TCAD simulations for rad-hard sensors

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on behalf of INFN and University of Perugia (Italy), CNR-IOM, and INFN and University of Torino (Italy) groups

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Outline

- Motivations and Challenges
- Radiation damage effects in silicon sensors
- TCAD modeling of rad-hard sensors
- TCAD radiation damage modeling approaches
  - LGAD
  - Compensated LGAD
  - DC-RSD
- Conclusions

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Motivations and Challenges

- Semiconductor detectors will face increasing radiation levels
  - $>1x10^{16}$ 1MeV n_{eq}/cm^2 (HL-LHC);
  - $>5x10^{17}$ 1MeV n_{eq}/cm^2 (FCC-hh);
    - detectors used at LHC cannot be operated after such irradiation.
- New requirements lead to new detector technologies
  - Need to be optimized for radiation hardness and/or 4D tracking capabilities.
- Modern TCAD simulation tools can have a crucial role in radiation-hard device design
  - Reducing costly and time-consuming physical testing.
  - Deep understanding of physical device behavior.
  - Combined Bulk and surface radiation damage can be considered.
    - deep-level radiation-induced traps whose parameters are physically meaningful and whose experimental characterization is feasible.
  - Within a hierarchical approach, increasingly complex models can be considered, by balancing complexity and comprehensiveness.

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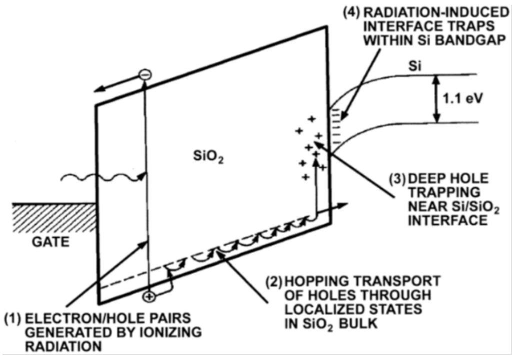
Radiation damage effects

Two main types of radiation damage in detector materials:

√ SURFACE damage ← Ionizing Energy Loss (IEL)

- build-up of trapped charge within the oxide;
- bulk oxide traps increase;
- interface traps increase;
- Q_{OX}, N_{IT}.

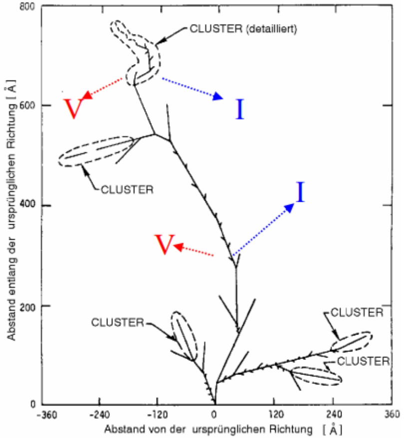


T. R. Oldham, F. B. McLean, *Total Ionizing Dose Effects in MOS Oxides and Devices*, IEEE Trans. on Nuclear Science, vol. 50, no. 3, June 2003

√ BULK damage ← Non-Ionizing Energy Loss (NIEL)

- silicon lattice defect generations;
- point and cluster defects;
- deep-level trap states increase;
- change of effective doping concentration;
- N_T.

van Lint 1980



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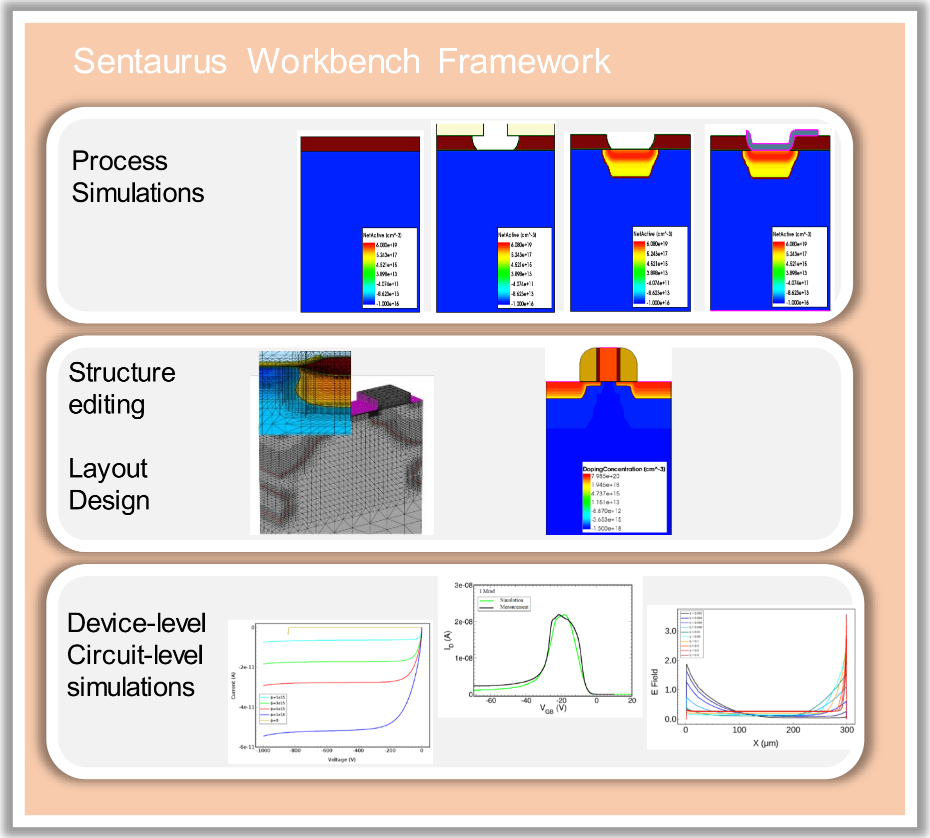
The Technology-CAD modeling approach



√ TCAD simulation tools solve fundamental, physical partial differential equations, such as diffusion and transport equations for discretized geometries (finite element meshing).

√ This deep physical approach gives TCAD simulation predictive accuracy.

✓ Synopsys© Sentaurus TCAD & Silvaco

$$\begin{cases} \nabla \cdot (-\varepsilon_s \nabla \varphi) = q\left(N_D^+ - N_A^- + p - n\right) & \text{Poisson} \\ \dfrac{\partial n}{\partial t} - \dfrac{1}{q}\nabla \cdot \vec{J}_n = G - R & \text{Electron continuity} \\ \dfrac{\partial p}{\partial t} + \dfrac{1}{q}\nabla \cdot \vec{J}_p = G - R & \text{Hole continuity} \end{cases}$$

$$\vec{J}_n = -q\mu_n n \nabla \varphi + qD_n \nabla n$$

$$\vec{J}_p = -q\mu_p p \nabla \varphi - qD_p \nabla p$$

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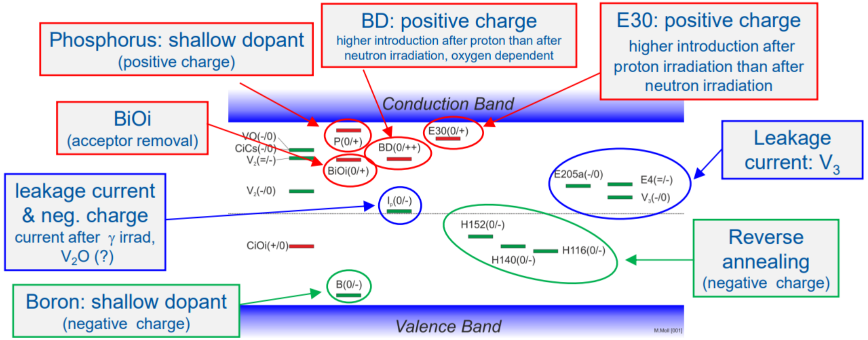
TCAD models - an overview

Different approaches to TCAD radiation damage modeling:

- ✓ EVL Model (2 levels)
- ✓ Delhi-2014 (2 levels)
- ✓ KIT (Eber) (2 levels)
- ✓ New Univ. Of Perugia Bulk+Surface (3 levels)
- ✓ Folkestad (CERN model)/LHCb (3 levels)
- ✓ Hamburg Penta Trap Model (HPTM) (5 levels)



RD50 map of most relevant defects for device performance near RT

Different modeling approaches (traps, energy levels and related parameters), often tailored to specific datasets and devices.

GOAL: General purpose TCAD model

- Not over specific
  → set of "effective" defects within the semiconductor bandgap.
- Accounts for different irradiation levels and particle types.

