Uses of SYNOPSYS in high-energy physics experiments

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Outline

- Introduction
- Process simulation
- Structure generation
- Electrostatic simulations
- Transient simulations
- Summary

Selective, non-complete set of examples from High Energy Physics (HEP)

Introduction

Challenging requirements for future High Energy Physics (HEP) silicon tracking detectors

Requirements for future HEP tracking detectors: *CERN-OPEN-2018-006*

Exp. Parameter	LHC	HL-LHC	SPS	FCC-hh	FCC-ee	CLIC 3 TeV
Fluence [n_{eq}/cm^2/y]	N x 10^{15}	10^{16}	10^{17}	10^{16} - 10^{17}	<10^{10}	<10^{11}
Max. hit rate [s^{-1}cm^{-2}]	100 M	2-4 G****)	8 G****)	20 G	20 M ***)	240k
Surface inner tracker [m^2]	2	10	0.2	15	1	1
Surface outer tracker [m^2]	200	200	-	400	200	140
Material budget per detection layer [X_0]	0.3%*) - 2%	0.1%*) - 2%	2%	1%	0.3%	0.2%
Pixel size inner layers [µm^2]	100x150-50x400	~50x50	~50x50	25x50	25x25	<~25x25
BC spacing [ns]	25	25	>10^9	25	20-3400	0.5
Hit time resolution [ns]	<~25–1k*)	0.2**)–1k*)	0.04	~10^{-2}	~1k ***)	~5

*) ALICE requirement **) LHCb requirement ***) At Z-pole running ****) max. output rate for LHCb/high intensity flavour experiments: 300-400 Gbit/s/cm^2

→ Extreme radiation tolerance

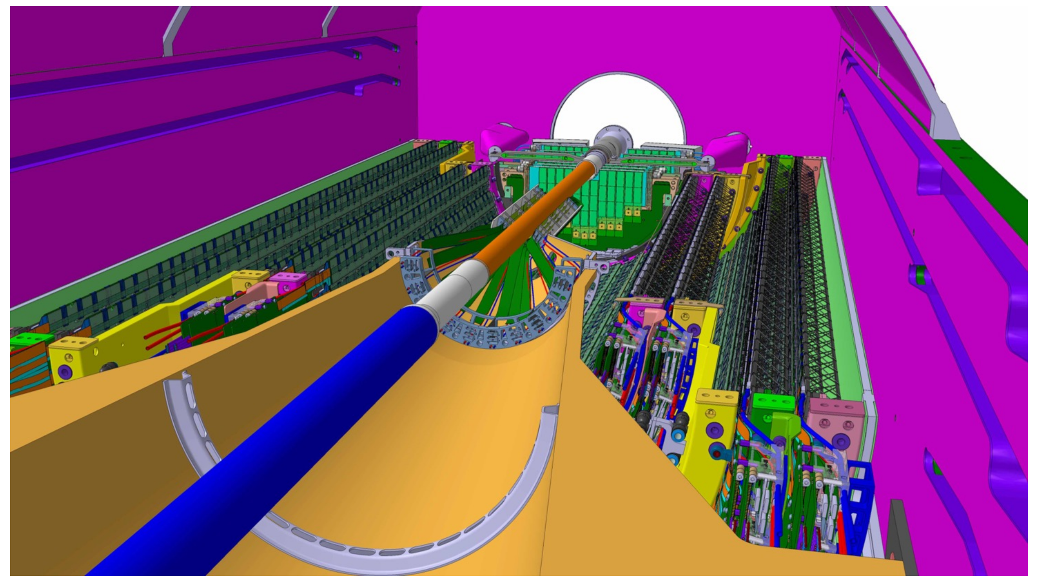
→ Very fast

→ Very large surface

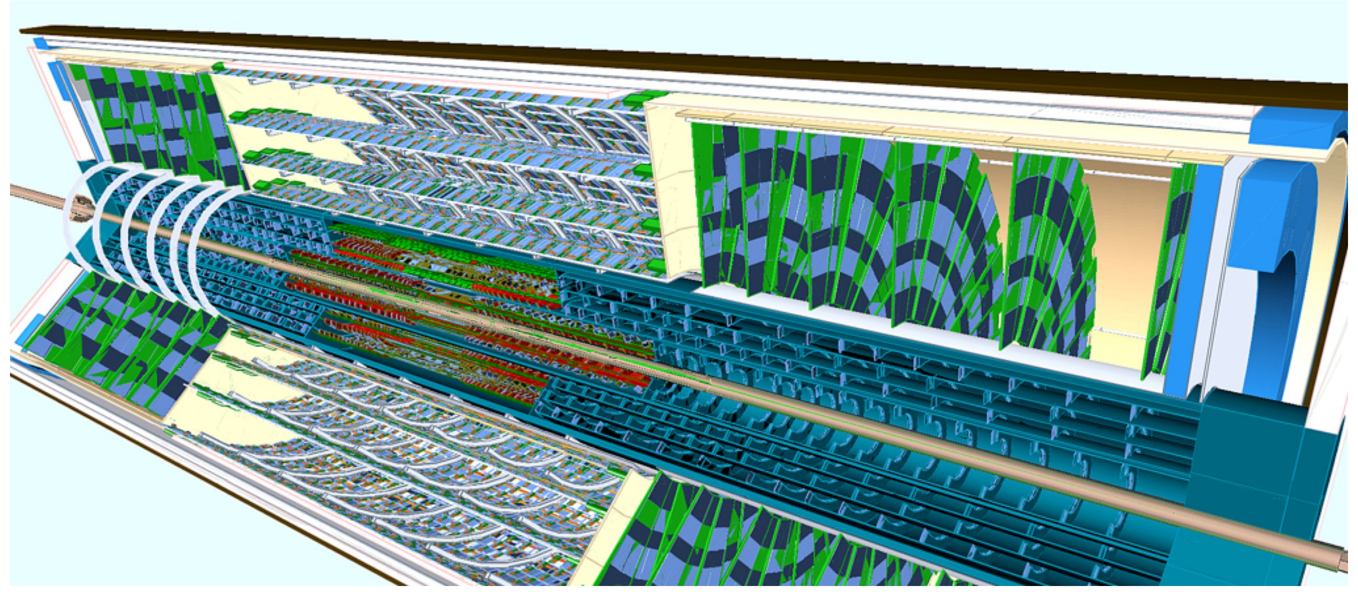
→ Very thin

→ Ultimate granularity

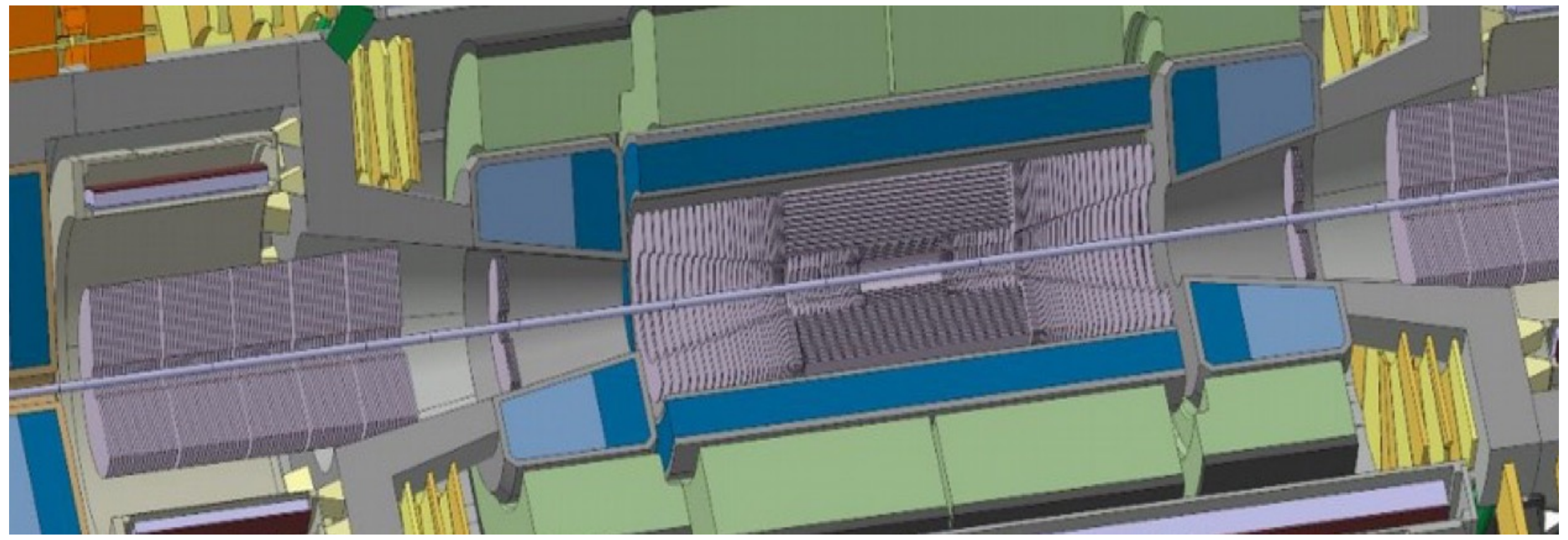
ALICE ITS4:



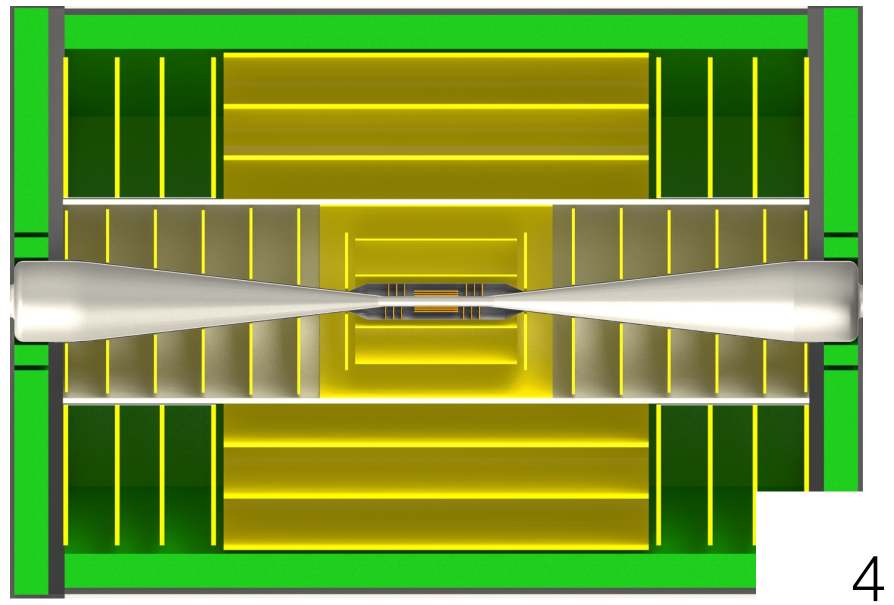
ATLAS ITK:



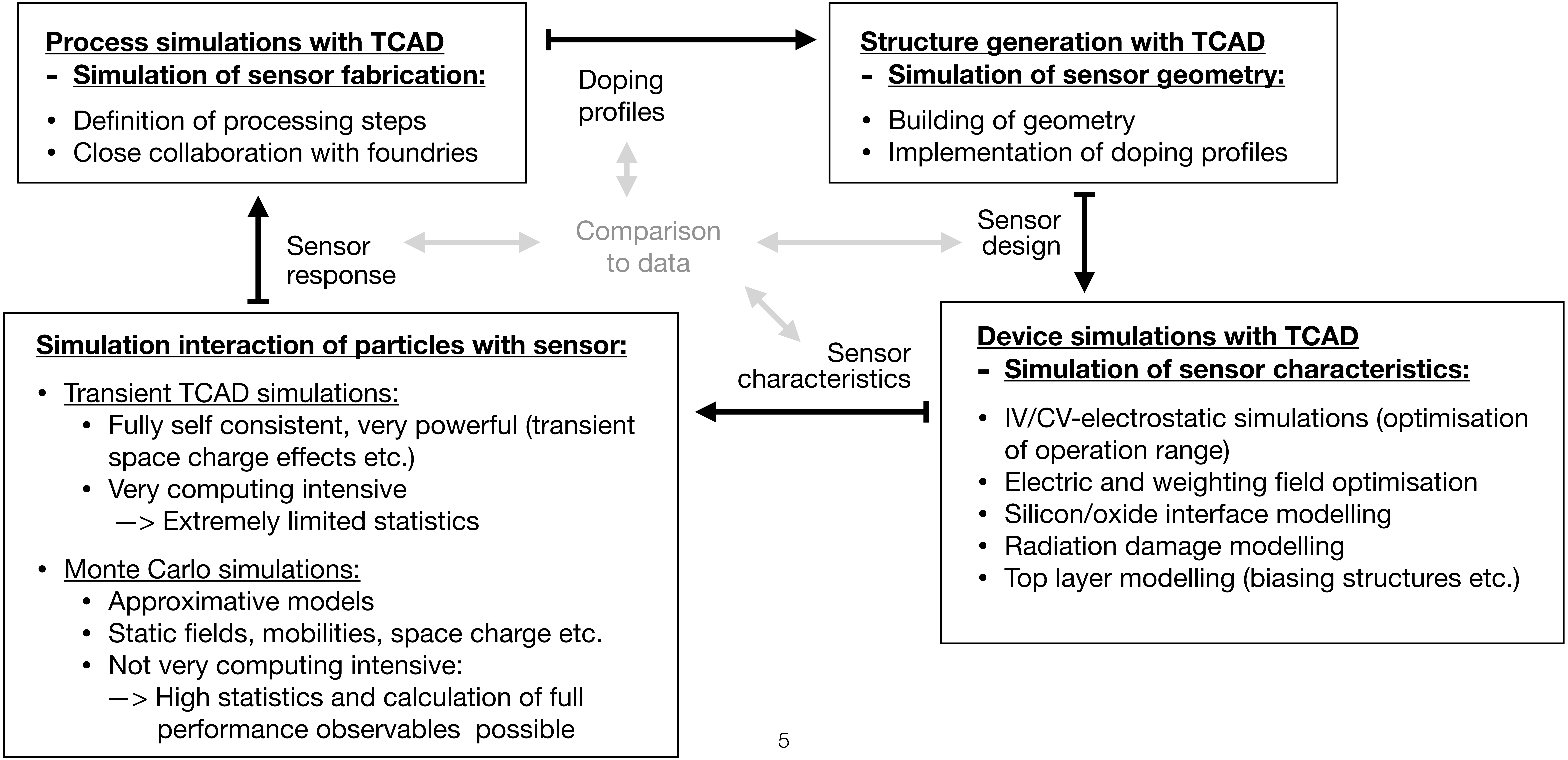
FCC hh:



CLIC 3TeV:



Overview of silicon detector simulations



Process simulations with TCAD
- Simulation of sensor fabrication:

- Definition of processing steps
- Close collaboration with foundries

Doping profiles

Structure generation with TCAD
- Simulation of sensor geometry:

- Building of geometry
- Implementation of doping profiles

Sensor design

Device simulations with TCAD
- Simulation of sensor characteristics:

- IV/CV-electrostatic simulations (optimisation of operation range)
- Electric and weighting field optimisation
- Silicon/oxide interface modelling
- Radiation damage modelling
- Top layer modelling (biasing structures etc.)

