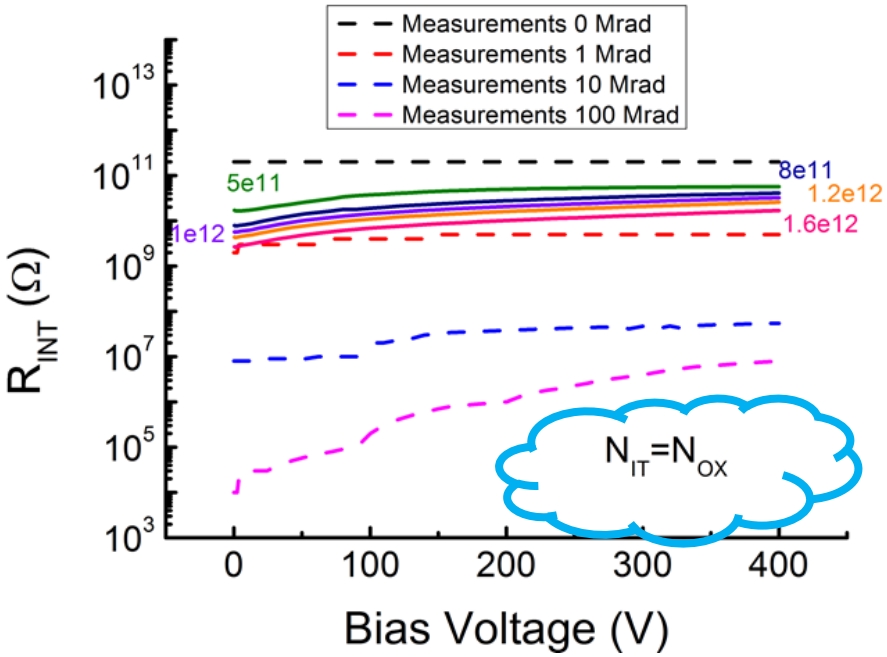
J. Zhang, DESY Thesis-2013, "X-ray radiation damage studies and design of a Si Pixel sensor for different fluences for science at the XFEL"

Effects of the surface

HPK process
- double p-stop structure
- Nsub = 3×10^{12} cm^{-3}
- Npeak = 5×10^{15} cm^{-3}







*Measurements after X-ray carried out by Anna Peisert and Hadi Behnamian at CERN and presented by R. Dalal at 25th RD50 Workshop