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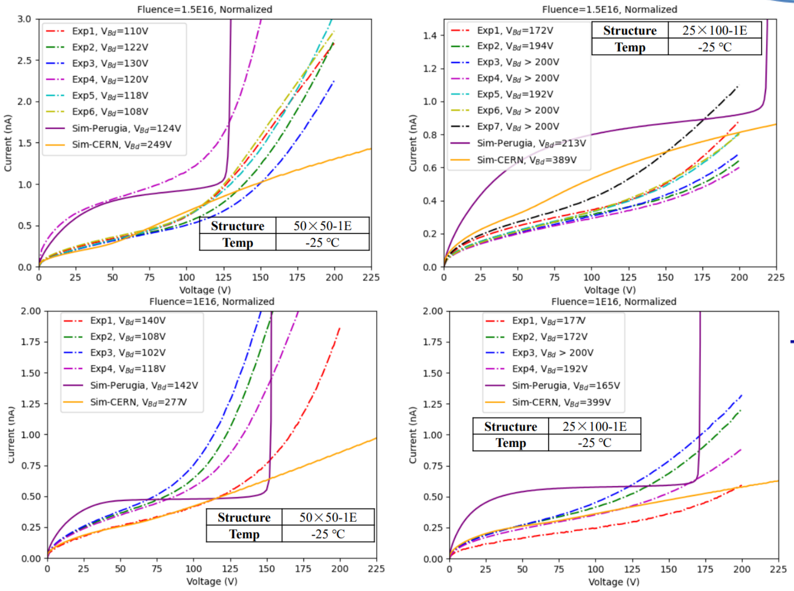
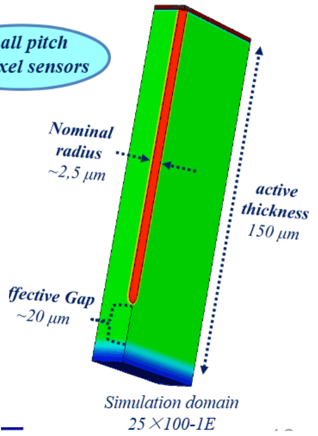
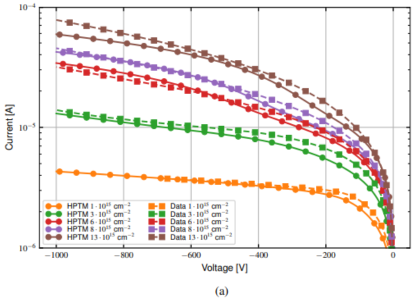
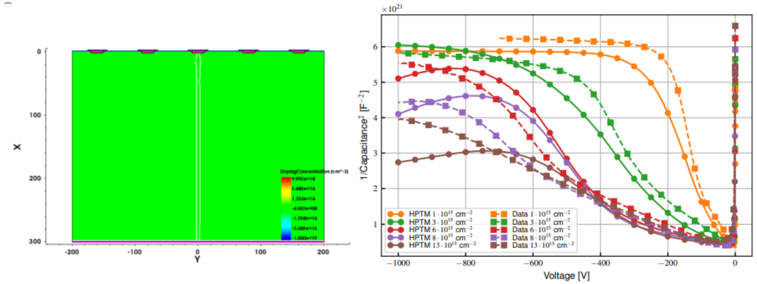
TCAD models - some applications









Simulation based on the **CERN Bulk Damage Model.**
Univ. of Trento Group.

Hamburg Penta Trap Model (**HPTM**).
Univ. of Hamburg group.

Ye, J.; Sensors 2023, 23, 4732, doi: 10.3390/s23104732

J. Schwandt et al., 2018 IEEE NSS/MIC, doi: 10.1109/NSSMIC.2018.8824412.

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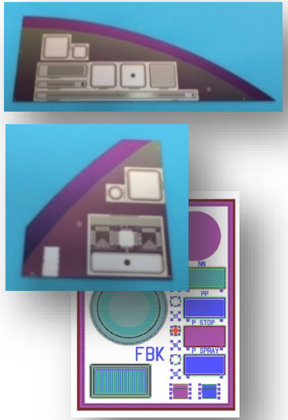
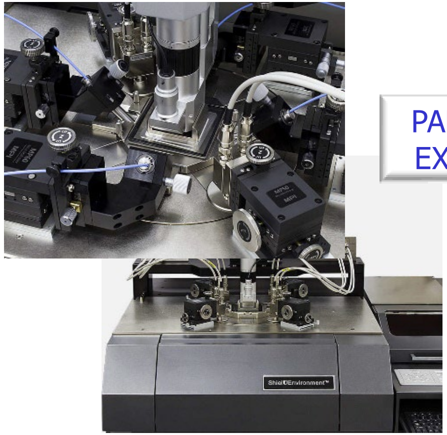
New University of Perugia model

The overall modelling approach pursued

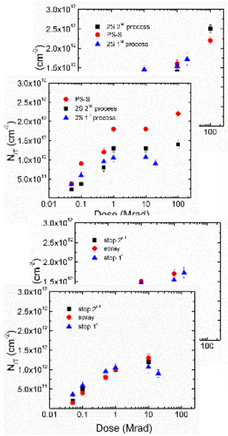


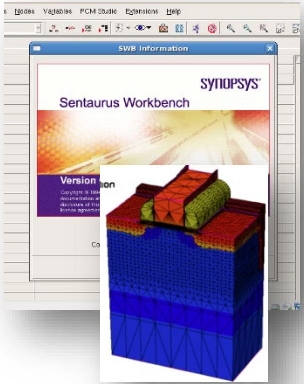
TEST STRUCTURE MEASUREMENTS



PARAMETERS EXTRACTION

MODEL





MODEL VALIDATION

DETECTOR OPTIMIZATION

CCE, I-V, C-V, …

- √ Modeling the effects of the radiation damage.
- √ Predictive insight into the behavior of detectors, aiming at their performance optimization.

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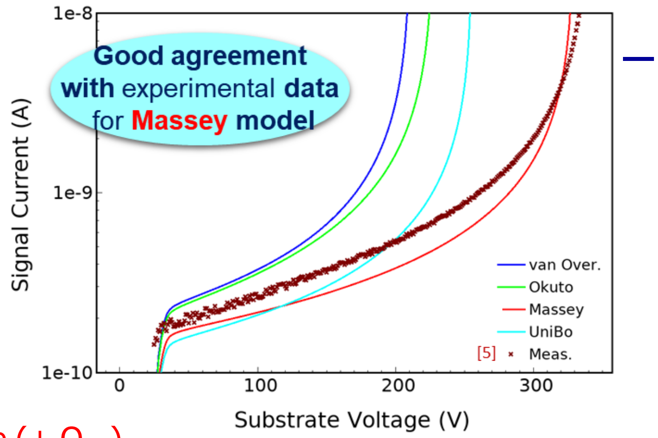
TCAD simulation of LGAD devices

✓ **Physical models**
- **Generation/Recombination rate**
  - Shockley-Read-Hall, Band-To-Band Tunneling, Auger
  - **Avalanche Generation => impact ionization models,** *van Overstraeten-de Man, Okuto-Crowell, Massey*[1], *UniBo*
- **Fermi-Dirac statistics**
- **Carriers mobility variation** doping and field-dependent
- **Physical parameters**
  - e-/h+ recombination lifetime



✓ **Radiation damage models: "PerugiaModDoping"**
- **"New University of Perugia model"**
  - **Combined surface and bulk** TCAD damage modeling scheme[2]
  - Traps generation mechanism
- **Acceptor removal mechanism** => $N_{GL}(\phi) = N_A(0)e^{-c\phi}$
  - where
    - **Gain Layer (GL)**, **c** removal rate (**Torino parameterization**[3])
- **Acceptor creation**

$$N_{A,bulk} = \begin{cases} N_{A,bulk}(0) + g_c\phi, & 0 < \phi < 3E15\, n_{eq}/cm^2 \\ 4.17E13 \cdot \ln(\phi) - 1.41E15, & \phi > 3E15\, n_{eq}/cm^2 \end{cases}$$

where g_c = 0.0237 cm^{-1} (**Torino acceptor creation**)

Surface damage (+ Q_{OX})

Type	Energy (eV)	Band width (eV)	Conc. (cm^{-2})
Acceptor	$E_C \le E_T \le E_C$-0.56	0.56	$D_{IT} = D_{IT}(\Phi)$
Donor	$E_V \le E_T \le E_V$+0.6	0.60	$D_{IT} = D_{IT}(\Phi)$

Bulk damage

Type	Energy (eV)	η (cm^{-1})	σ_n (cm^2)	σ_h (cm^2)
Donor	E_C - 0.23	0.006	2.3×10^{-14}	2.3×10^{-15}
Acceptor	E_C - 0.42	1.6	1×10^{-15}	1×10^{-14}
Acceptor	E_C - 0.46	0.9	7×10^{-14}	7×10^{-13}

[1] M. Mandurrino et al., https://doi.org/10.1109/NSSMIC.2017.8532702.
[2] D. Passeri, AIDA2020 report, CERN Document Server.
[3] M. Ferrero et al., https://doi.org/10.1016/j.nima.2018.11.121.
[4] V. Sola et al., https://doi.org/10.1016/j.nima.2018.07.060.