Sensor characteristics

Simulation interaction of particles with sensor:

- Transient TCAD simulations:
  - Fully self consistent, very powerful (transient space charge effects etc.)
  - Very computing intensive
    —> Extremely limited statistics
- Monte Carlo simulations:
  - Approximative models
  - Static fields, mobilities, space charge etc.
  - Not very computing intensive:
    —> High statistics and calculation of full performance observables possible

Sensor response

Comparison to data

Technology Computer Aided Design - TCAD

Poisson equation:

$$\nabla \cdot \epsilon \nabla \phi = -\rho_{eff} \quad \text{with} \quad \rho_{eff} = q[p - n + N_D - N_A] - \rho_{traps}$$

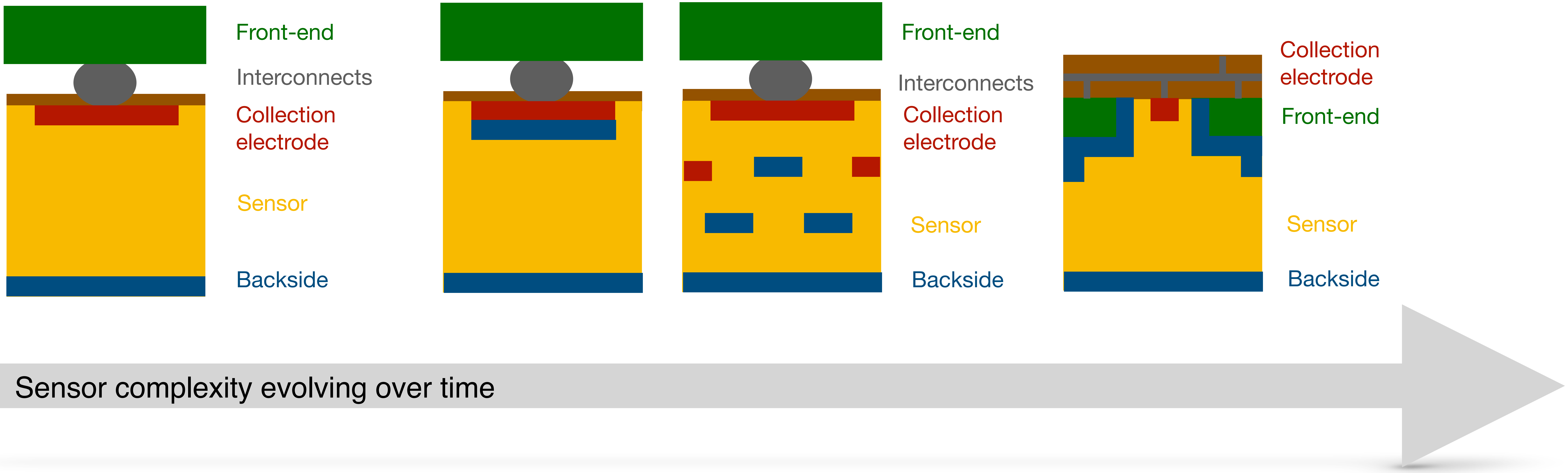
Continuity equations:

Electrons:
$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_n + R_{net} \quad \text{where} \quad \mathbf{J}_n = q n \mu_n \mathbf{E} + q D_n \nabla n$$

Holes:
$$\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{J}_p + R_{net} \quad \text{where} \quad \mathbf{J}_p = q p \mu_p \mathbf{E} - q D_n \nabla p$$

- Equations + boundary conditions are solved on discrete mesh points
- Various models and parameters selectable
- Extensive documentation in Synopsys Sentaurus manuals

Increasing relevance of TCAD simulations for silicon detectors in HEP



Hybrid planar sensors:

Front-end

Interconnects

Collection electrode

Sensor

Backside

Hybrid advanced sensors with complex well structures:

Front-end

Interconnects

Collection electrode

Sensor

Backside

Monolithic sensors with complex well structures:

Collection electrode

Front-end

Sensor

Backside

Sensor complexity evolving over time

Characteristics of complex sensors not analytically predictable anymore → increasing need of TCAD simulations.

Process simulations

- SPROCESS simulations for HEP in Synopsys Sentaurus -

Aim:
Extract and optimise doping profiles for realistic processing steps
—> *Close collaboration with foundry.*

Increasing relevant in HEP due to advanced sensor processes needed to reach ambitious requirements of future silicon detectors in HEP

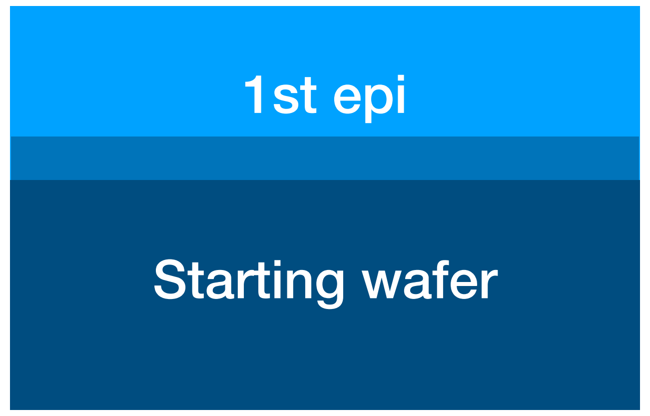
Process simulations for HEP

SPROCESS simulation in Synopsys Sentaurus

Example- deep sensor implants, very deep sensor implants usually realised by ‘successive epitaxial layer growth’:

Start with low resistivity wafer:

Growth of 1st epitaxial layer:

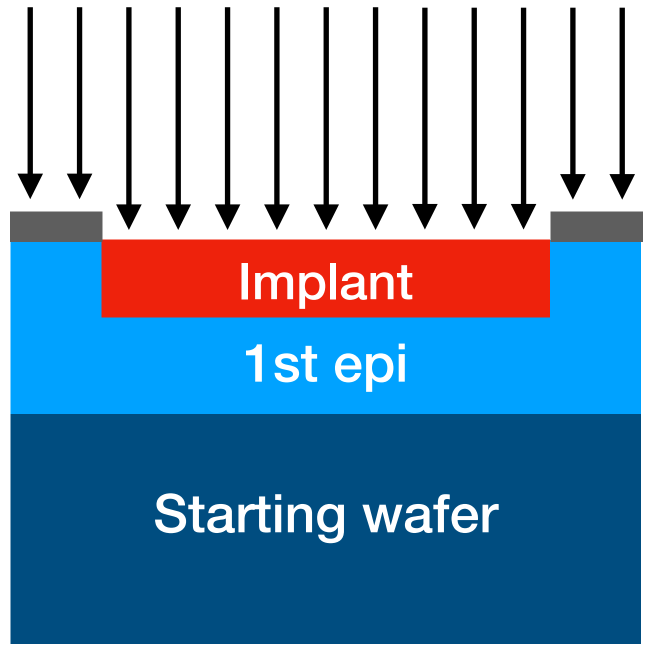


- Growth of first high resistivity epitaxial layer on low resistivity wafer with Chemical Vapour deposition CVD
- Definition of time and temperature in SPROCESS

→ Out-diffusion of starting wafer doping into epi

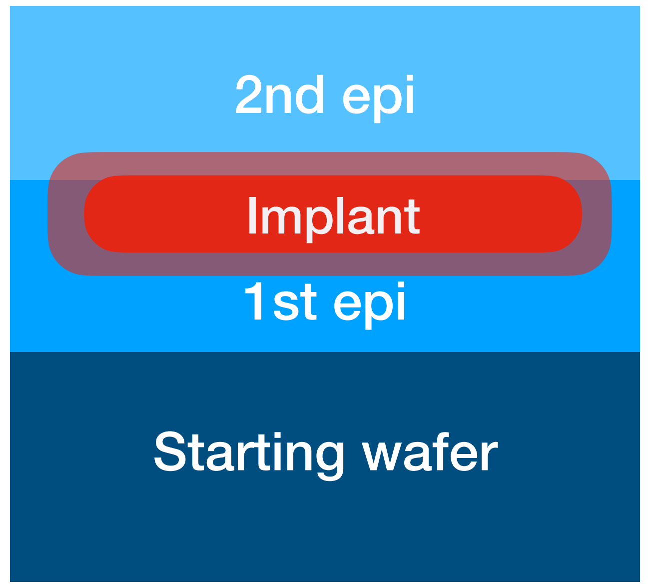
→ Reduced active thickness.

Implantation:



- Patterning of implant with mask
- Implantation in openings of mask
- Definition of dose, energy, type and incidence angle in Sprocess
- Etching/removal of mask

Growth of 2nd epitaxial layer:



- Growth of second high resistivity epitaxial layer
- Definition of time and temperature in Sprocess

→ Diffusion of implant

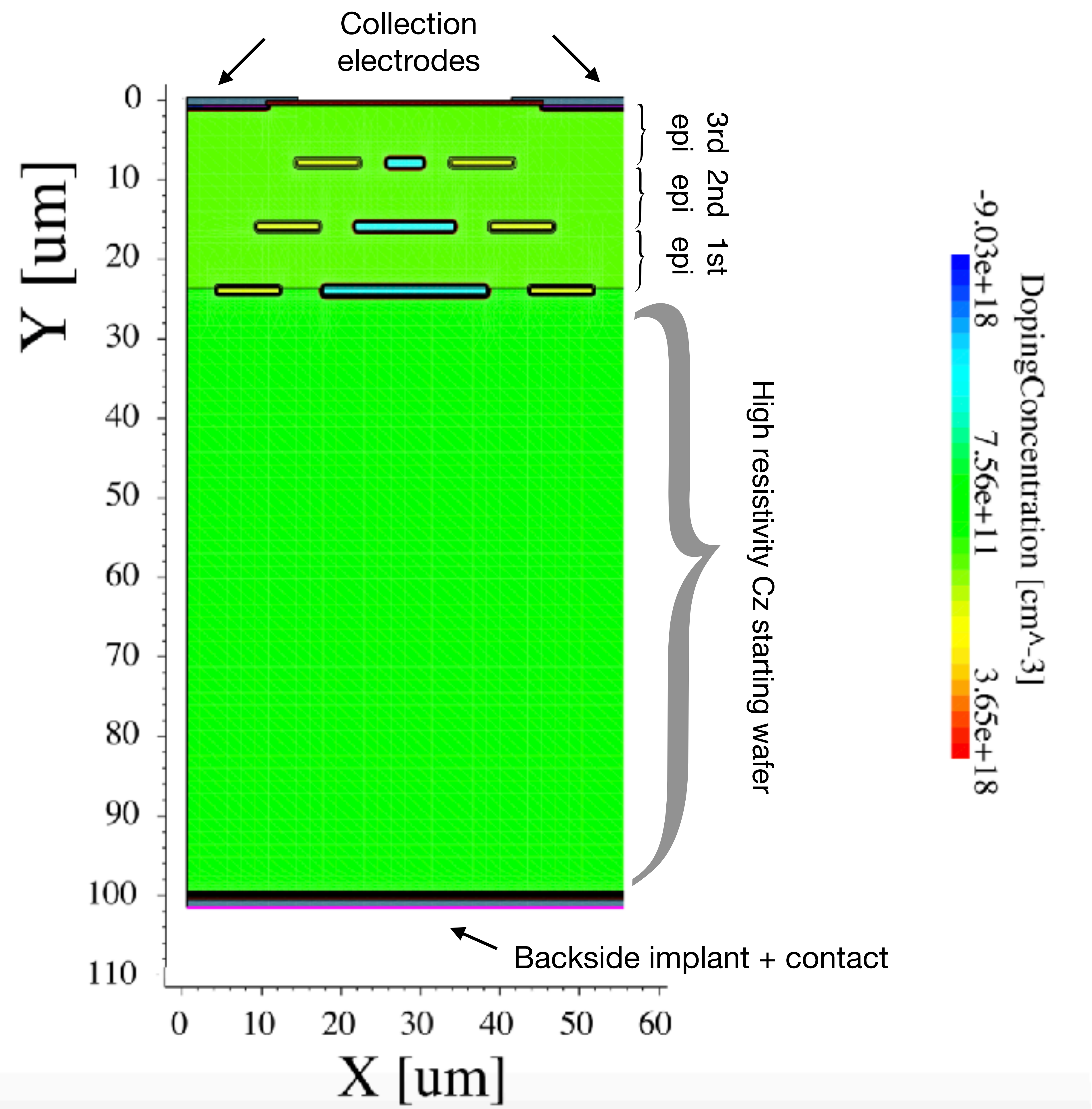
→ Reduced accuracy of implant

→ Impact on field shaping and breakdown.