Effects of the surface

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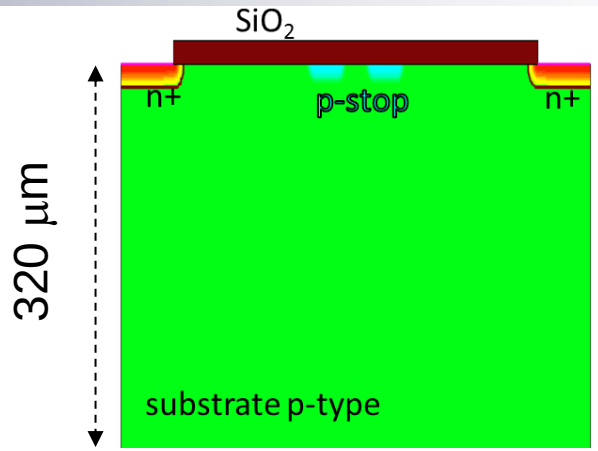
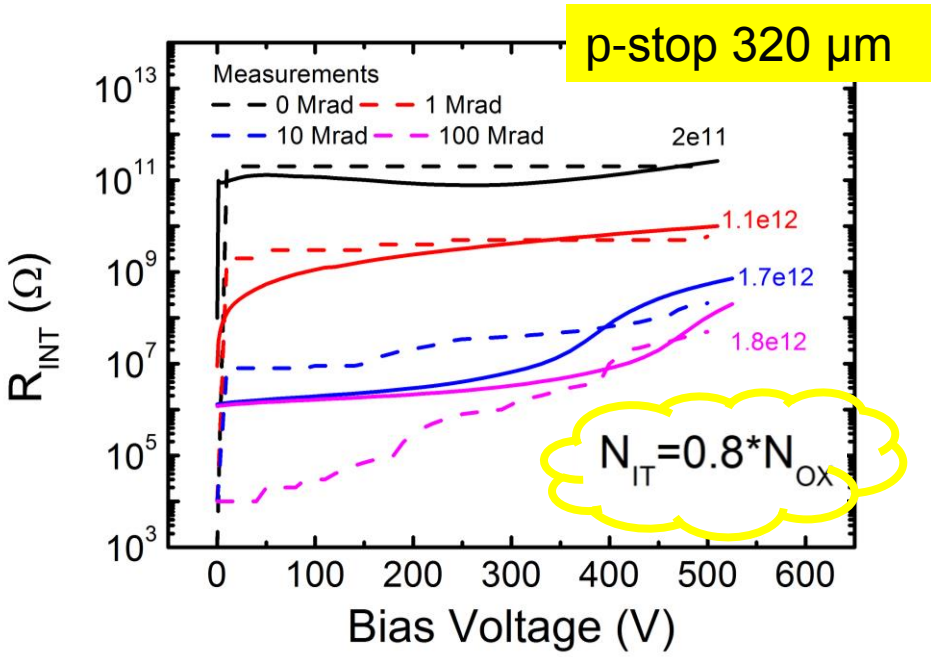
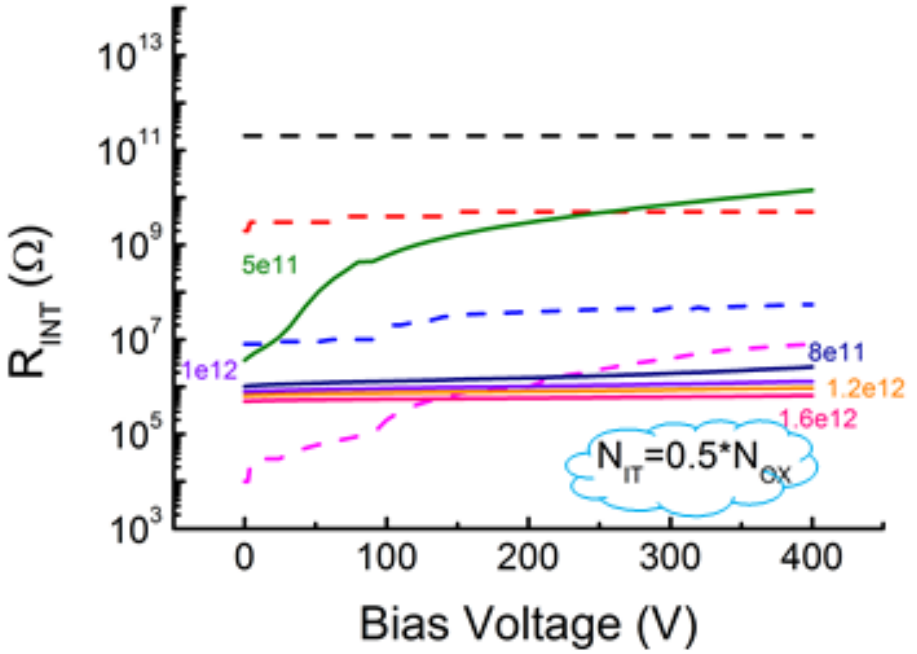






*Measurements after X-ray carried out by Anna Peisert and Hadi Behnamian at CERN and presented by R. Dalal at 25th RD50 Workshop