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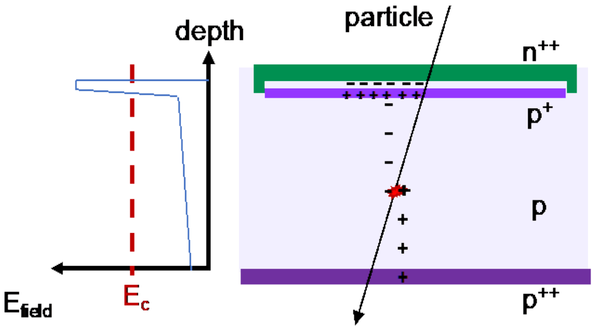
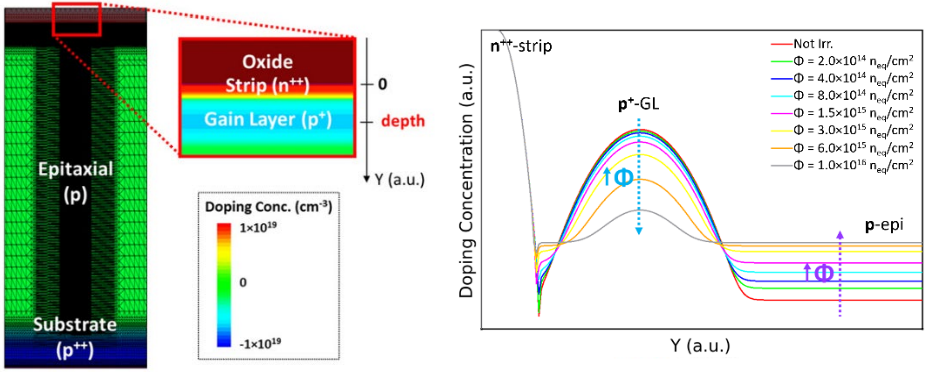
Low Gain Avalanche Diodes

- **Low-Gain Avalanche Diode (LGAD)**
  - **n-in-p silicon** sensors
  - Operated in **low-gain regime** (20 – 30)
  - **Critical electric field ~ 20 – 30 V/µm**
  - Good candidates for **4D tracking**
  - Mitigation of the radiation damage effects by exploiting the **controlled charge multiplication** mechanism.



- **Advanced TCAD** modeling
  - **Radiation damage effects** model implementation
  - Accounts for the acceptor removal mechanism[5] which deactivates the p^{+}-doping of the gain layer with irradiation.
  - Electrical behavior **prediction/ performance optimization** up to the highest fluences.

Layout and **doping profile**



[5] [M. Ferrero et al., doi:10.1016/j.nima.2018.11.121]

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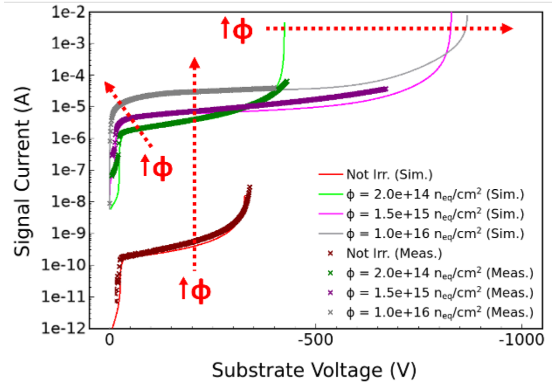
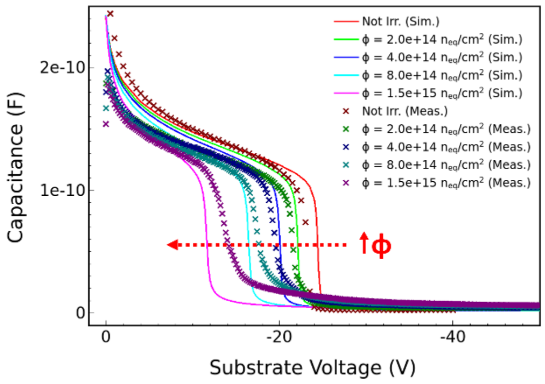
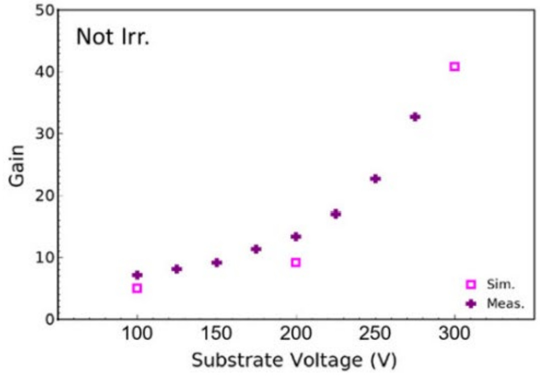
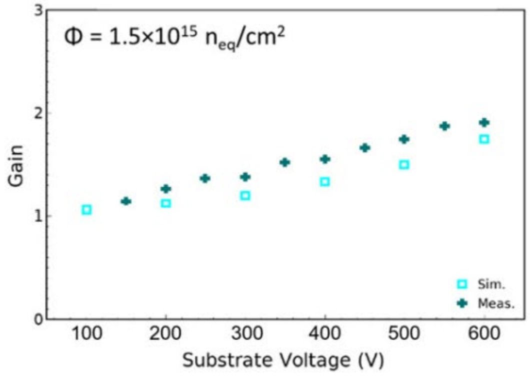
LGAD: Electrical behavior investigation (1)

- **FBK LGADs** (UFSD2, W1)
  - 55 μm thick
- Simulations-Measurements comparison for not irradiated and irradiated devices.
- TCAD settings:
  - "PerugiaModDoping"
  - Massey avalanche model.
  - Temperature sets as per experimental measurements (RT not irrad, 248 K irrad).
  - Electrical contact area $1 mm^2$.
  - Frequency 1 kHz for C-Vs.









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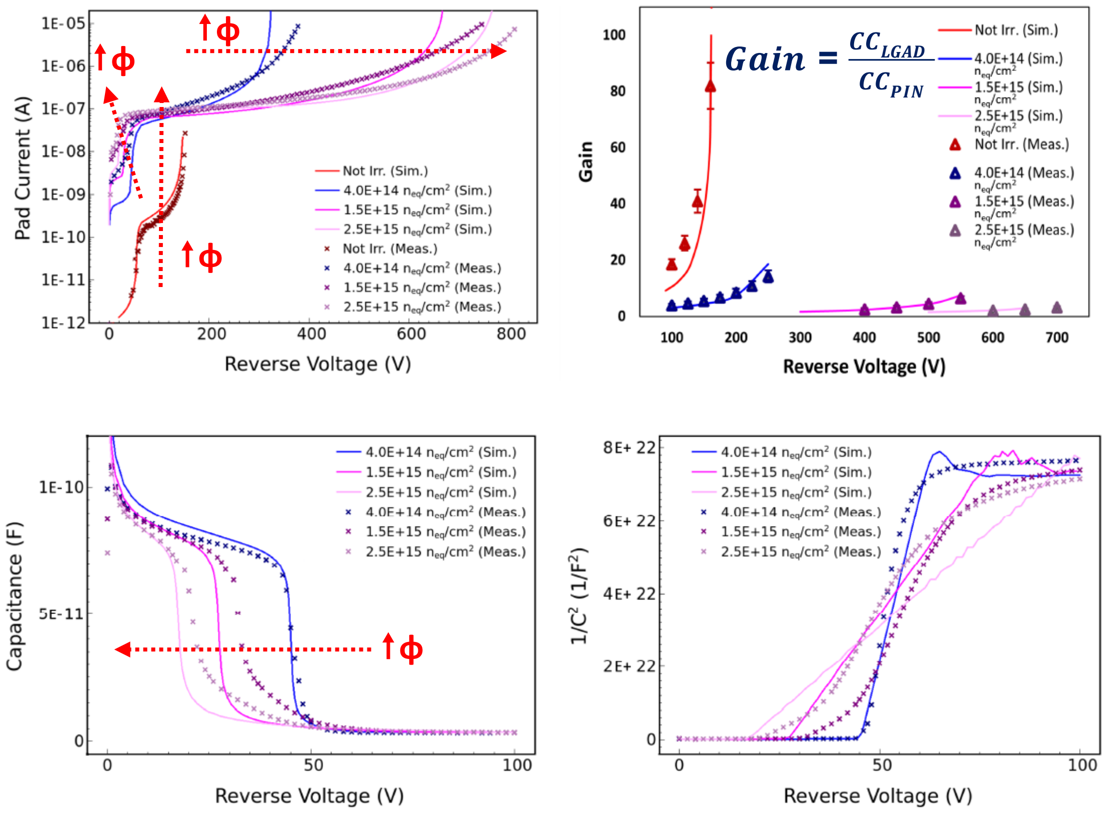
LGAD: Electrical behavior investigation (2)

- **HPK LGADs** (HPK2, split 1-2)
  - 50 μm thick
- Simulations-Measurements comparison for not irradiated and irradiated devices.
- TCAD settings:
  - "PerugiaModDoping"
  - vOv avalanche model.
  - Temperature sets as per experimental measurements (RT not irrad, 248 K irrad).
  - Electrical contact area 1.3×1.3 mm^2.
  - Frequency 2 kHz for C-Vs.