Process simulations for HEP - ELAD

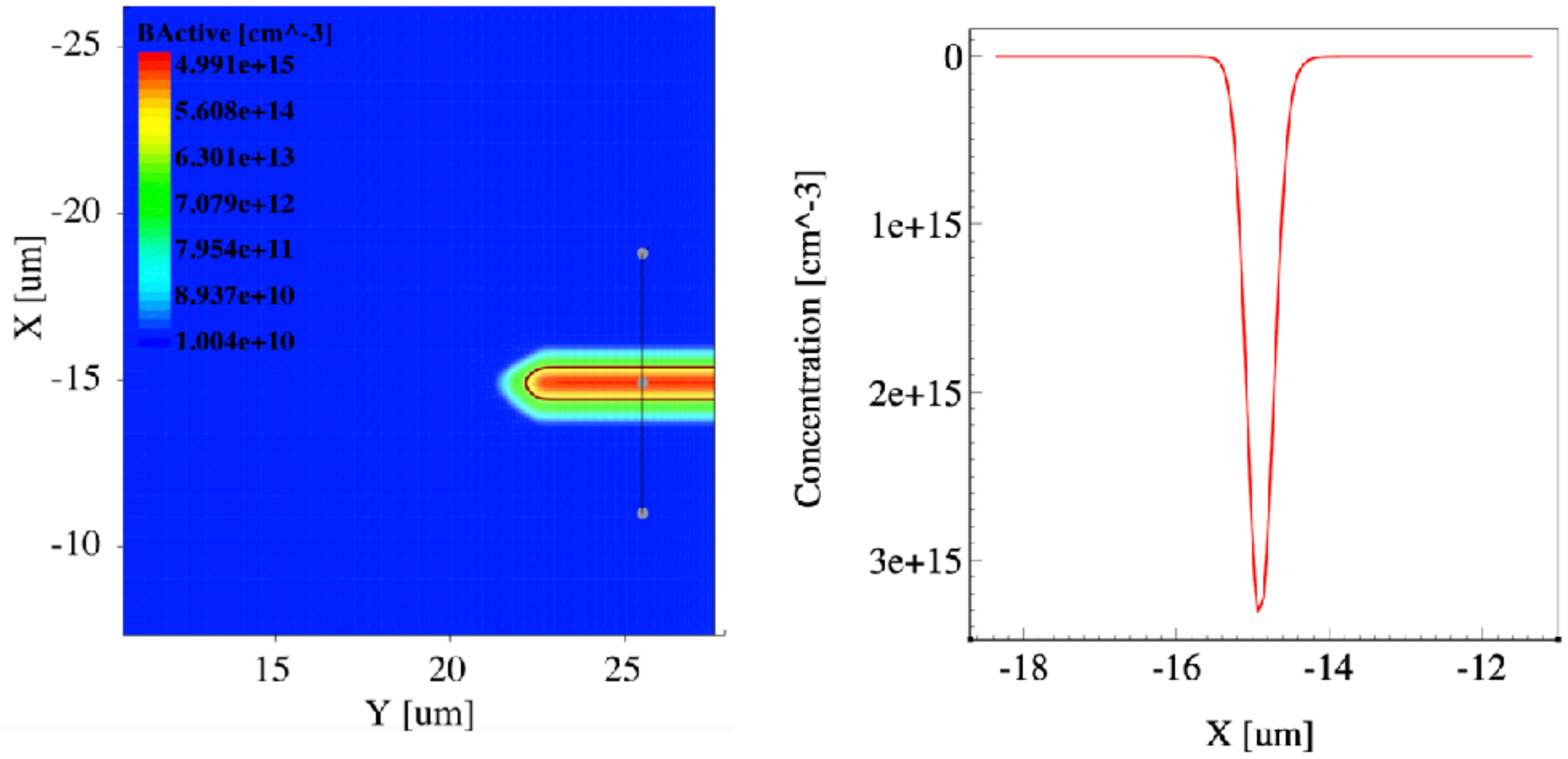
Example - Enhance Lateral Drift Sensors (ELAD):

- Field shaping with deep implants to increase charge sharing
- Increased charge sharing and improved spatial precision interesting for future HEP experiments, e.g. CLIC



From:
Concept and Development of Enhanced Lateral Drift (ELAD) Sensors, PhD Thesis Anastasiia Velyka

SPROCESS simulation of 2nd layer boron implant:



- SPROCESS simulations for different implants in different layers
- For each epi, simulation of CVD with 1100 °C for 20 minutes

→ Realistic width of implants crucial for field shaping

Structure generation

- SDE simulations for HEP in Synopsys Sentaurus -

Aim:
Model exact geometry of silicon detector prototype
—> *Close collaboration with foundry.*

Increasing relevant in HEP due to advanced sensor geometries needed to reach ambitious requirements of future detectors

Advanced geometrical shapes in Synopsys Sentaurus

Predefined functions allow for advanced/complex geometries in 2D and 3D:

- Predefined functions for structure building, e.g. complex polygons

—> *Easy implementation of advanced shapes, e.g. hexagonal 3D shape with arbitrary cutout, …*

Hexagonal pixels:

- Mitigate electric field edge effects
  —> Relevant for small pixels, timing, electric field breakdown!
- Reduce charge sharing (2 neighbours instead of 3)
  —> Improved efficiency for thin sensors

—> *Attractive for future HEP experiments*

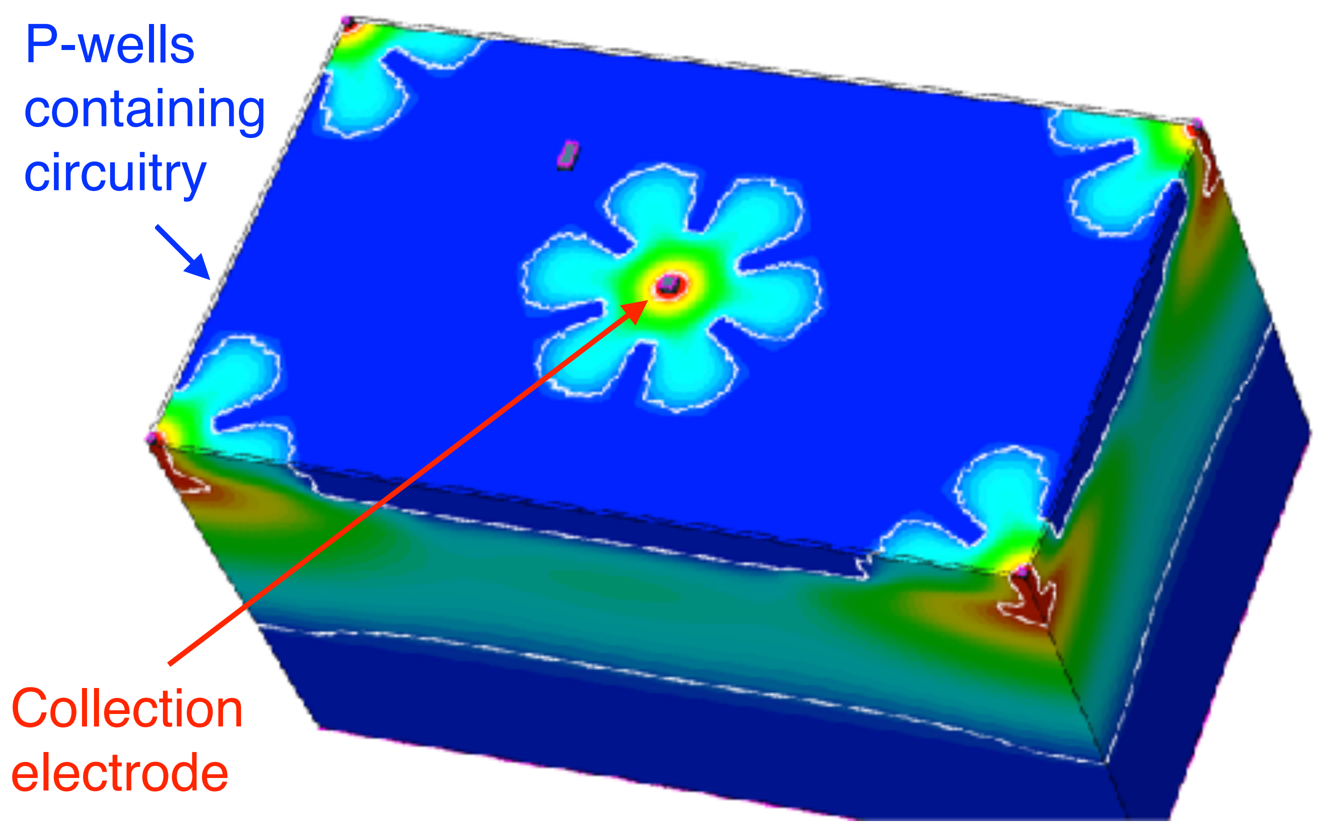
Examples from HEP R&D:

FASTPIX: sub-nanosecond radiation tolerant CMOS pixel sensors 10.1016/j.nima.2020.164461

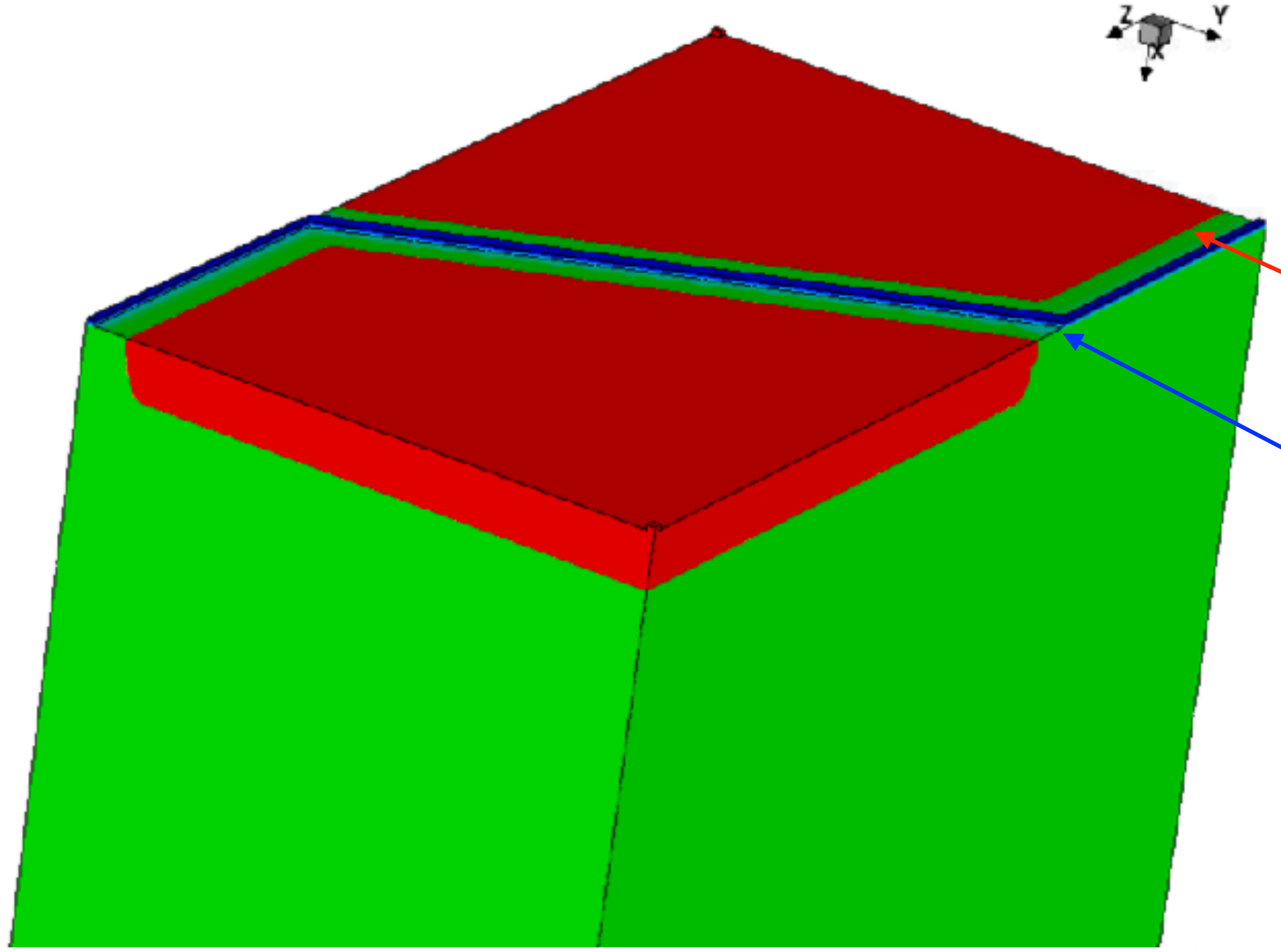
The MONOLITH ERC Advanced Project d10.1109/MIM.2021.9620045