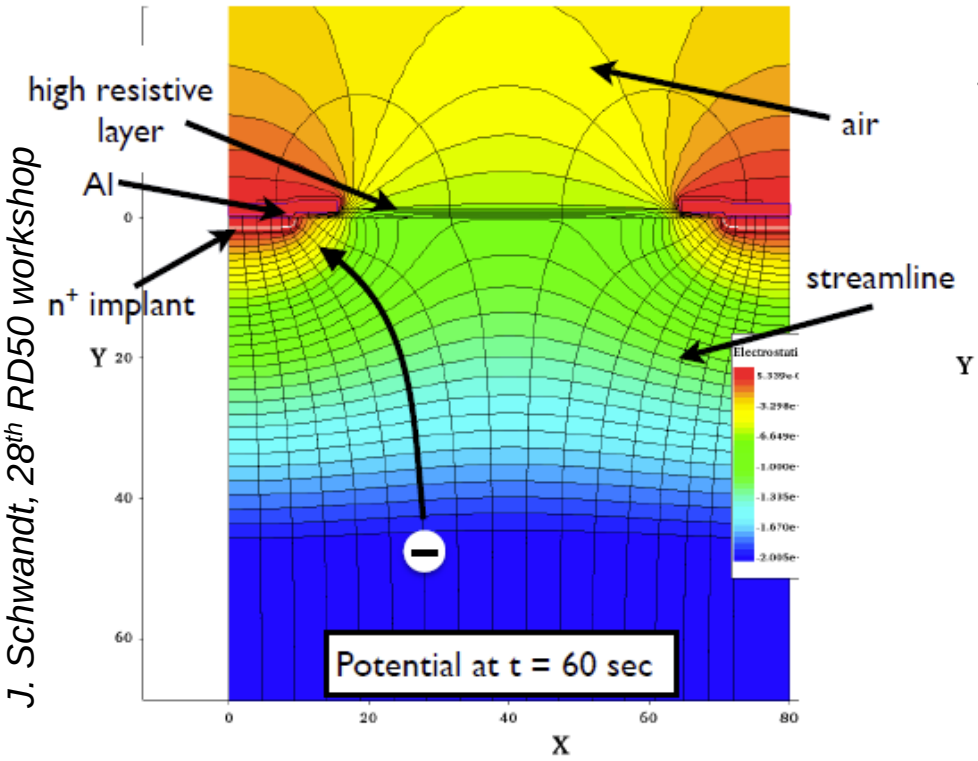
Outer surface charges (humidity)

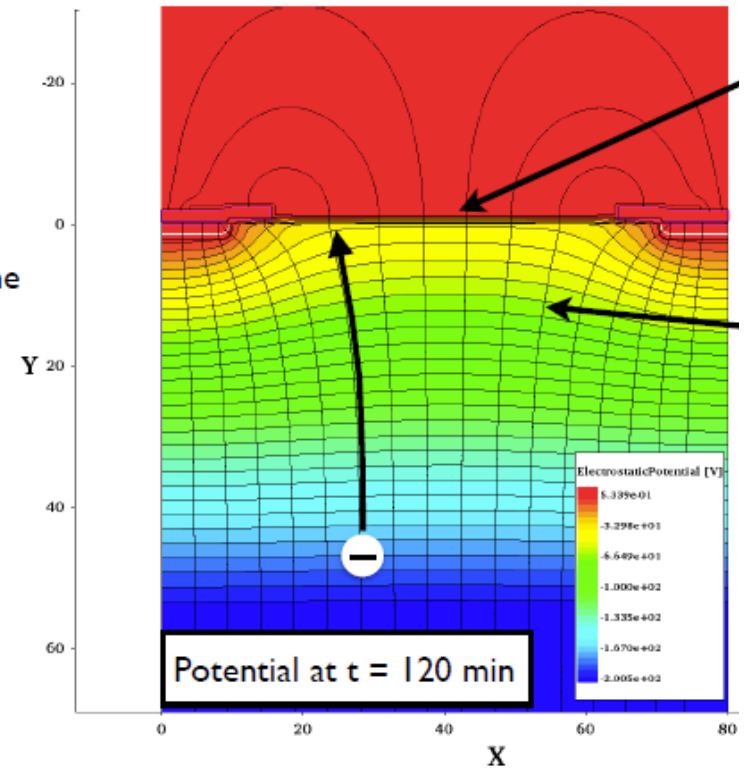
Explanation of long-term changes (w.o. radiation damage)*):

- Biasing → longitudinal E-field component on o.s. → rearrangement of Q_{os}
- until $E_{long} = 0$ and $V_{os} = const$ → time constant depends R_{sq},
- which changes by many orders of magnitude with humidity (and T)

Humidity changes R_{sq} by factor of 50 from (46%-30%) in CGD measurements !

n^+-p sensor with p-spray ($N_{p\text{-}spray} = 5 \cdot 10^{11}$ cm^{-2}), $N_{ox} = 1 \cdot 10^{10}$ cm^{-2}
High resistive layer of 10 nm on top of passivation with $R_{sq} \approx 7 \cdot 10^{14}\ \Omega$
Voltage ramp: -10V/s up to -600V and than constant -600V





J. Schwandt, 28th RD50 workshop

discussed already in A.Longoni et al., NIM-A288(1990)35

Signal Simulation Tools

- **What is their main feature?**
  - they solve Poisson Equation for an input N_{eff} rather that calculating N_{eff} from microscopic defects as in TCAD.
  - charge drift is considered in a static electric field and is done in steps – never a 4D problem (as in relaxation of non-equilibrium carriers) – much, much faster and allows minimization
  - the induced current is calculated by Ramo's theorem directly

- These tools are in many ways complementary to TCAD.