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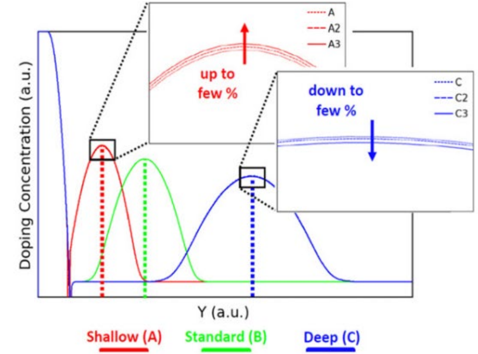
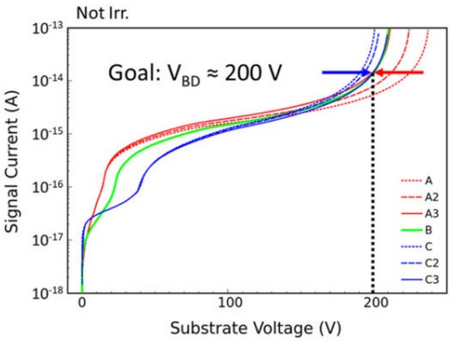
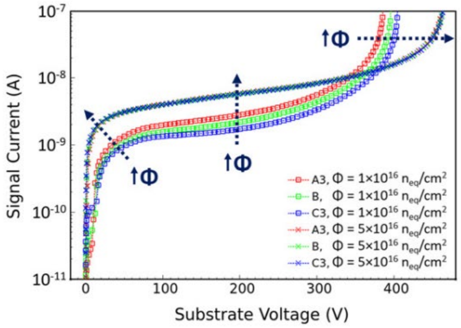
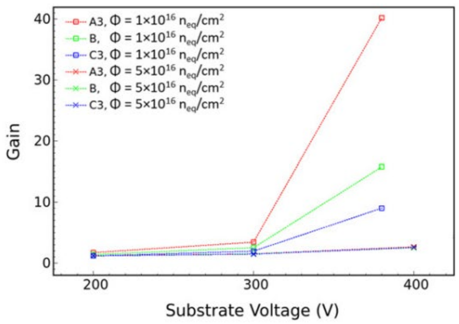
Gain layer sensitivity analysis

- Three different doping profiles considered
  - Shallow, Standard, Deep.
  - **Gain layer** peak:
    a variation of a few percentages affects the breakdown voltage (V_{BD}).
  - Effect on the gain layer depletion voltage.
  - **Predictive** analysis on sensor performance considering the **radiation damage effects**.









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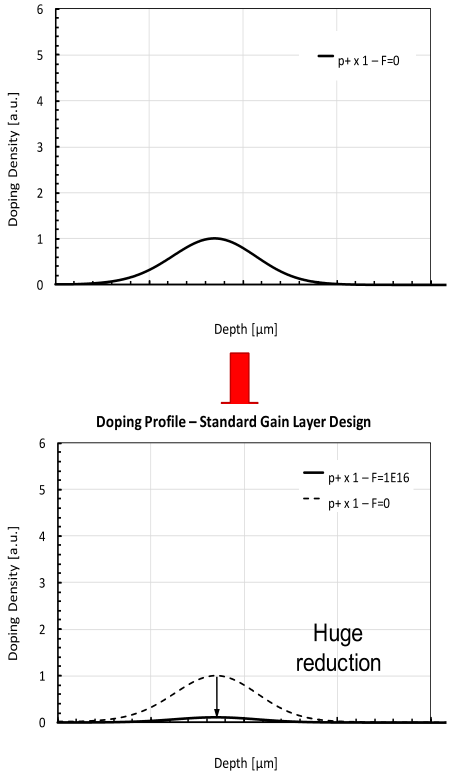
Compensated LGAD: innovation for extreme fluences

- Difficult to operate silicon sensors above 10^{16} n_{eq}/cm^2 due to:
  - defects in the silicon lattice structure → dark current increase
  - trapping of the charge carriers → charge collection efficiency decrease
  - change in the bulk effective doping → impossible to fully deplete the sensors
- In standard LGAD
  - acceptor removal mechanism → $\Phi > 1\text{–}2 \cdot 10^{15}$ n_{eq}/cm^2 lose the multiplication power and behave as standard n-in-p sensors .
- Overcome the present limits above extreme fluences[6]:
  - saturation of the radiation damage effects above $5 \cdot 10^{15}$ n_{eq}/cm^2
  - the use of thin active substrates (20 – 40 mm)
  - extension of the charge carrier multiplication up to $5 \cdot 10^{17}$ n_{eq}/cm^2



Standard LGAD design

[6] V. Sola et al, "A compensated design of the LGAD gain layer", NIMA 1040 (2022) 167232

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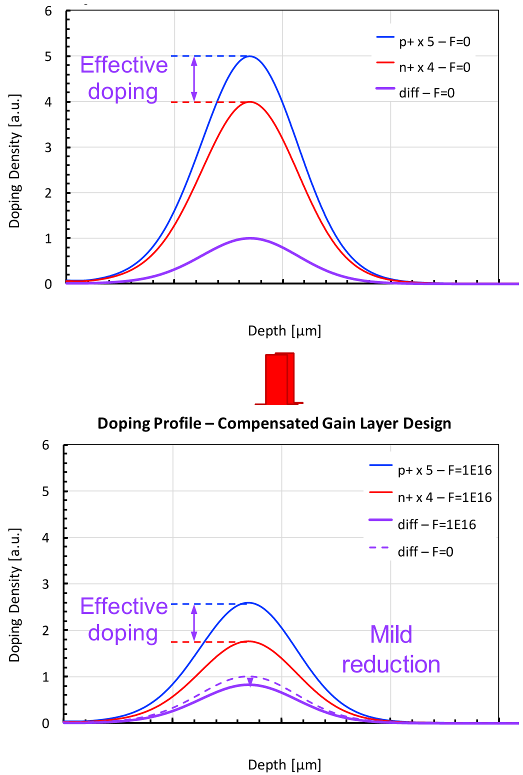
Compensated LGAD: innovation for extreme fluences

- **Goal**: extreme fluences $\Phi = 5\cdot10^{17}\ n_{eq}/cm^2$
- Impossible to reach the design target with the present design of the gain layer.
- Use the interplay between acceptor and donor removal to keep a constant gain layer active doping density.
  Compensated LGAD: Technology under development (FBK EXFLU1 R&D)
- Many unknowns:
  - donor removal coefficient,
  - interplay between donor and acceptor removal (c_D vs c_A)
  - effects of substrate impurities on the removal coefficients

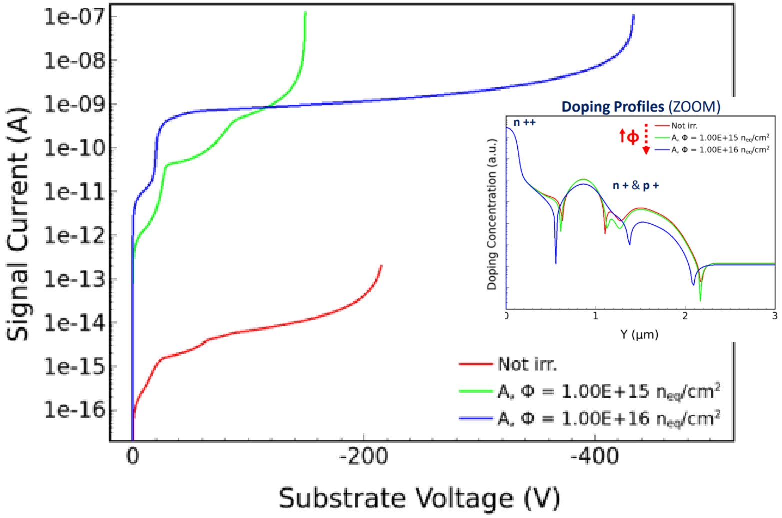


Compensated LGAD

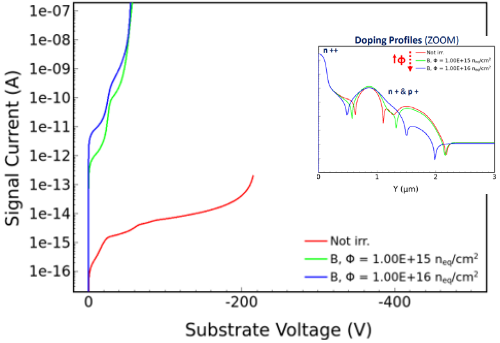
Compensation – doping evolution with fluence

- Three scenarios of net doping evolution are possible, according to the acceptor and donor removal interplay:

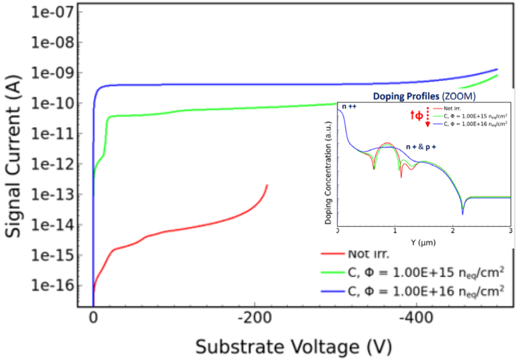
1. $c_A \sim c_D$
   p+-n+ effective doping remains almost constant → unchanged gain with irradiation.



2. $c_A < c_D$
   rapid increase of the net p+-doping → the gain increases with irradiation.
   Co-implantation of oxygen might mitigate the donor deactivation rate.



3. $c_A > c_D$
   effective doping disappearance is slower than in the standard design.
   Co-implantation of carbon atoms can mitigate the p+-doping removal.