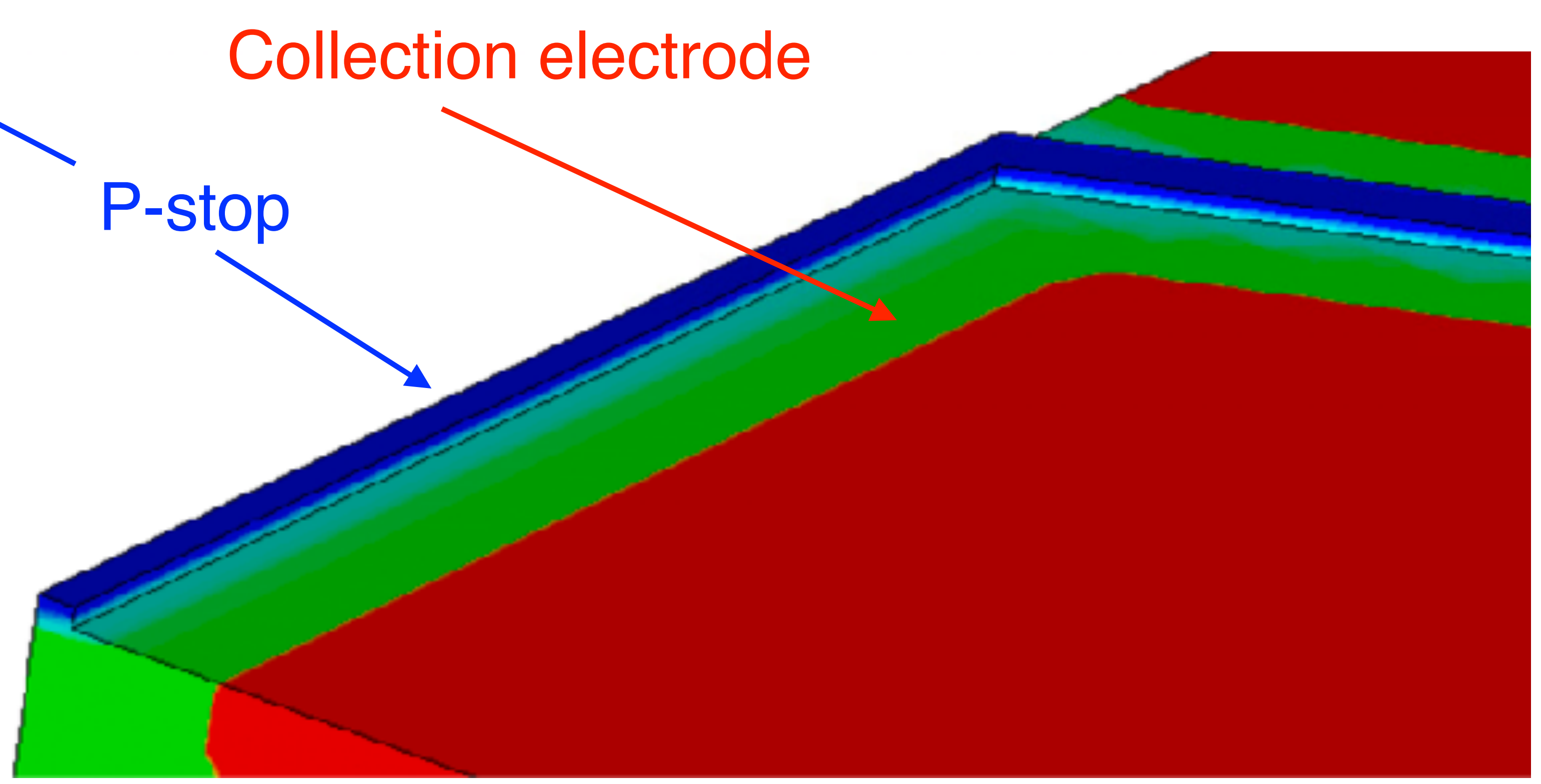
TIMESPOT https://doi.org/10.1016/j.nima.2020.164491

Example - 3D hexagonal pixel simulation with small collection electrode and 'flower-shaped' wells:



Example - 3D hexagonal pixel simulation with large collection electrode separated by p-stops:





→ Advanced shapes very useful for development of novel silicon pixel detectors.

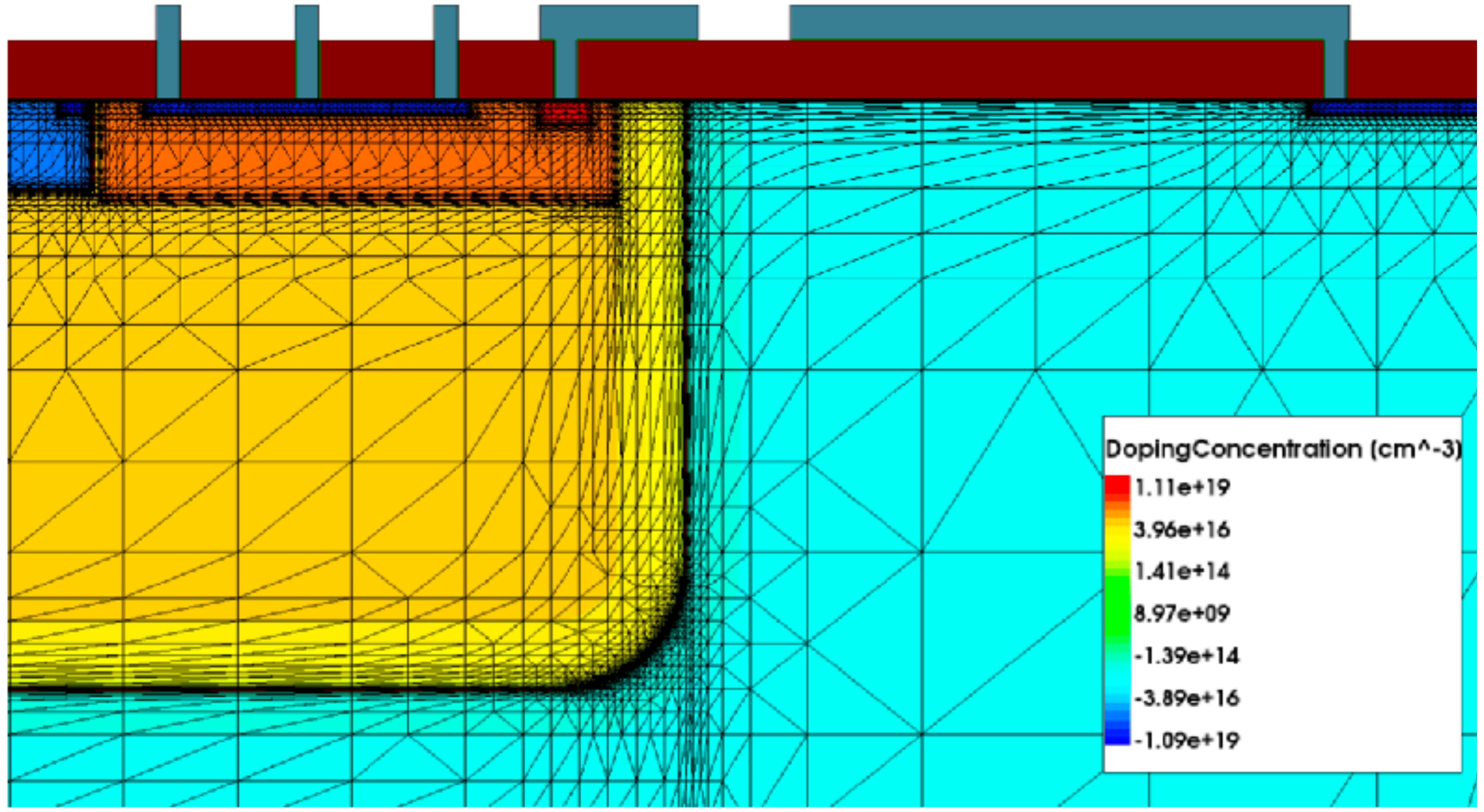
Advanced geometrical shapes in Synopsys Sentaurus

Predefined functions allow for advanced/complex geometries in 2D and 3D:

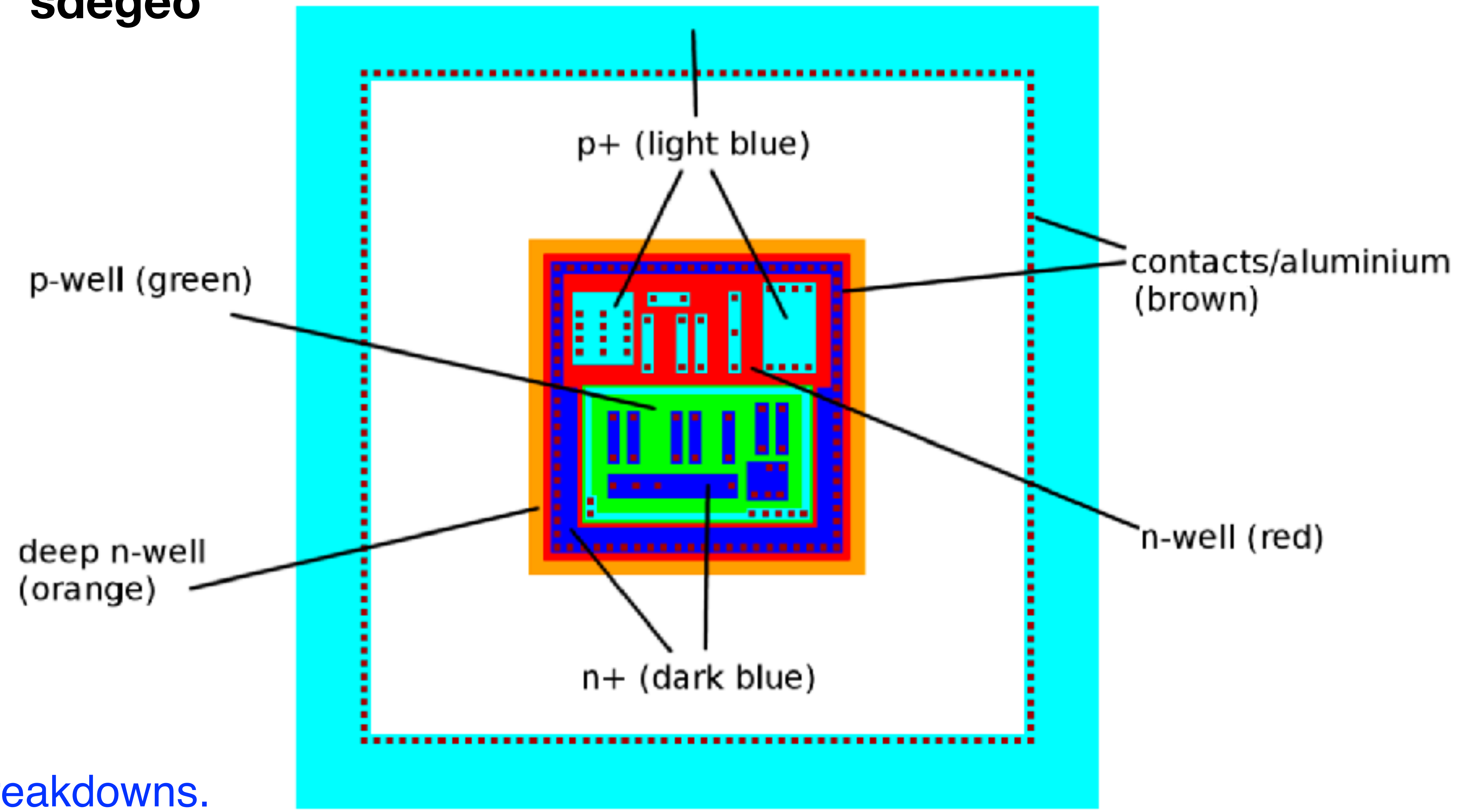
- Predefined functions for layer deposition and mask generation
- Relevant for modelling of top-side metal structures
- Increasingly important for monolithic sensors (more complex top-side processing)

From:
Simulation and evaluation of HV-CMOS pixel sensors for the CLIC vertex detector, PhD Thesis
Matthew Buckland

Example - HV-CMOS top-layer modelling:



sdegeo



—> Top-layer modelling is very relevant e.g. to avoid electric field breakdowns.

Electrostatic simulations

- SDEVICE simulations for HEP in Synopsys Sentaurus -

Aim:
Electrostatic characterisation of silicon detector prototypes
—> *IV, CV, field shaping, field breakdown optimisation etc…*

Increasing relevance in HEP due to advanced sensor geometries with multiple voltage terminals, needed to reach ambitious requirements of future silicon detectors in HEP

—> Not possible to analytically calculate electrostatic performance

3D vs. 2D TCAD simulations

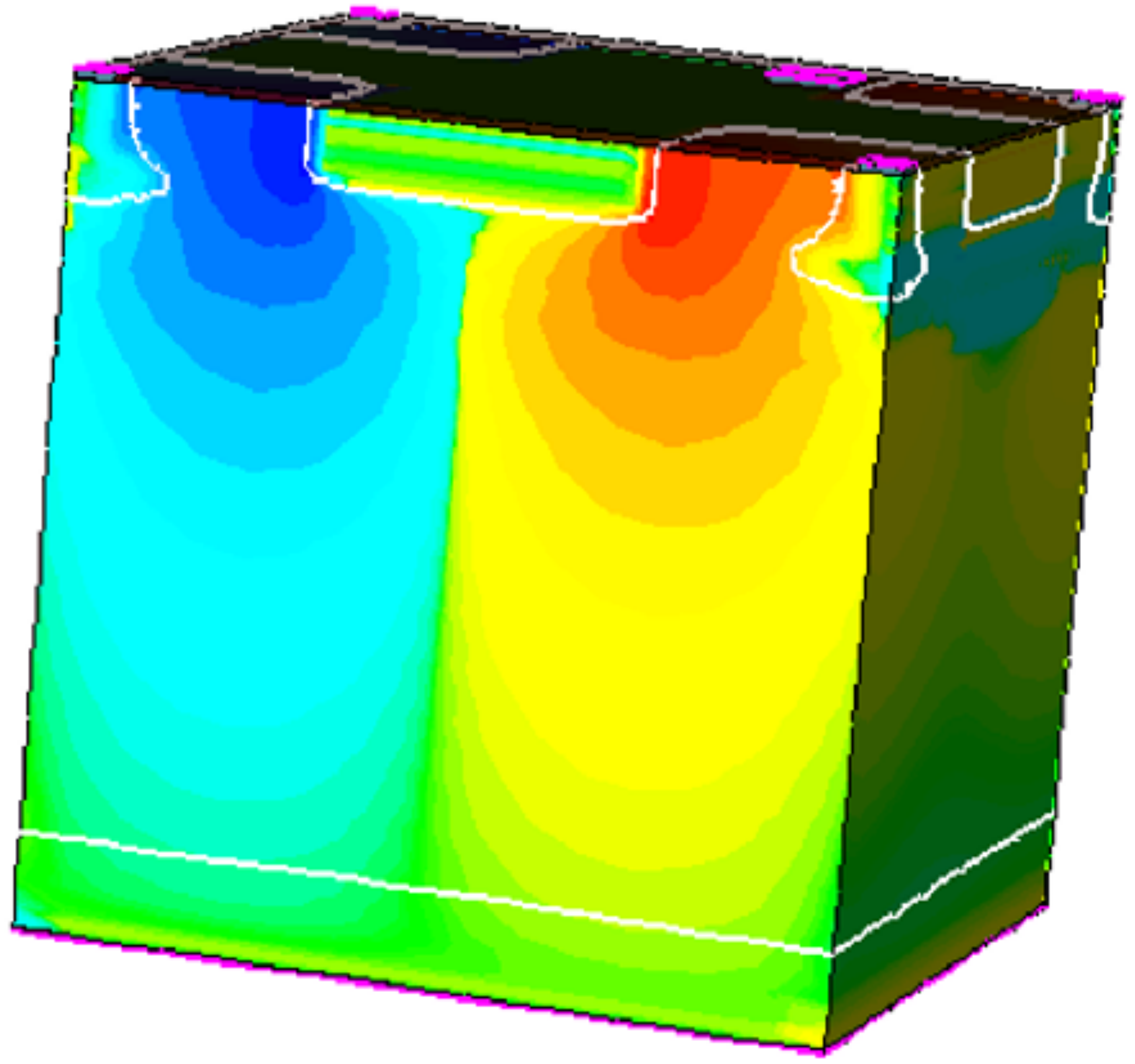
Disadvantage of 3D:

Extremely computing intensive —> better avoid whenever possible…

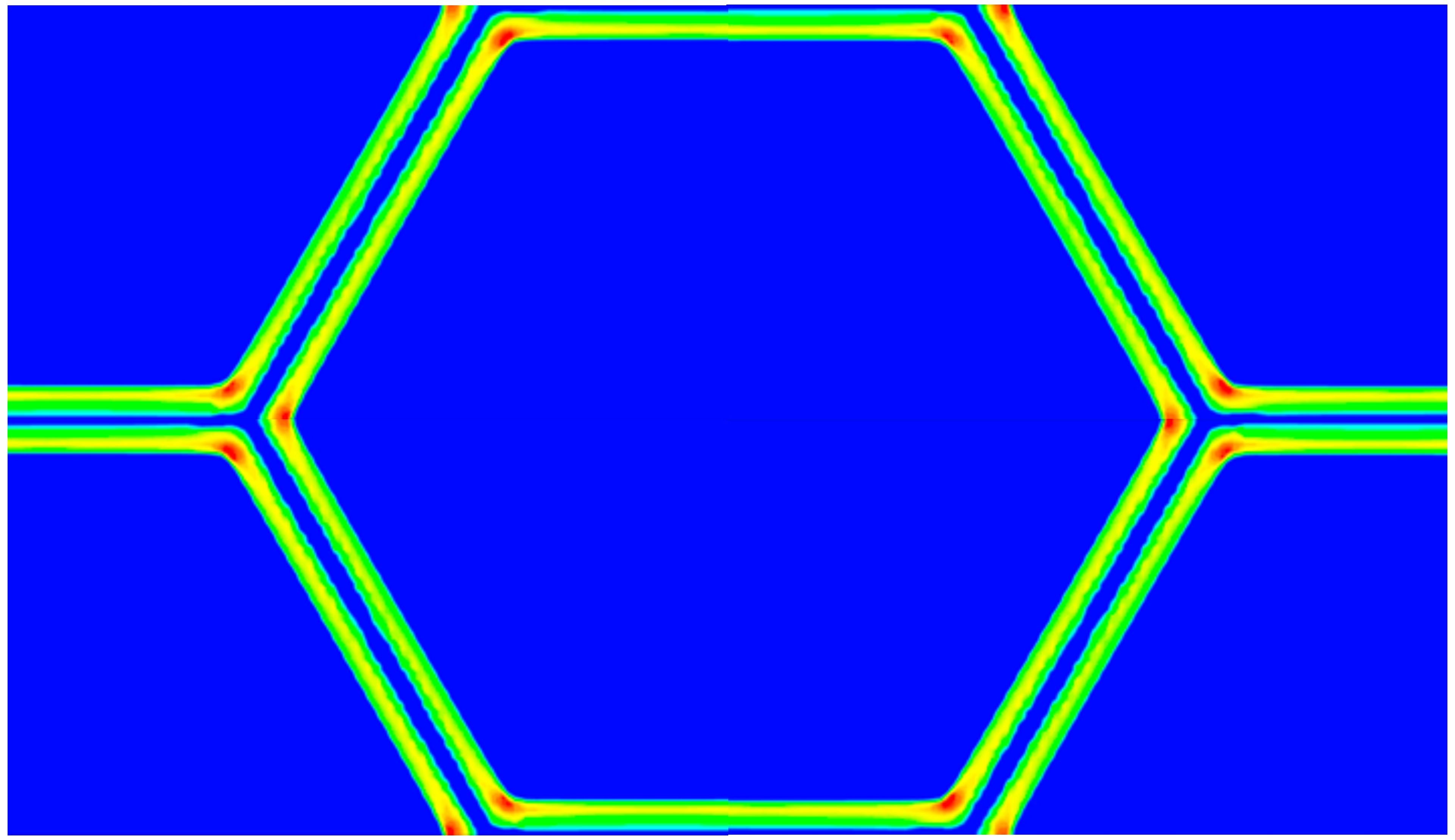
But, we need 3D TCAD whenever we have a dependance of our solution on the 3rd dimension:

Example - Modelling of pixel corner effects:

Highly in-homogenous lateral electric field in small collection electrode CMOS sensors:



Electric field close to sensor surface in large collection electrode CMOS sensors:



→ Crucial for field breakdown determination.

3D sensors - TIMESPOT

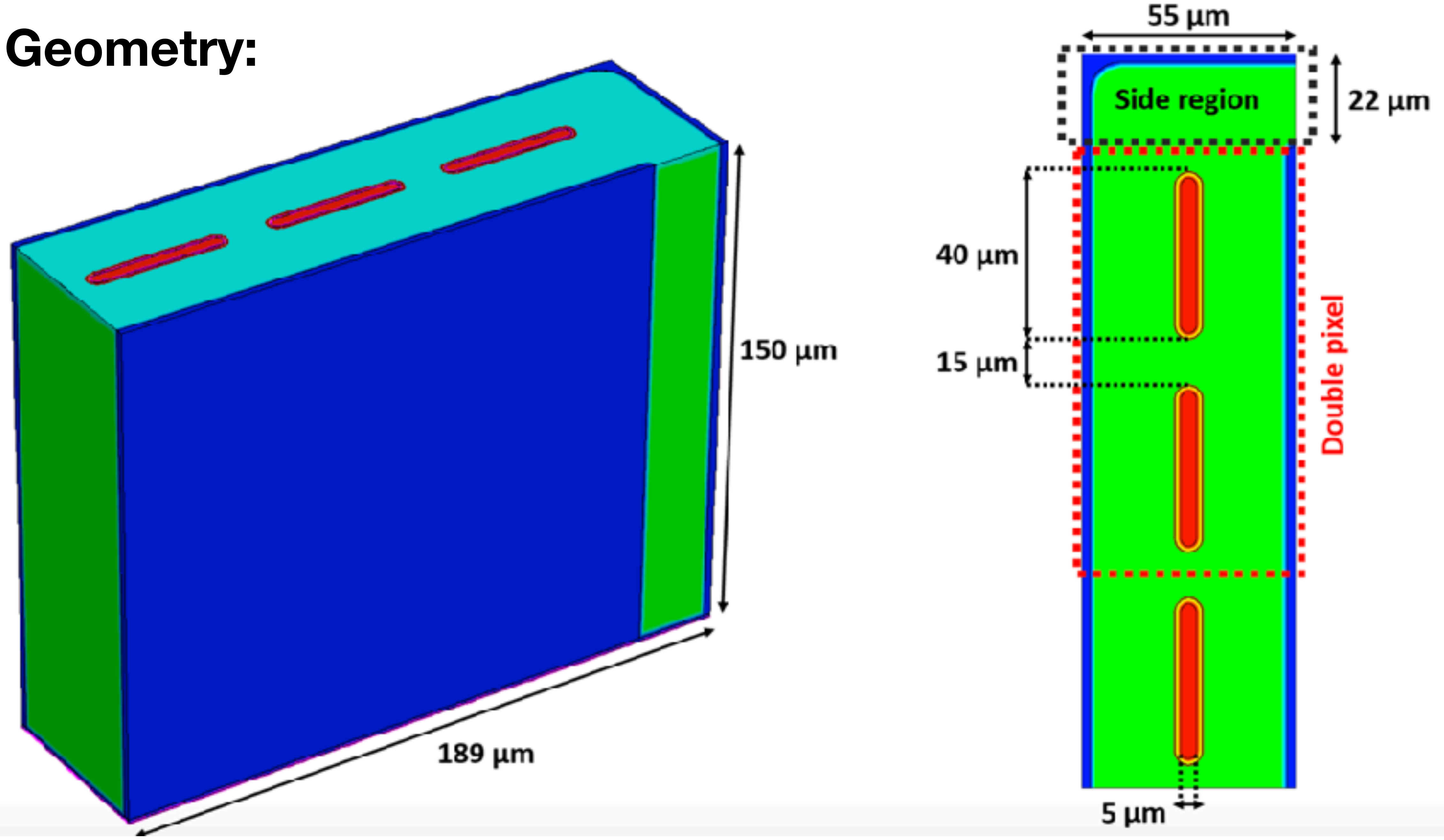
3D sensors:

- 3D sensors already used for ATLAS IBL
- TIMESPOT: Optimisation of 3D sensors for picosecond time stamping

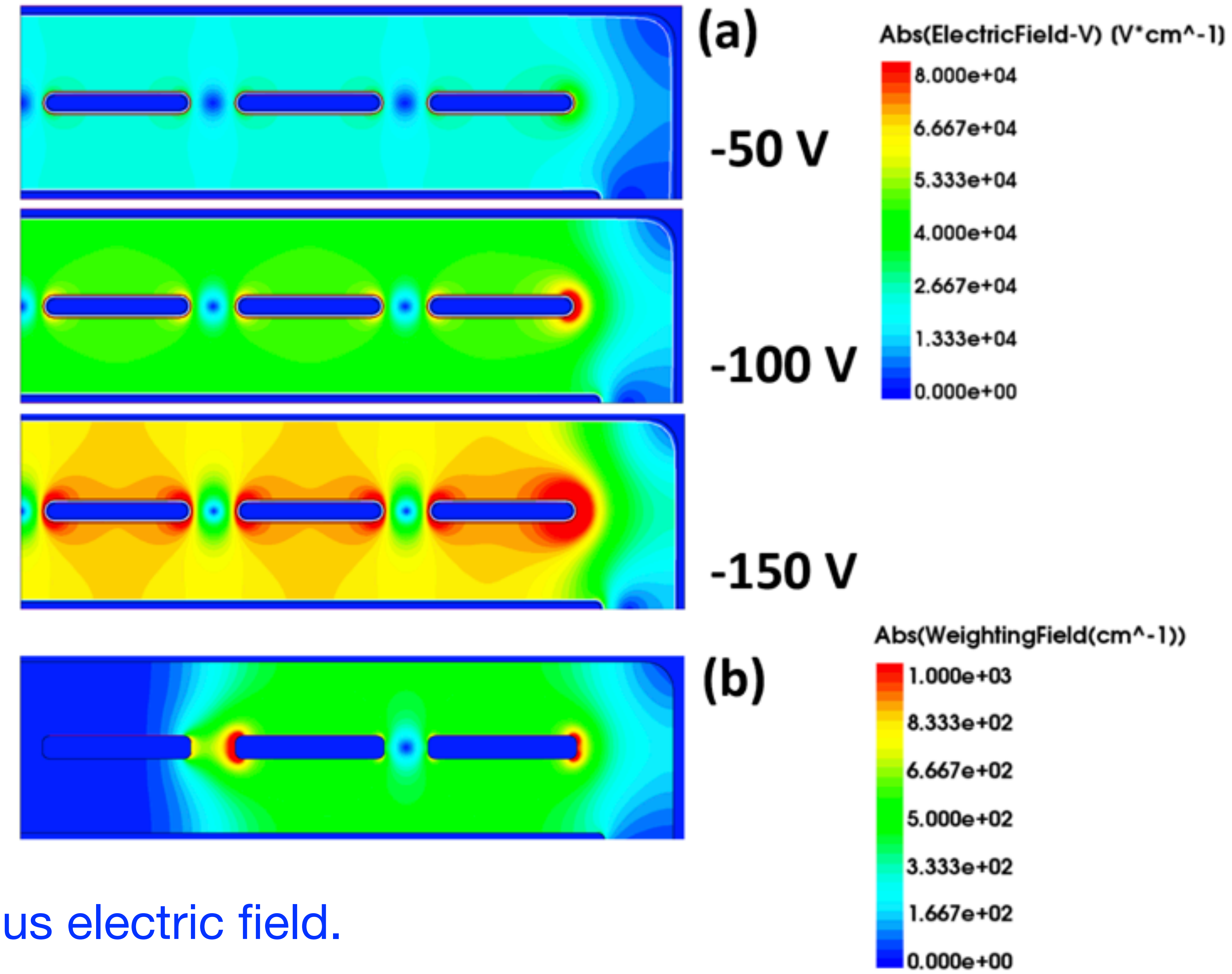
From:
D. Brundu et al 2021 JINST 16 P09028