  - are more suitable for multi-electrode systems by taking weighing field into account.
  - allow simpler carrier generation which can be any distribution – i.e. coupling to other software packages e.g. GEANT4.
  - are well suited for Monte Carlo Studies of detector performance (charge sharing, magnetic field, position resolution …)
  - are available on the level of source code – very high flexibility
  - are fast and therefore allow for modeling and fitting of the field parameters to the measurements
  - allow in principle TCAD fields to be imported for Monte-Carlo studies

Signal Simulation Tools – review of them

Overview of non-commercial tools (not all) that have been developed within RD50:

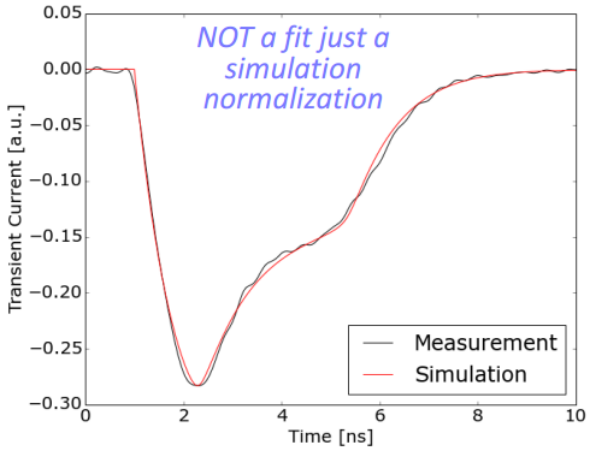
- Weightfield 2 (Torino, UCSC-SCIPP, …)
  https://indico.cern.ch/event/273880/session/4/contribution/59/attachments/493722/682260/cenna_ufsd_simulator.pdf
- TRACS (CERN, Santander…)
  https://indico.cern.ch/event/334251/session/1/contribution/25
- KDetSim (JSI)
  https://indico.desy.de/getFile.py/access?contribId=26&sessionId=3&resId=0&materialId=slides&confId=12934

	WF2	TRACS	KDetSim
Dimensions	2D	2D	3D
E field from	$\Delta U = -\frac{\rho}{\varepsilon\varepsilon_0}$	$\Delta U = -\frac{\rho}{\varepsilon\varepsilon_0}$	$\nabla(\varepsilon\nabla U) = -\frac{\rho}{\varepsilon_0}$
Meshing	Custom (variable, orthogonal semi adaptive)	Open FEM library FENICS (adaptive, advanced), parallel processing	Custom (variable ,not adaptive)
Physics	drift, diffusion, B, trapping,	drift, trapping (not MC wise)	drift, diffusion, B, trapping, impact ionization*
Electronics	More advanced	Basic (RC…)	Basic (preamp,CR,RC)
OS/Framework	Mac, Linux (partially ROOT based-compile from scratch)	Mac, Linux	Linux,Mac,Windows, ROOT based
User interface/IO	GUI (batch file)	GUI / CLI	CLI (ROOT GUI)

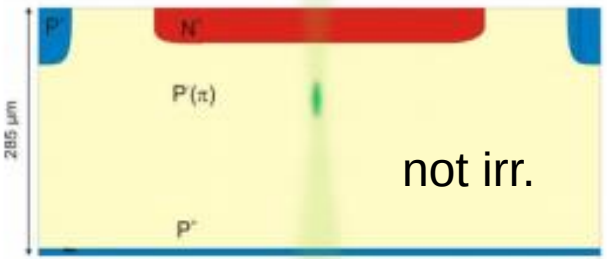
These packages are mostly used to explain TCT measurements and to extract effective models!