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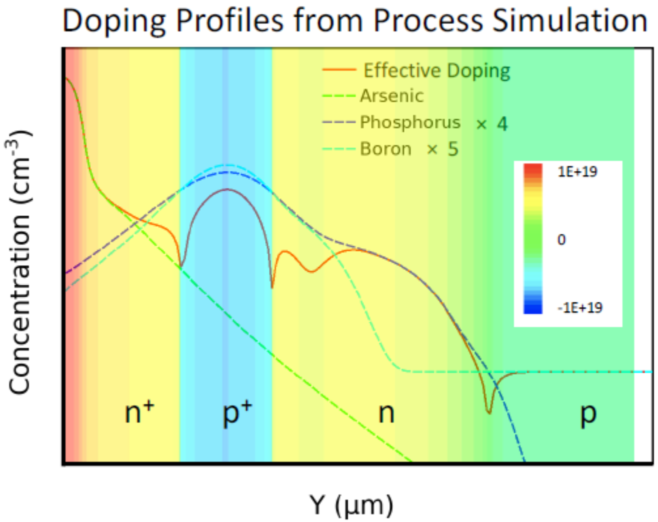
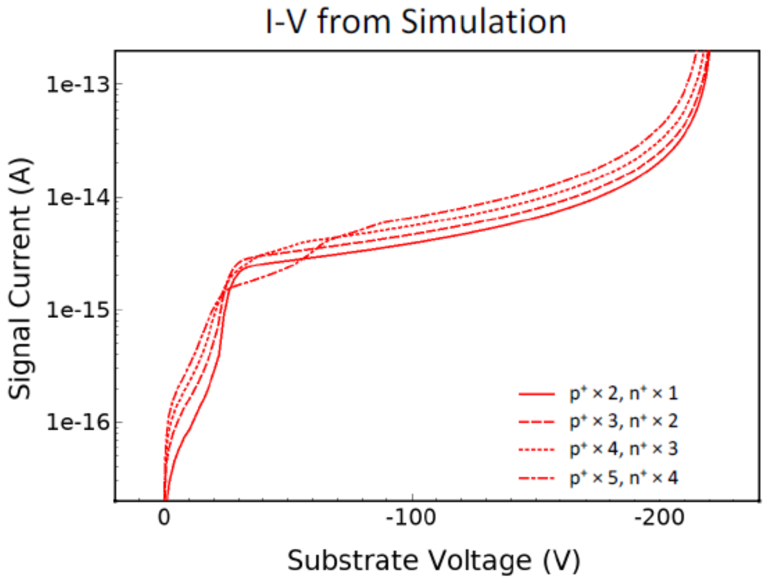
Compensation - simulation

- Process simulations of Boron (p+) and Phosphorus (n+) implantation and activation reveal the different shapes of the two profiles (TCAD Silvaco).





- The simulation of electrostatic behavior illustrates that attaining similar multiplication is achievable with diverse initial compensation values (TCAD Synopsys).

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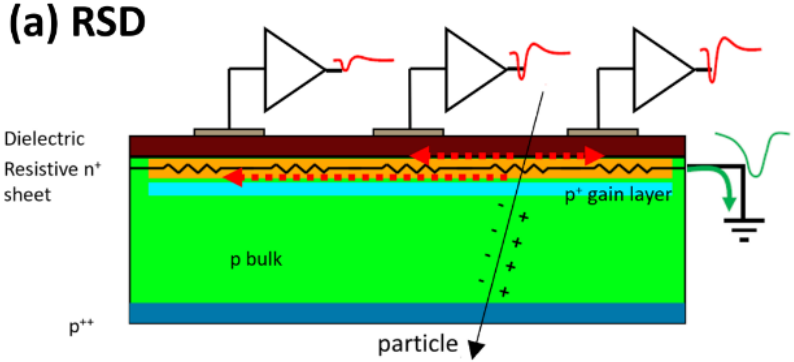
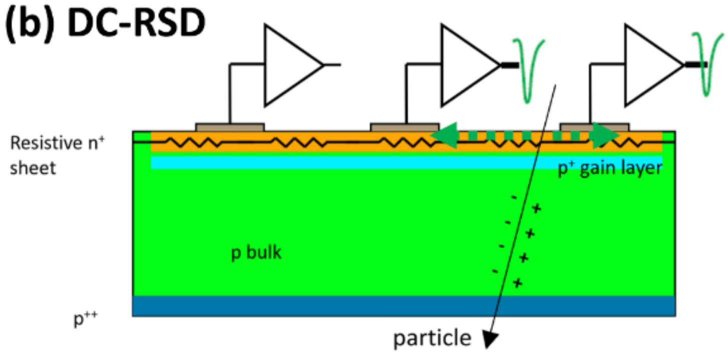
Resistive Silicon Detector: AC-RSD and DC-RSD





- ✓ This design has been manufactured in several productions by FBK, BNL, and HPK.

See Luca Menzio talk & poster

- ✓ This design is presently under development by FBK.
- ✓ The main advantage of the DC-RSD design is to limit the signal spread;
- ✓ A promising solution to simultaneously meet all the specifications required for the next generation of colliders;
- ✓ Evaluation of different layouts and technologies for future DC-RSD production using TCAD tools;

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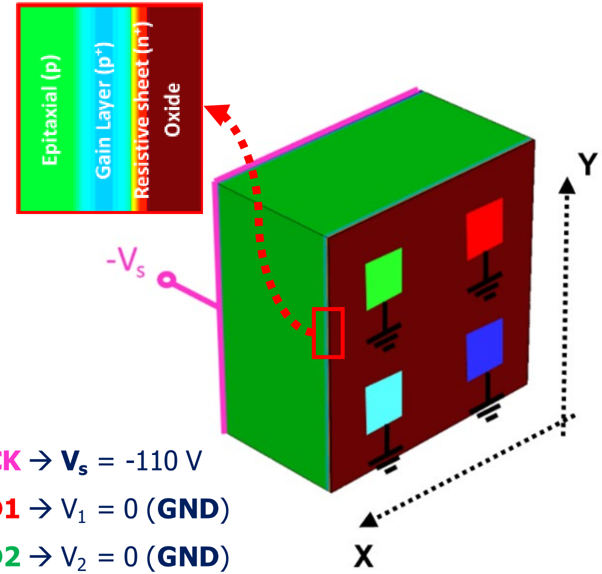
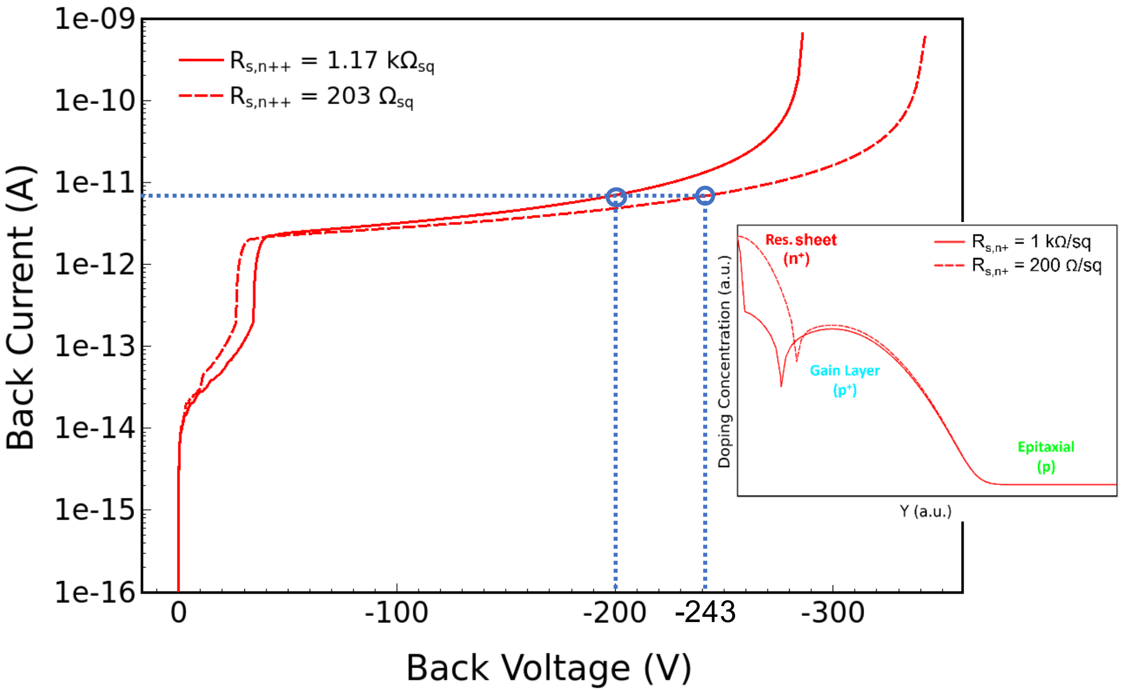
Different n++ layer resistance

- ✓ 3D structure, 2x2 PADs => LGAD



- ❑ **BACK** → $\mathbf{V_s}$ = -110 V
- ❑ **PAD1** → V_1 = 0 (**GND**)
- ❑ **PAD2** → V_2 = 0 (**GND**)
- ❑ **PAD3** → V_3 = 0 (**GND**)
- ❑ **PAD4** → V_4 = 0 (**GND**)

I-V, not irr.