TIMESPOT 3D TCAD simulations:

Geometry:



Electric field from SDEVICE simulation in Synopsys - top view:

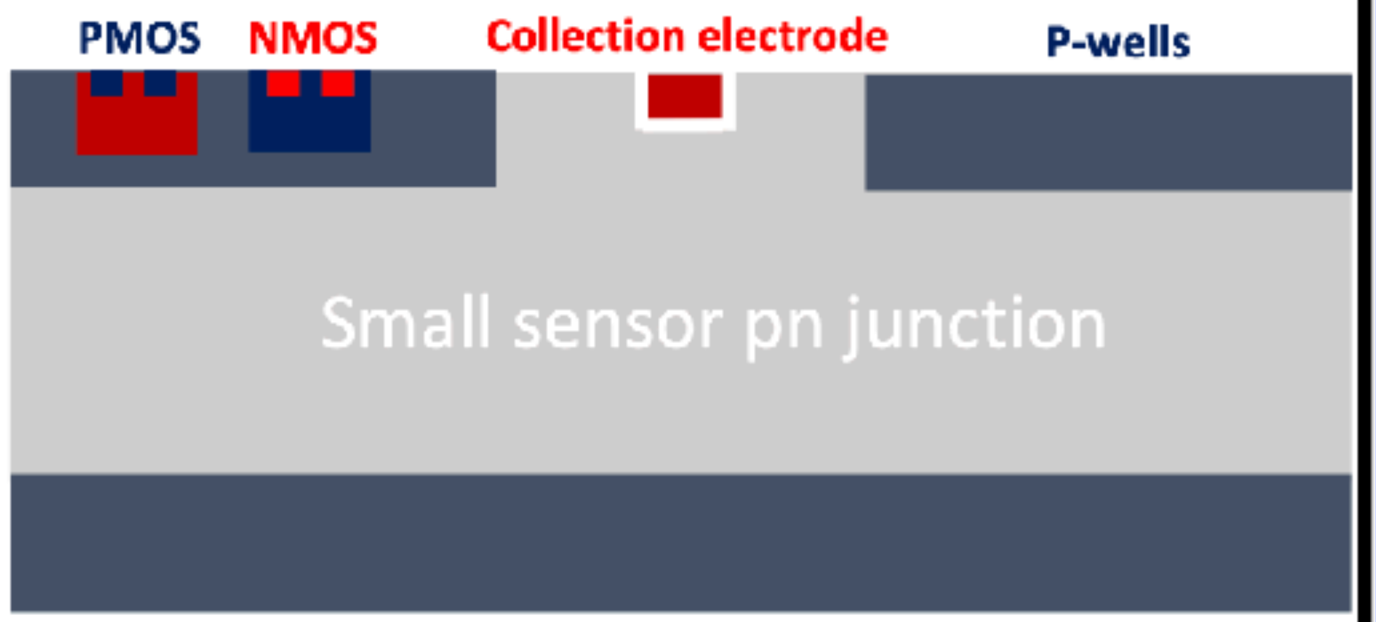


→ Relevance of 3D simulations to correctly model highly non-homogenous electric field.

Small c-electrode CMOS optimisations

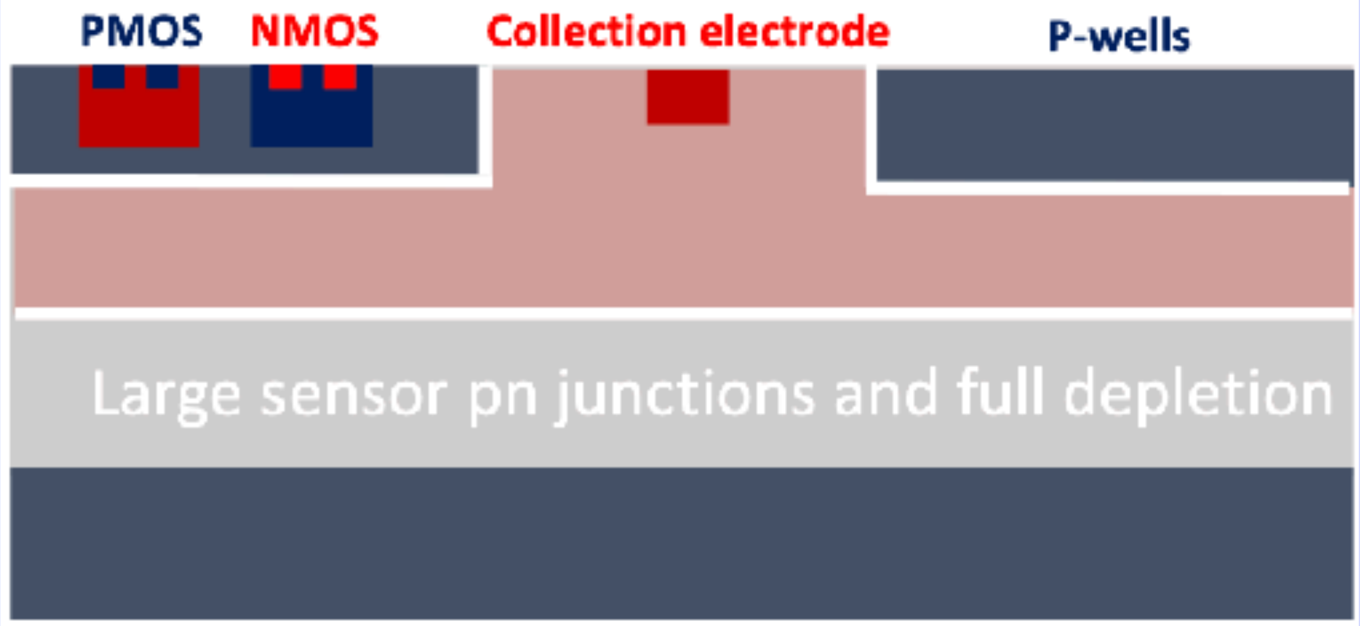
Process cross sections:

Standard process cross section:



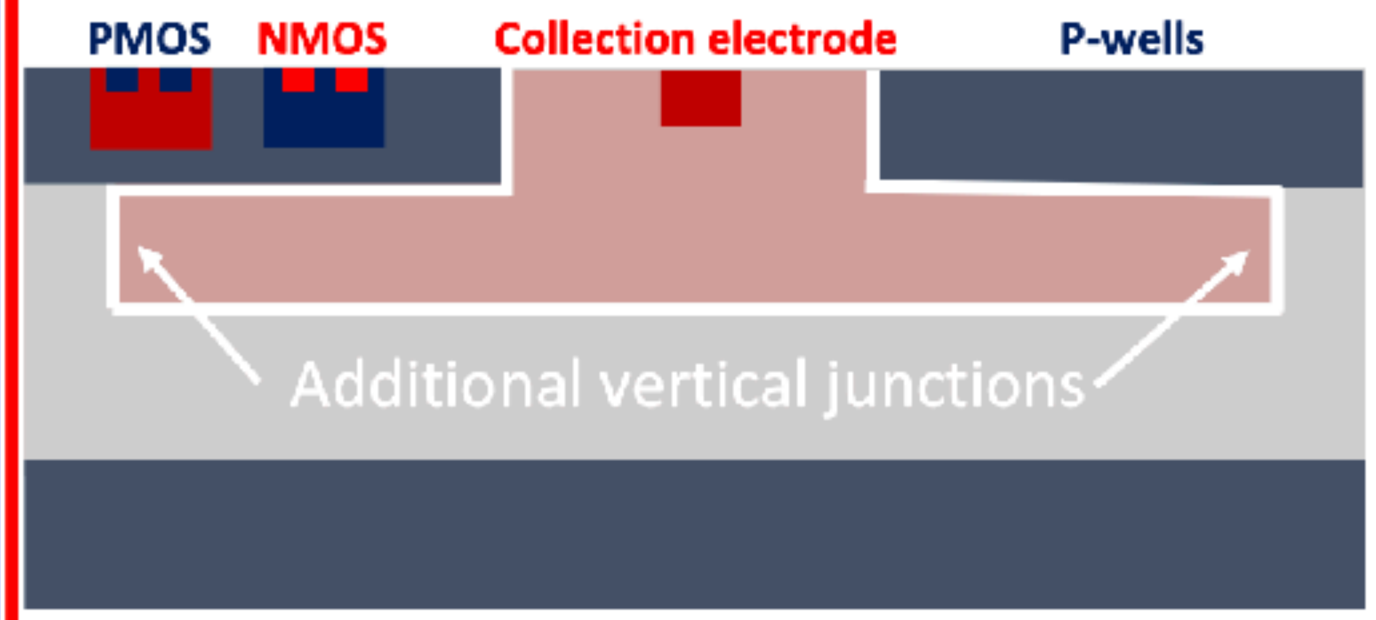
Small sensor junction
→ limited depletion and field

Modified process cross section with deep n-implant:



Large sensor junction
→ full depletion, low field in corners

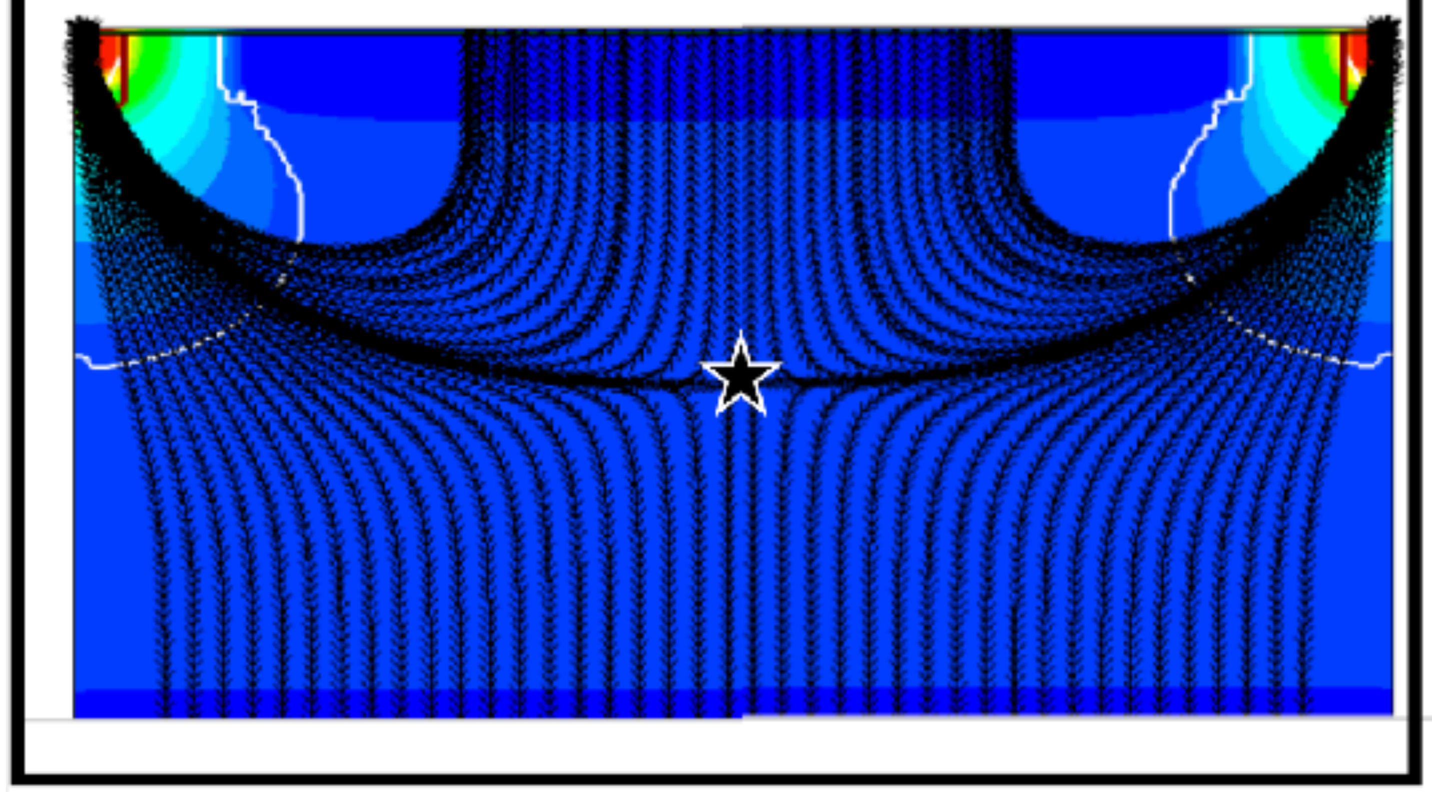
Process cross section with gap in deep n-implant:



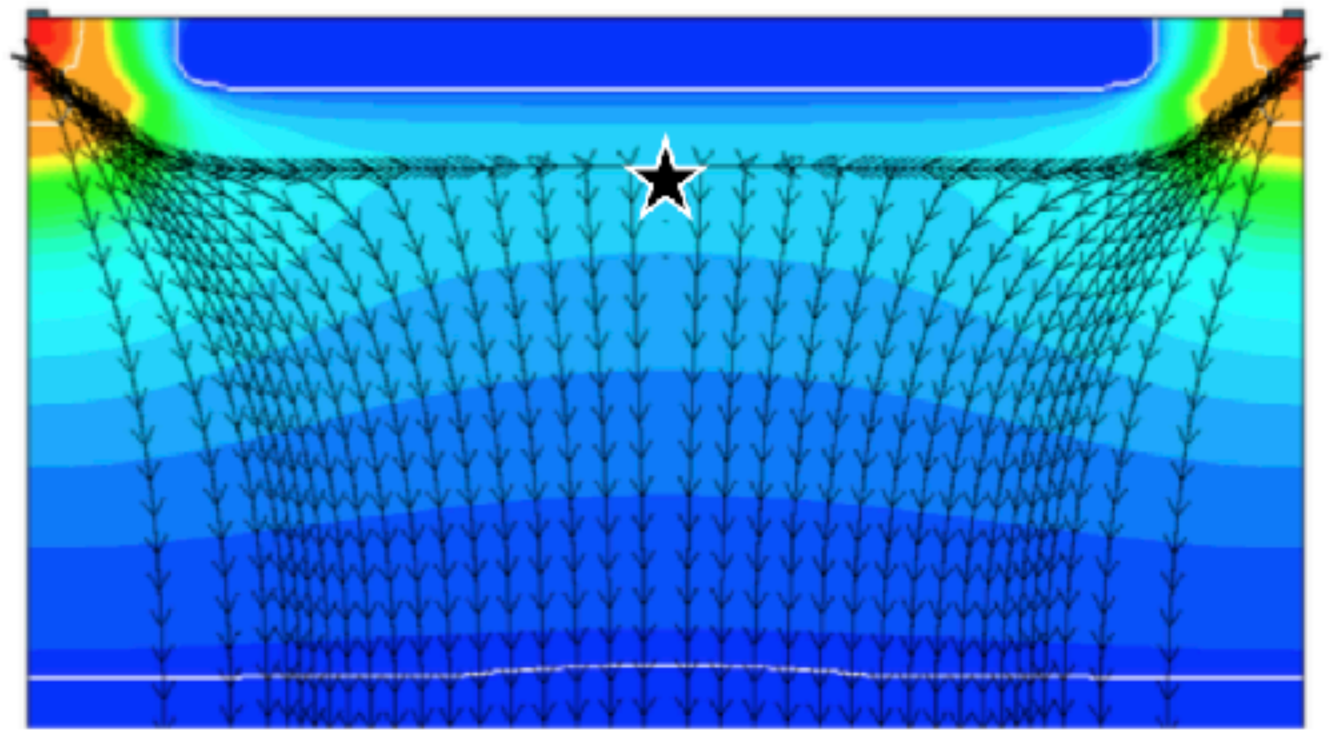
Additional vertical junctions in corners
→ Increased field towards c-electrode

Electrostatic potential, depletion, electric field streamlines and electric field minimum:

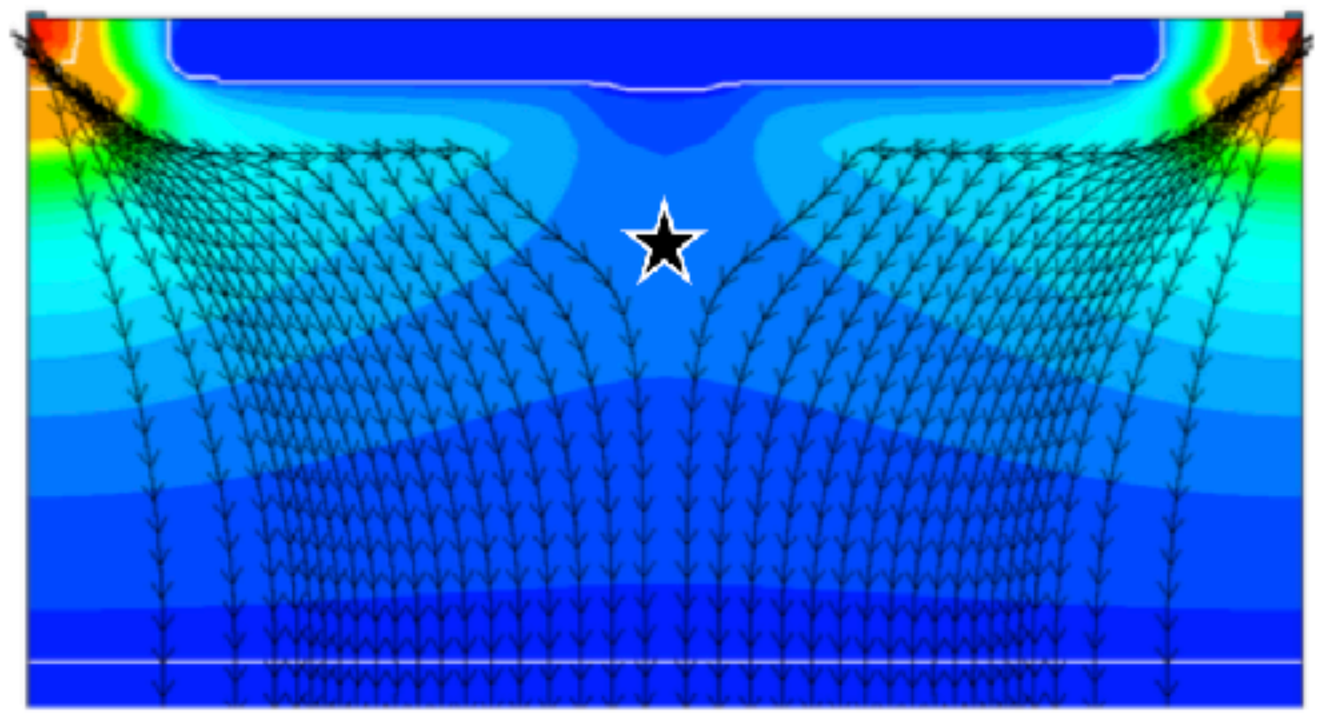
Standard process:



Modified process:



Gap in deep n-implant:



Pitch of 36.4µm, voltage p-well/substrate = -6V/-6V

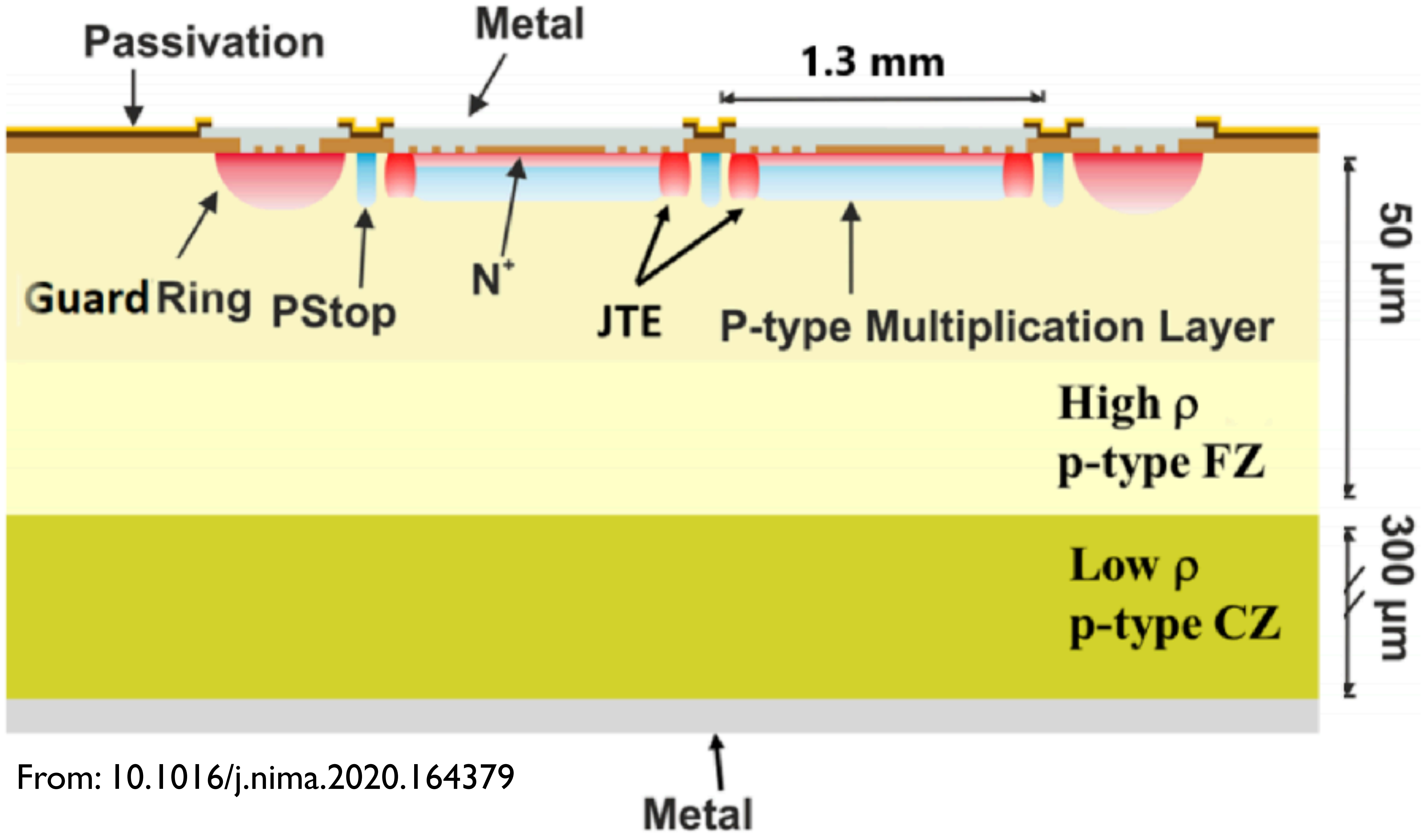
Evolution of technology towards HEP requirements (radiation tolerance, fast charge collection) based on 3D TCAD

LGAD - UFSD

From:
An Introduction to Ultra-Fast Silicon Detectors,
Marco Ferrero, Roberta Arcidiacono, Marco Mandurrino, Valentina Sola, Nicolò Cartiglia

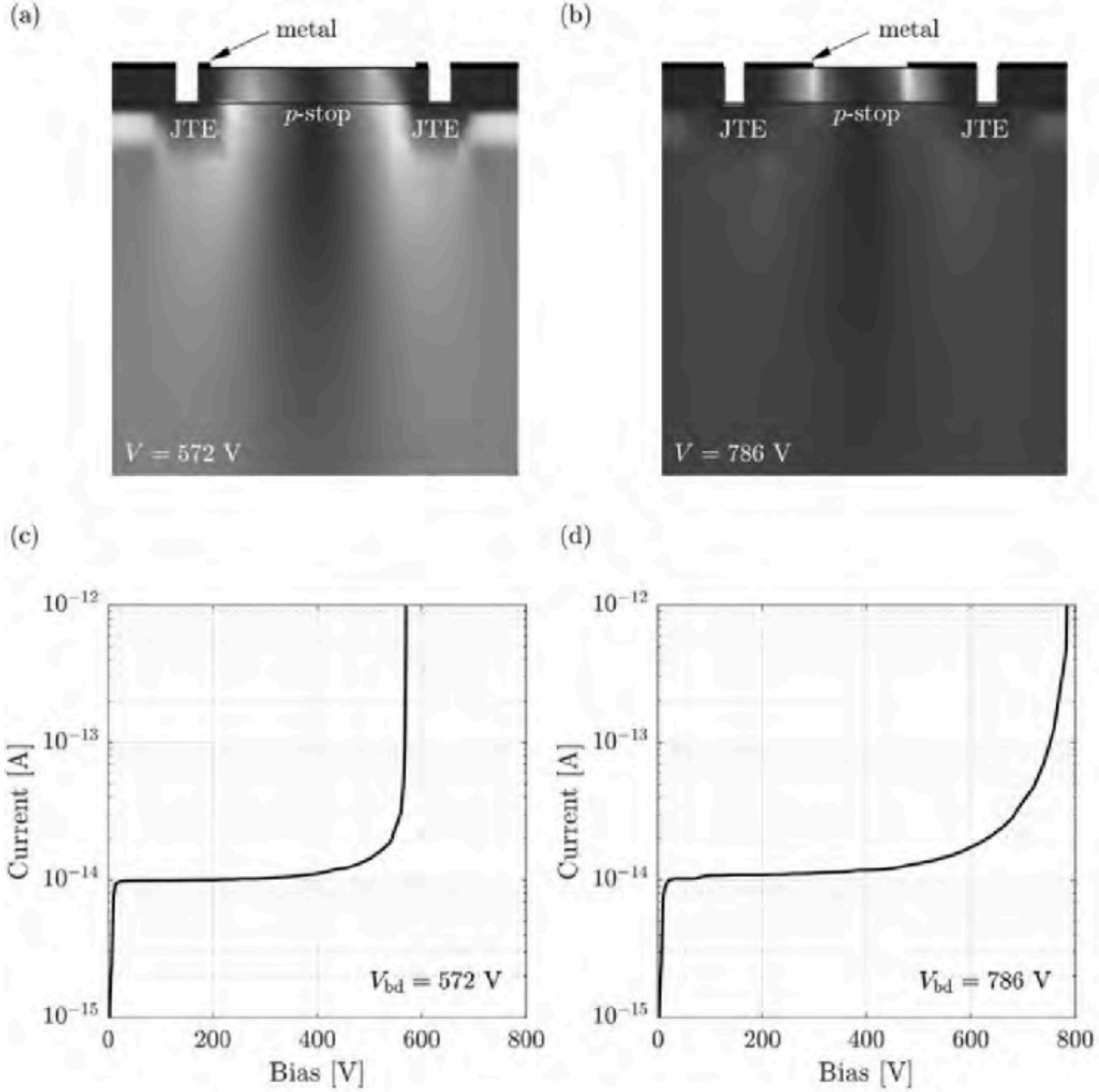
Ultra Fast Silicon Detectors UFSD:

Pixelated LGAD sensors with Junction Termination Extension (JTE) at pixel edges:



From: 10.1016/j.nima.2020.164379

Electric field from SDEVICE TCAD simulations:



→ Earlier breakdown for smaller metal overhang → TCAD used to significantly improve performance.