Signal Simulation Tools – some examples

TRACS – TPA simulations



see S. Wonsak talk

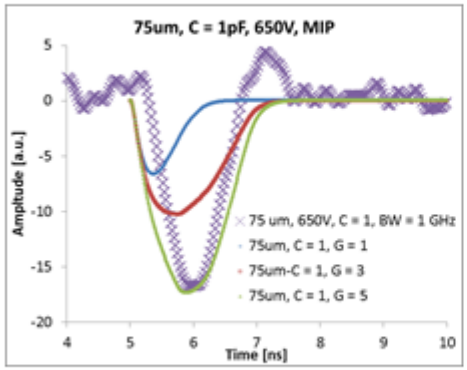


Two photon absorption TCT simulation – a novel state of the art technique!

(I. Vila et al, 26th RD50 Workshop)

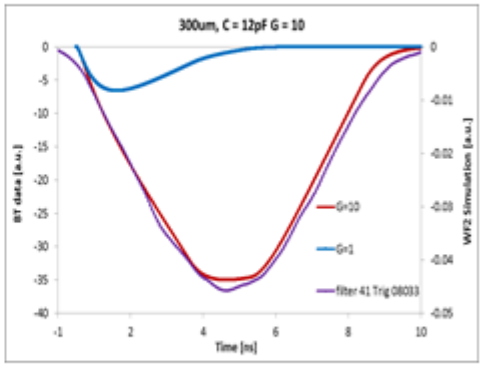
WF2 simulation - timing performance of LGAD detector (good agreement with test beam)

75 µm LGAD, β's

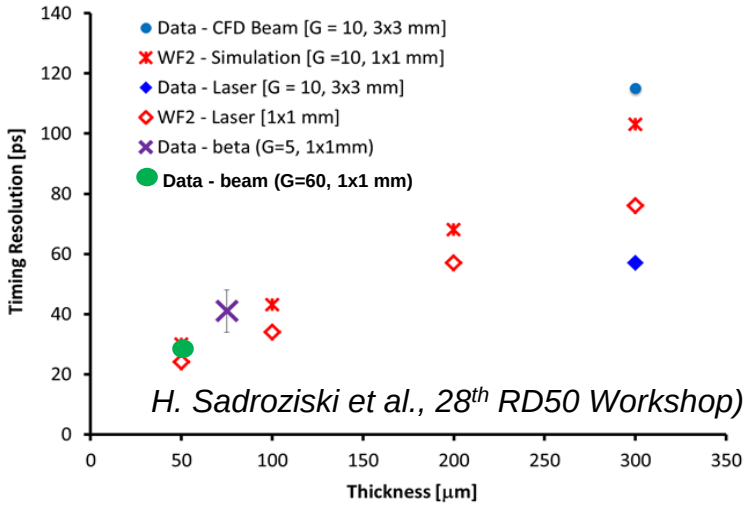


$G \sim 5$, $\tau_{Rise} = 500ps$

300 µm LGAD, 120 GeV π's



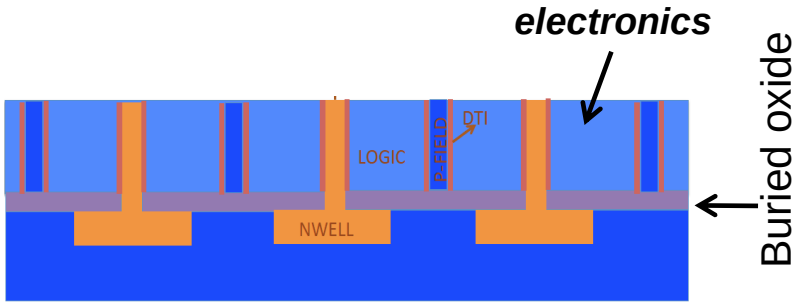
$G \sim 10$, $\tau_{Rise} = 5ns$



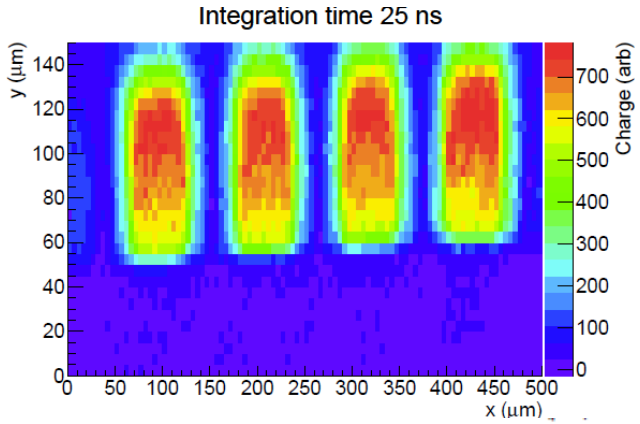
H. Sadroziski et al., 28th RD50 Workshop)