Avalanche model: **Massey**. Temperature **300 K**

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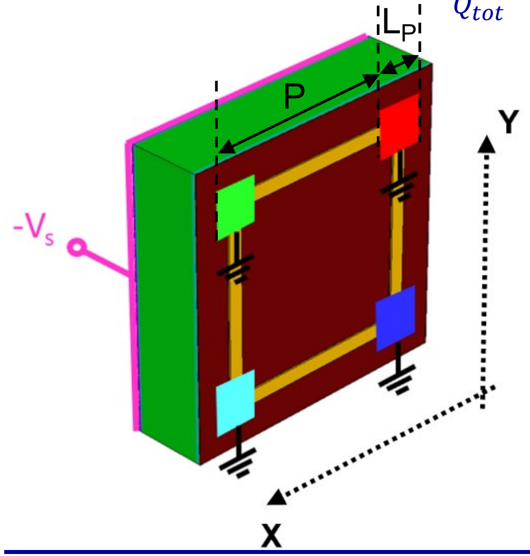
Reconstruction

- ✓ Stimulus MIP
- ✓ The position is reconstructed using the charge imbalance

$$x_i = \frac{Q_{top\ right} + Q_{bottom\ right} - Q_{top\ left} - Q_{bottom\ left}}{Q_{tot}}$$

$$z_i = \frac{Q_{top\ right} + Q_{top\ left} - Q_{bottom\ left} - Q_{bottom\ right}}{Q_{tot}}$$



L_P = 15 μm

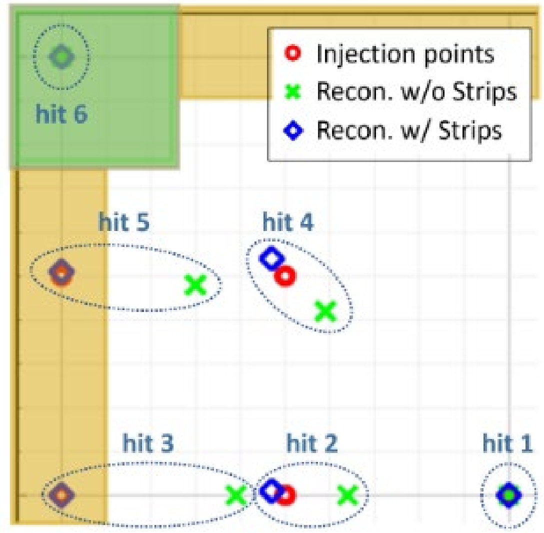
P = 105 μm

@ V_{Back} = -110 V

$R_{s,n++} \approx 721\ \Omega_{sq}$

$R_{s,strip} \approx 15$ mΩ/μm

Results from *TCAD* simulations



Avalanche model: **Massey**. Temperature **300 K**

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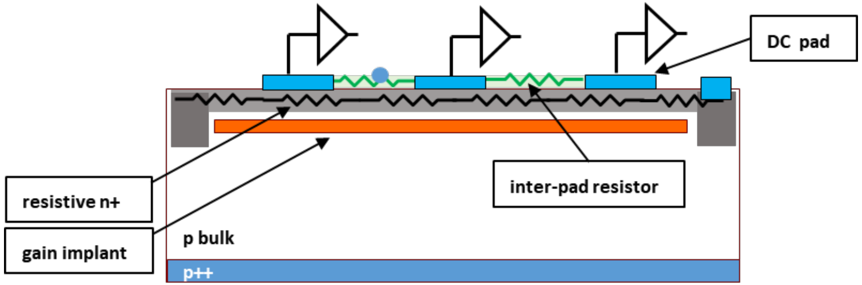
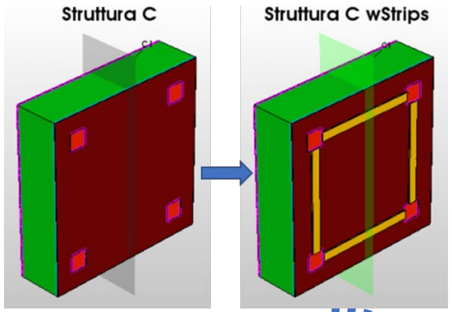
DC-RSD with strips

- The DC-RSD design can consider resistors between the read-out electrodes.

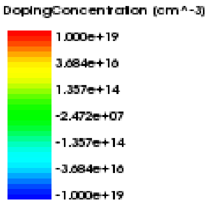
→ these resistors could improve the position resolution of the sensors

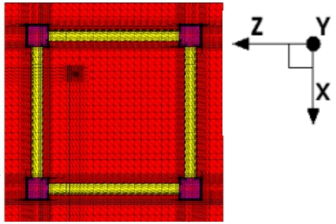


3D structure, **2x2 PADs => LGAD**



~ 280 kpoints

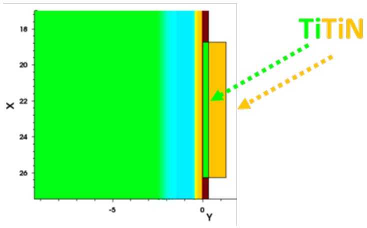




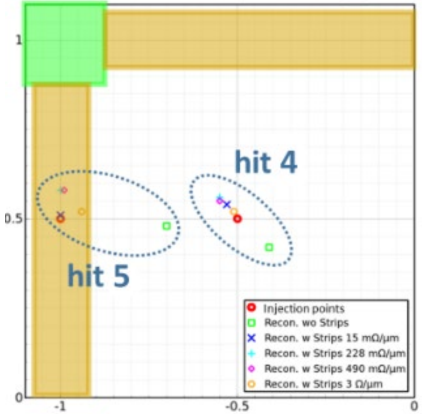
@ $R_{s,n++} \approx 721\ \Omega_{sq}$

~ 350 kpoints

Y-Cut



R_{TiTiN}
- 3,06 Ω/µm
- 228 mΩ/µm
- 490 mΩ/µm
- 15 mΩ/µm



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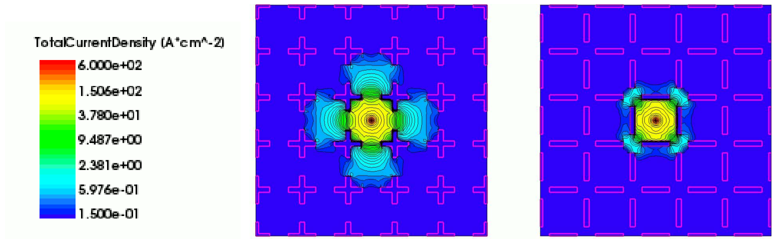
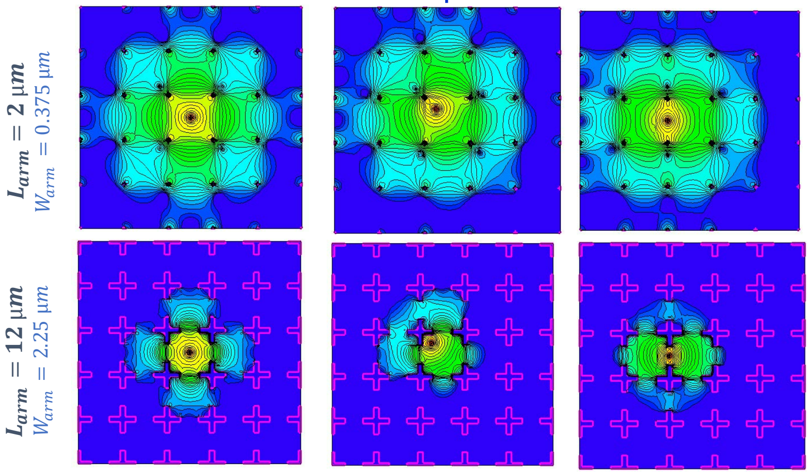
Charge sharing and signal confinement

- Investigation of the signal confinement within the TCAD environment.
- Minimum Ionizing Particle (MIP): various hit points considered.
- Different pad geometries
  - Cross or bar-shaped;
  - Better confinements in larger pads;
  - Error in reconstruction by associating any point covered by metal with the center of the pad;
  - Need small, circular-shaped electrodes and strategy to confine the signal (e.g., trenches);

Cross- vs bar-shaped pads



Three hit points



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Conclusions

- ✓ Strategy for TCAD numerical simulation of rad-hard devices
  - Bulk + Surface radiation damage effects need to be considered in the modeling scheme.
  - "New University of Perugia Model" + Acc removal/creation mechanism→ "PerugiaModDoping"
    - LGAD, compensated and RSD LGAD → optimization for their use in the future HEP experiments

- ✓ TCAD plays a pivotal role in the design/optimization of rad-hard devices
  - Modelling radiation damage effects is a tough task!
  - New guidelines for future production of radiation-resistant options.
  - Modeling dopant removals, impact ionization, carriers' mobility, traps dynamics

- ✓ A General-purpose TCAD modeling scheme for extreme fluences doesn't exist yet
  - Predictive capabilities to be extended $\Phi > 10^{16}\ n_{eq}/cm^2$.
  - Application to the optimization of advanced (pixel) detectors (3D detectors, LGADs, …)


VERTEX 2023
Thanks for your kind attention

BACKUP SLIDES

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Low-Gain Avalanche Diodes (LGADs)