KDetSim - importance of biasing scheme in HVCMOS detectors

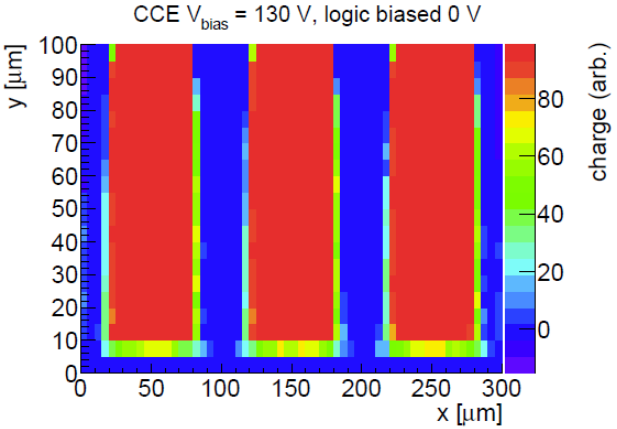
Mandić et al,
28th RD50 Workshop



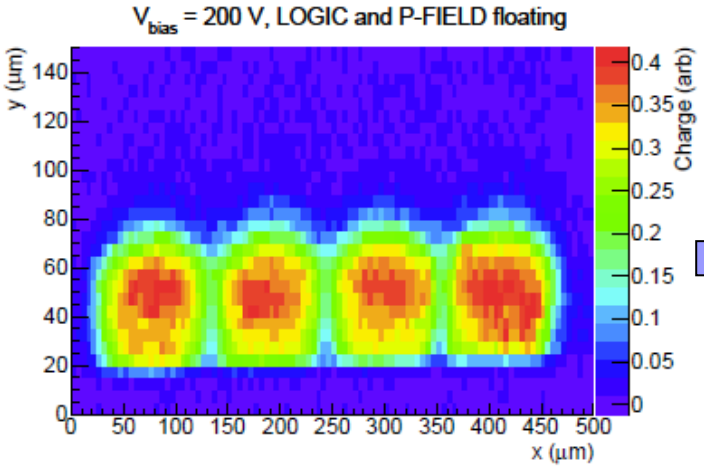
made on SOI by XFAB



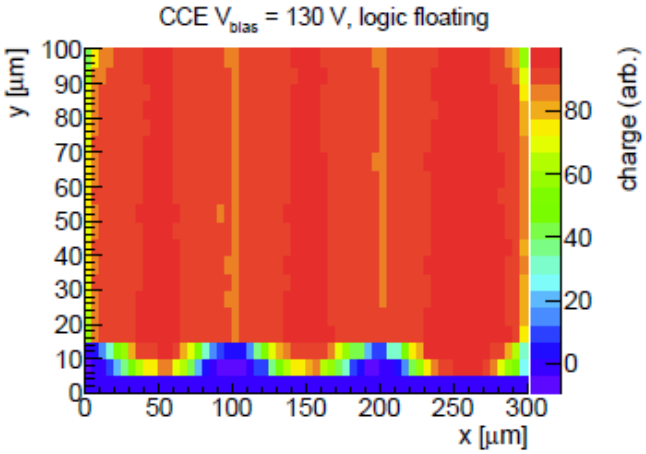
Logic at 0V



qualitive agreement



Logic floating

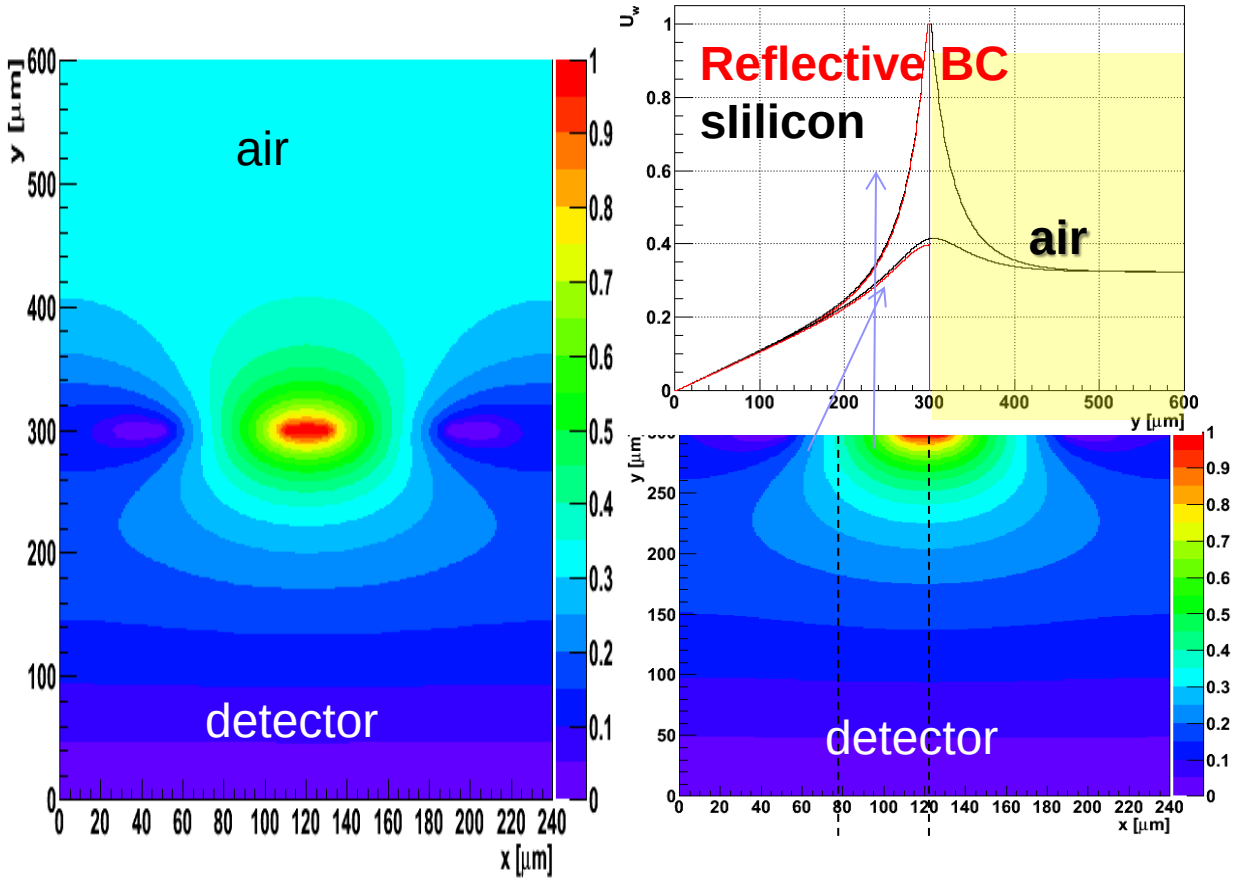


Conclusions

- TCAD simulations are the main tool for designing and simulating detector performance -> very successful.
- Simulation of radiation damage is still a problem – a model that satisfactory describes the whole set of measured detector properties is sought. Due to computational issues all models now are based on 2 or 3 mostly effective levels.