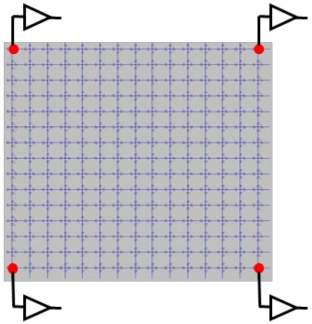
- Most promising devices to cope with the high spatial density of particles hits due to the increasing radiation fluence expected in the HL-LHC at CERN.
- **LGAD structure**: pin diode with the additional inclusion of a p+-type layer just below the n-contact, which is commonly called *multiplication layer.*
- By applying a reverse-bias, this layer is responsible for a **multiplication of carriers**.

$$\mathrm{G}_{\mathrm{aval}} = \boldsymbol{\alpha_n} n v_n + \boldsymbol{\alpha_p} p v_p \qquad \boldsymbol{\alpha} = \frac{E}{E_{th}} e^{-\frac{E_i}{E}}$$

- By accurately chosing the **peak and shape of the implanted p+ profile**, it is possible to control the **avalanche mechanism** in order to obtain the required internal gain with a sufficiently high breakdown voltage.
- One of the best tools **for predicting the behaviour of the avalanche process** is **device-level simulation**

Reconstruction (3/3)

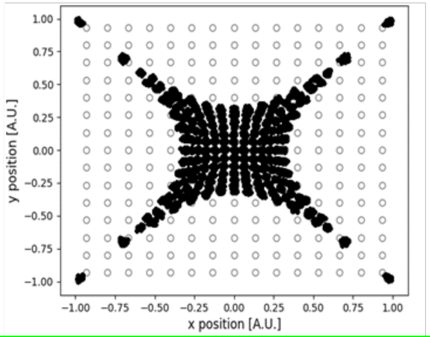
Results from *Spice* simulations **VS.** **Results** from *TCAD* simulations



AMPLITUDE imbalance

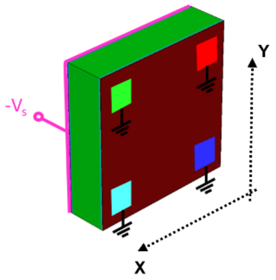
$$x_i = \frac{A_{top\ right} + A_{bottom\ right} - A_{top\ left} - A_{bottom\ left}}{A_{tot}}$$

$$z_i = \frac{A_{top\ right} + A_{top\ left} - A_{bottom\ left} - A_{bottom\ right}}{A_{tot}}$$



Empty circles: injection points

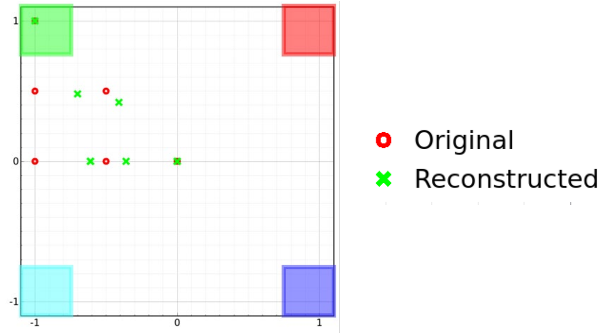
Filled circles: reconstructed points



CHARGE imbalance

$$x_i = \frac{Q_{top\ right} + Q_{bottom\ right} - Q_{top\ left} - Q_{bottom\ left}}{Q_{tot}}$$

$$z_i = \frac{Q_{top\ right} + Q_{top\ left} - Q_{bottom\ left} - Q_{bottom\ right}}{Q_{tot}}$$



From **L. Menzio et al.**, 17th "TREDI" Workshop 03/03/22.

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The "New Perugia" model

√ Surface damage (+ Q_{OX})

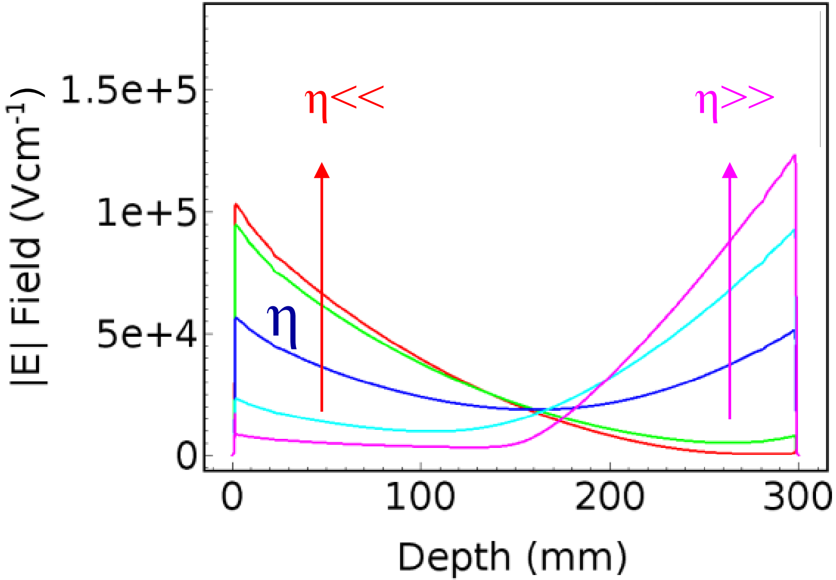
Type	Energy (eV)	Band width (eV)	Conc. (cm^{-2})
Acceptor	$E_C \le E_T \le E_C$-0.56	0.56	$D_{IT} = D_{IT}(\Phi)$
Donor	$E_V \le E_T \le E_V$+0.6	0.60	$D_{IT} = D_{IT}(\Phi)$

√ Bulk damage

Avalanche ON: Van Overstraeten–De Man (default)

Type	Energy (eV)	η (cm^{-1})	σ_n (cm^2)	σ_h (cm^2)
Donor	E_C - 0.23	0.006	2.3×10^{-14}	2.3×10^{-15}
Acceptor	E_C - 0.42	1.6	1×10^{-15}	1×10^{-14}
Acceptor	E_C - 0.46	0.9	7×10^{-14}	7×10^{-13}

- ✓ Traps concentrations dependence upon fluences ~ $\eta \times \phi$.
- ✓ Strong sensitivity to the introduction rate (defects concentration).
- ✓ @ 1.0×10^{16} n_{eq}/cm^2.



Methodology

DC / AC analysis	Transient analysis	Gain calculation
• **DC biasing (static)** ○ n cathode: 0 V ○ p anode: *sweep* ✓ start = 0 V ✓ step = - 25 V (from 100 V) ✓ stop = - 1000 V ○ Temperature ✓ 300 K for not irr., 253 K for irr. [7] • **AC biasing (small-signal)** ○ For each DC bias step, superimposition of a 1 V_{pp}, 1 kHz sinusoid ○ Impedance matrix for each node of the discretized grid ○ Temperature 300 K for not irr. / irr.	• For each DC bias step, one **Time-Variant (TV)** simulation of impinging particle (**MIP**), following the **“HeavyIon” model** ○ instant of penetration 1 ns ○ through the whole device ○ Linear Energy Transfer (LET) $LET_f = \frac{E_{LOSS}}{E} \; \frac{pC}{\mu m}$ where $E = 3{,}68 \; eV$ [5] $E_{LOSS} = 0{,}027 \log(y) + 0{,}126 \; \frac{keV}{\mu m}$	• Leakage current calculation ○ instant = 0,9 ns • Leakage current offset subtracted from the simulated I(t) curve • Calculation of **Collected Charge (CC)** as the **integral of the current** $Gain = \frac{CC_{LGAD}}{CC_{PIN}}$ [6]

[5] S. Meroli et al., *Energy loss measurement for charged particles in very thin silicon layers*, JINST 6 P06013, 2011
[6] V. Sola et al., *First FBK production of 50 µm ultra-fast silicon detectors*, Nucl. Instrum. Methods Phys. Res. A, 2019
[7] A. Chilingarov, *Temperature dependence of the current generated in si bulk*, JINST 8 P10003, 2013.

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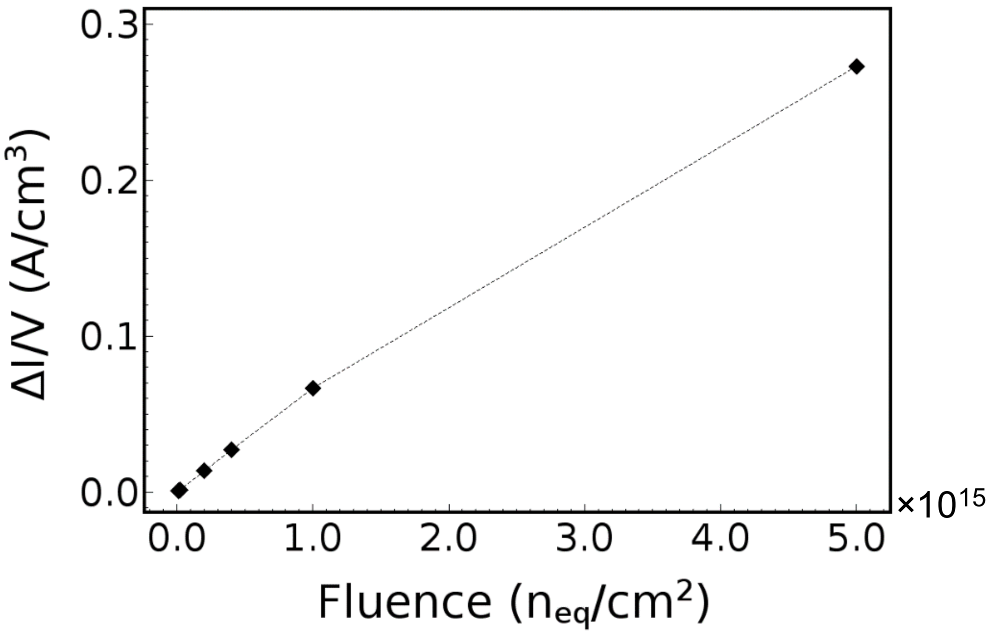
Leakage current vs fluence

- ✓ Leakage current measured/simulated at -20°C and scaled to +20°C [3].
- ✓ p-type susbstrate devices.
- ✓ Leakage current over a detector volume is proportional to the fluence with a proportionality factor α :
  - ✓ MEASUREMENTS: $\alpha \sim 4 \div 7 \times 10^{-17}$ A/cm^3 depending on the annealing time/temperature [4].
  - ✓ SIMULATIONS: $\alpha = 5.4 \times 10^{-17}$ A/cm^3.



$$\alpha = \frac{\Delta I}{V \cdot \Phi_{eq}}$$

[3] A. Chilingarov, Generation current temperature scaling, RD50 technical note.