- For the surface damage effects , determination of N_{it} is the main challenge.
- One of the important questions is initial dopant removal models – removal rates, removal fractions – for different irradiation particles. Is it required?
- Signal simulation tools can be very effective for many applications and allow Monte Carlo studies as well as direct modeling of the electric field.

BACKUP

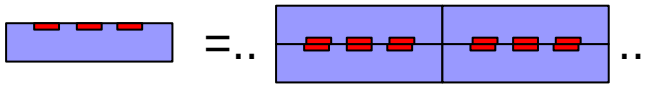
Choice of boundary conditions - U_w



Reflective BC (von Neumann) at non-electrode surfaces

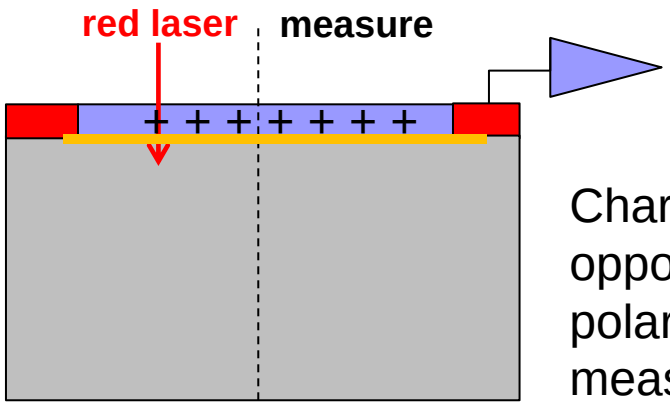
$$\nabla U_w = 0$$

No field lines escape the sensors – hence the structure is fully symmetrical in all directions