[4] A. Dierlamm, KIT Status, CMS Outer tracker Meeting, March 2019.

The "New Perugia" model

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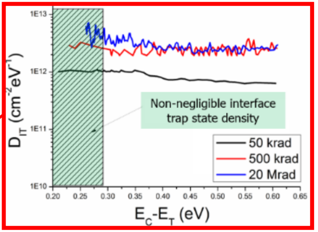

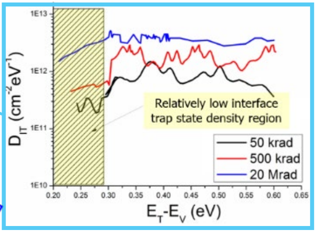

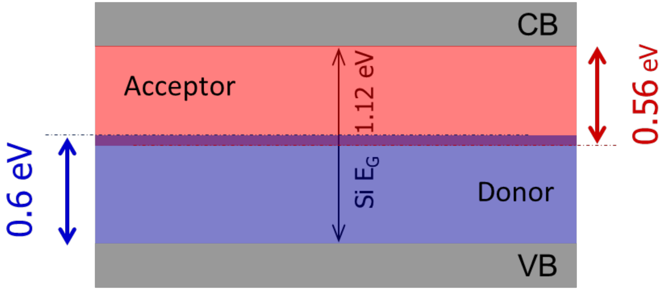

√ Bulk damage

Avalanche ON: Van Overstraeten–De Man (default)

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Donor	E_C - 0.23	0.006	2.3×10^{-14}	2.3×10^{-15}
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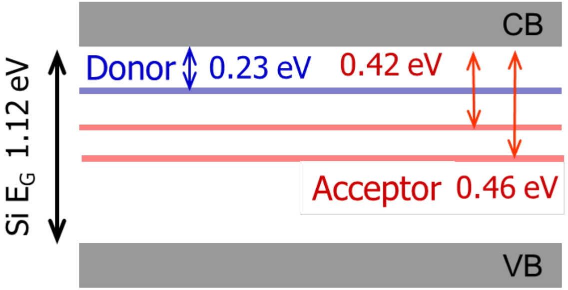

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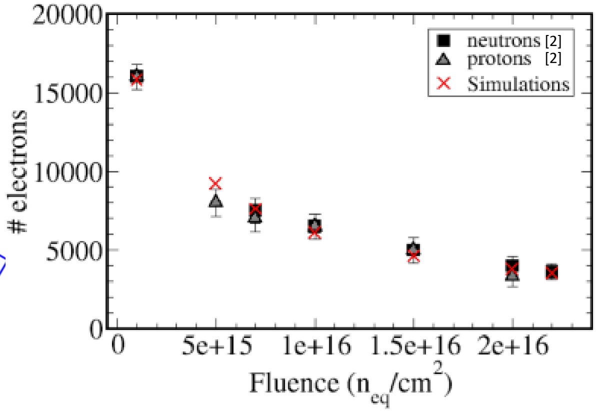
Acceptor	E_C - 0.46	0.9	7×10^{-14}	7×10^{-13}

AIDA 2020

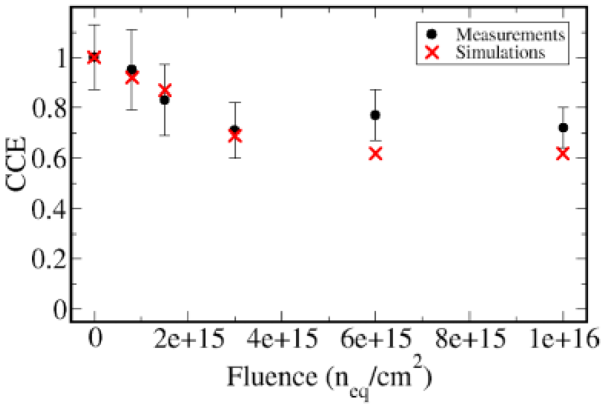
Charge Collection for silicon strips.



[2] A. Affolder et al., NIMA Vol. 623 (2010), pp. 177-179.

F. Moscatelli et al., *Effects of Interface Donor Trap States on Isolation Properties of Detectors Operating at High-Luminosity LHC*, IEEE Transactions on Nuclear Science, 2017, Vol. 64, Issue: 8, 2259 – 2267.

Charge Collection for PiN diodes.



M. Ferrero, 34th RD50 Workshop, June 12-14 2019

Measurements conditions:
- Room temperature
- Measurements with laser 1064nm
- Measurements at 3 laser intensity
- Reference diode to check laser stability

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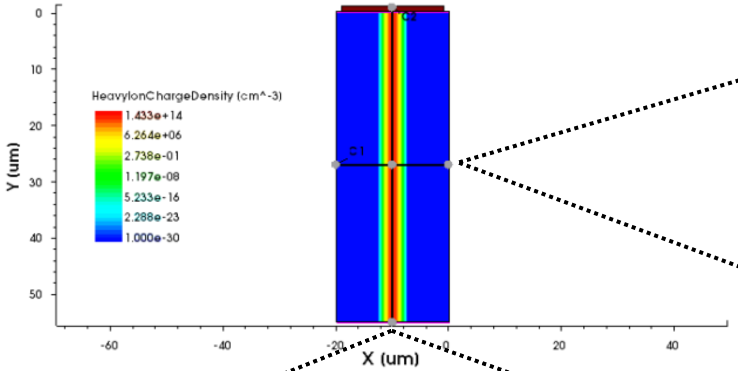
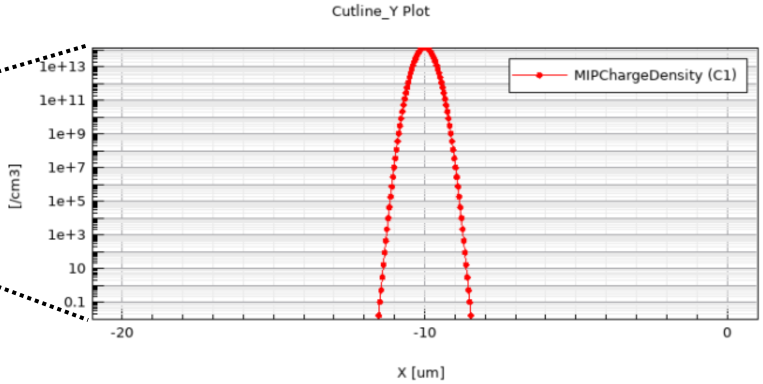
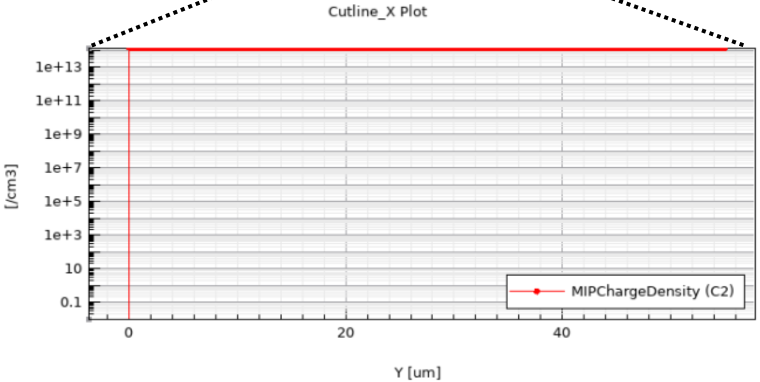
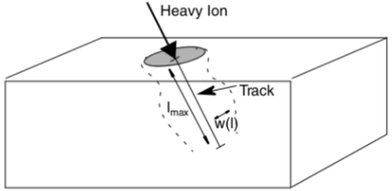
Transient responce: "HeavyIon" model









$$G(l,w,t) = G_{LET}(l)\, R(w,l)\, T(t)$$ → **Gaussian**

$$G_{LET}(l) = a_1 + a_2 l + a_3 e^{a_4 l} + k' [c_1 (c_2 + c_3 l)^{c_4} + LET\_f(l)]$$

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