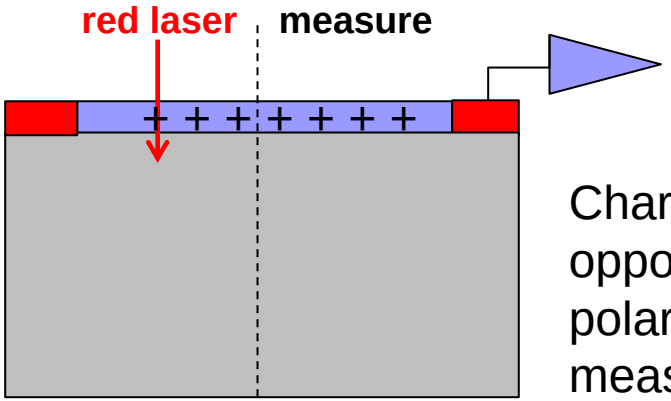


- For ATLAS geometry detectors the effect of reflective boundary conditions on the surface to weighting field is small – few % at most in the interstrip region. Should be looked individually for each structure.
- Same applys for electric field calculation.

Examples of surface damage simulations

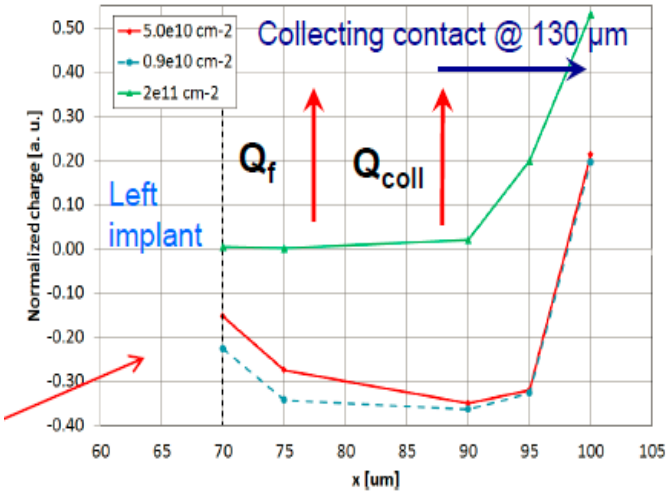


Charge of opposite polarity measured

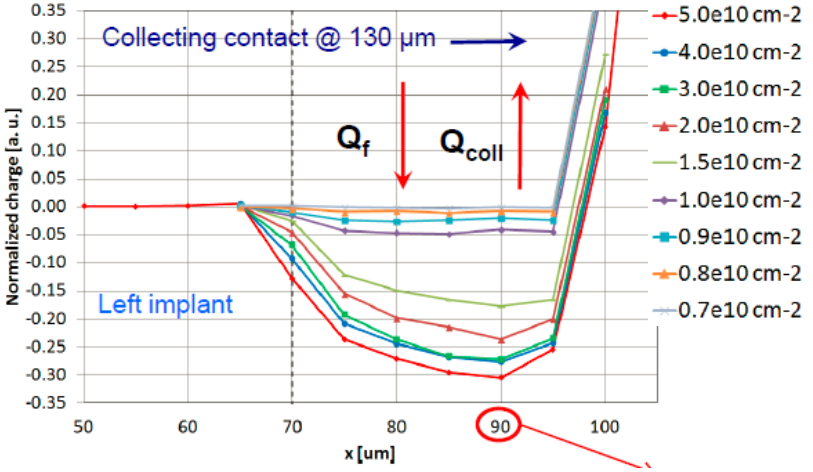


Charge of opposite polarity measured

n-p detector



p-n detector



Strip border

T. Pentola et. al. , 26th RD50 workshop