PicoAD - electric field

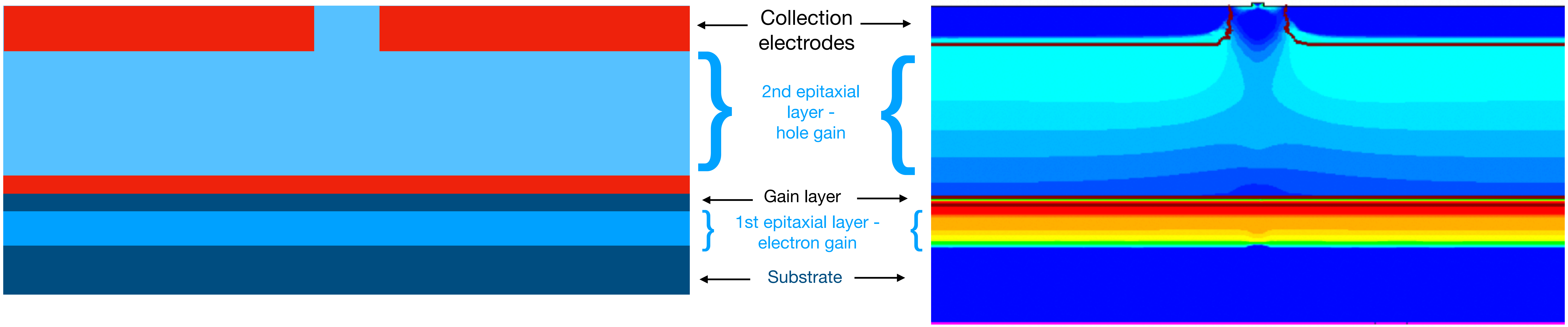
Picosecond Avalanche Detector (PicoAD): EU Patent EP18207008.6

Picosecond time stamping combined with high spatial precision in a fully monolithic design:

Realised by Hetrojunction Bipolar Transistors HBTs transistors and deep multi-junction sensor concept:

Schematic process cross section:

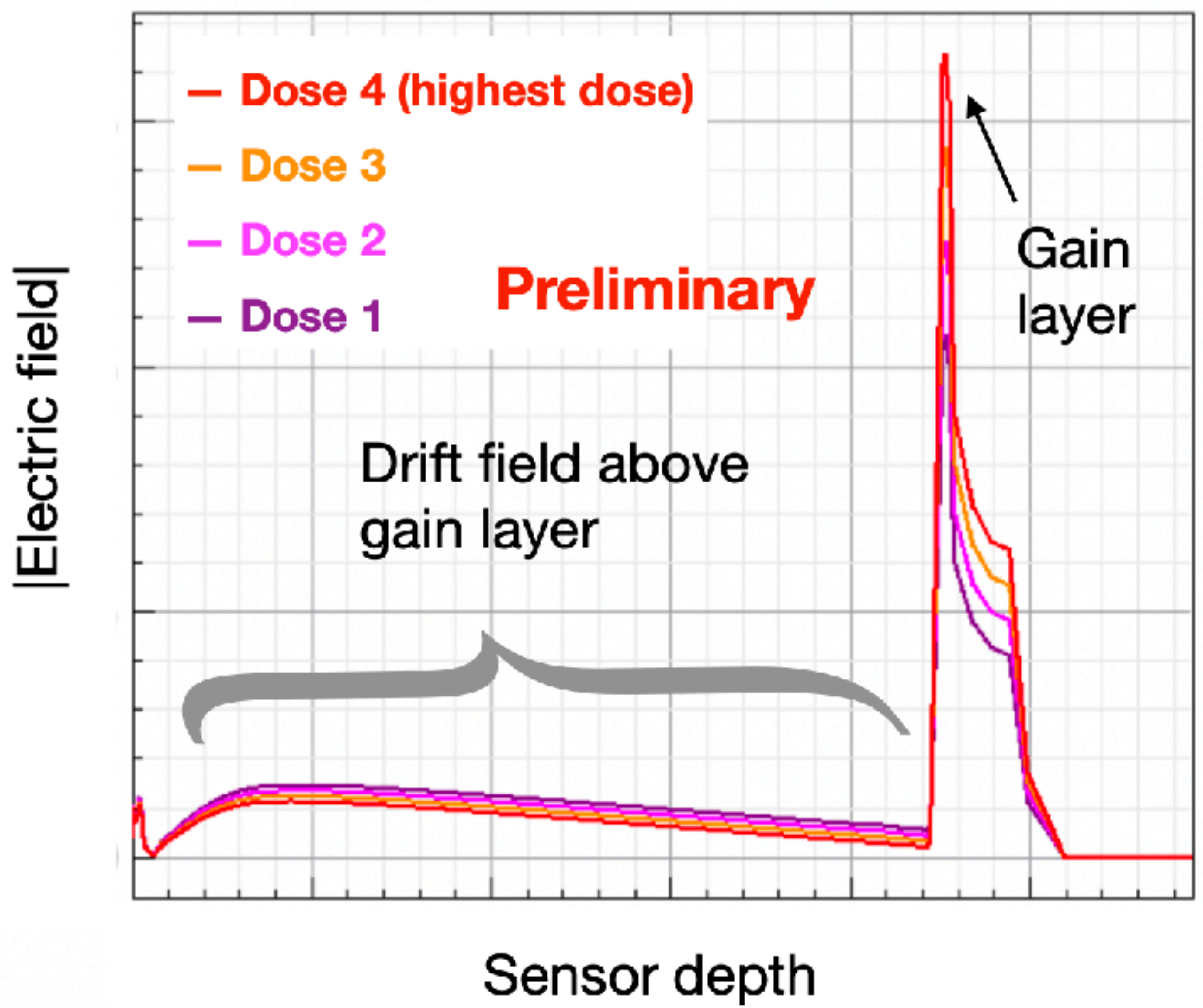
Cross section through 3D TCAD simulations - electric field:



→ Complex electric field due to multi-junction process, needs to be modelled in 3D TCAD.

PicoAD - gain layer optimisation

Electric field for different gain layer doses at -240V:



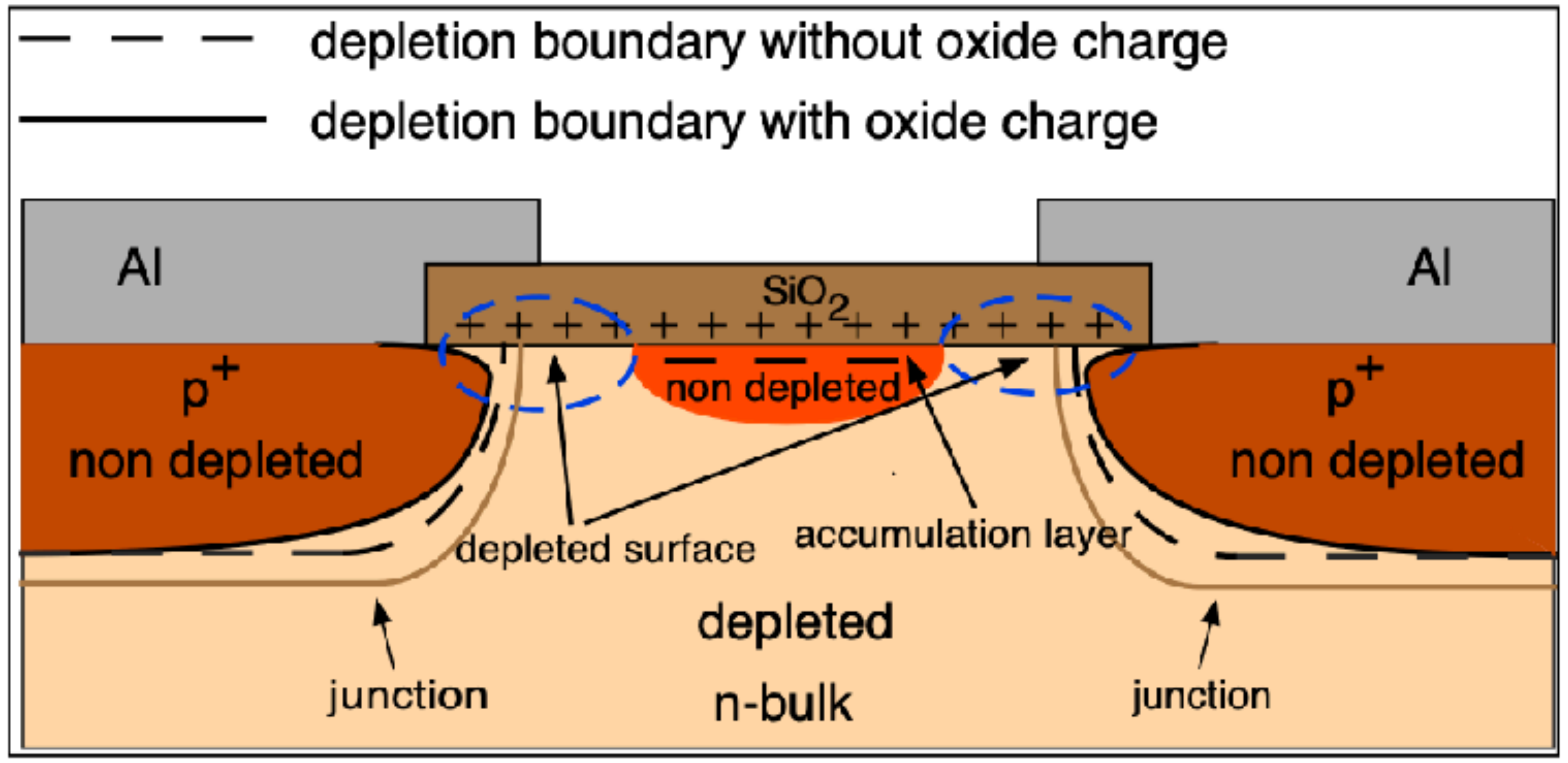
At a fixed sensor bias voltage:

- Field in the gain layer is higher for higher gain layer doses
- Field in drift region is lower for higher gain layer doses

→ If the field breakdown is limited by the breakdown in the gain layer it is best to go to the lowest gain layer dose possible to build up the electric field in the drift region

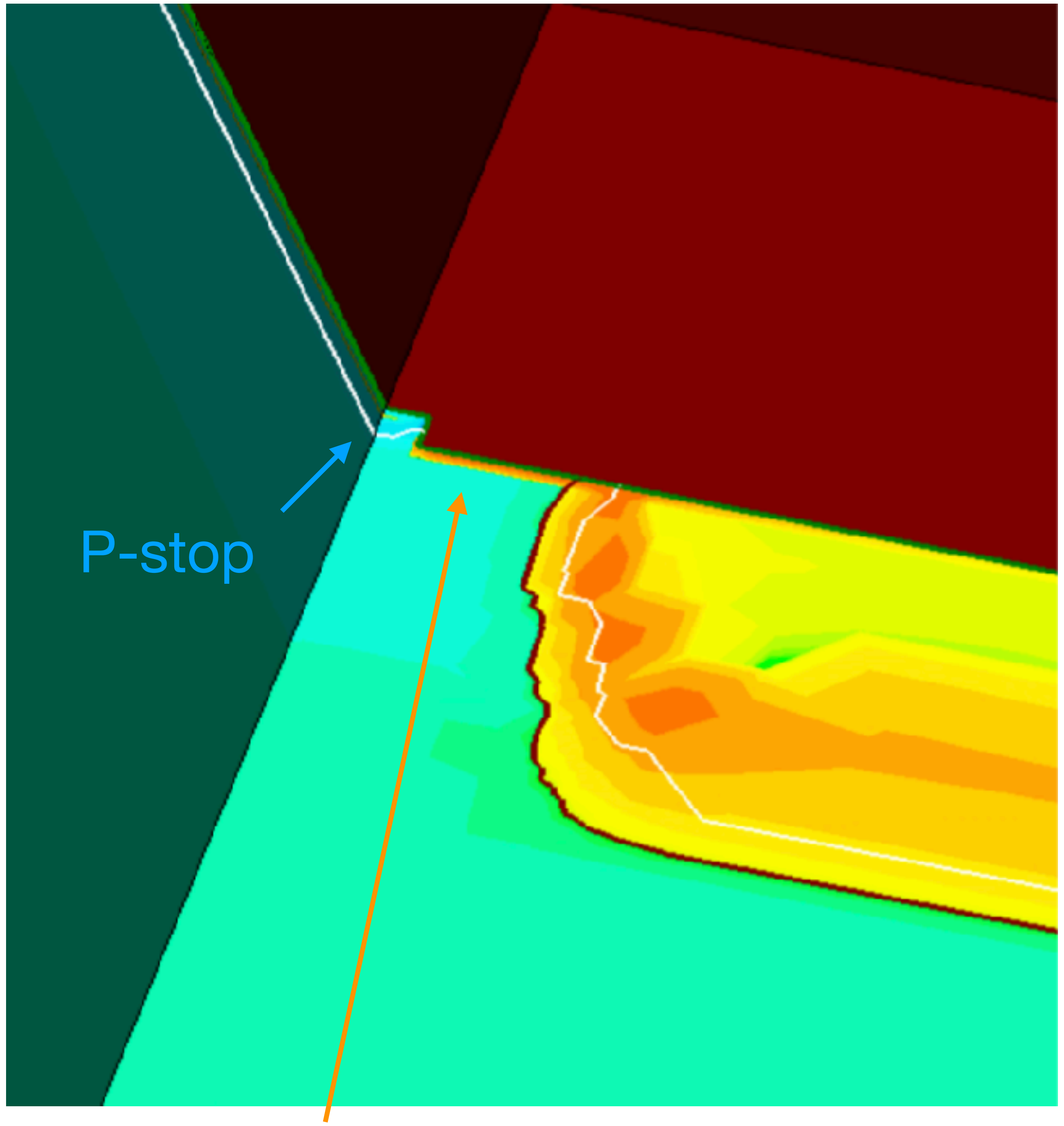
Silicon/oxide interface

Schematic cross section of inter pixel region:



- Depending on ratio of oxide charge to silicon doping at interface also relevant before irradiation
- Thin inversely doped channel can change filed, depletion, surface current and breakdown voltage

3D TCAD - space charge in inter pixel region:



← Oxide

← Collection electrode

Thin channel of high negative space charge, attracted by positive space charge in oxide

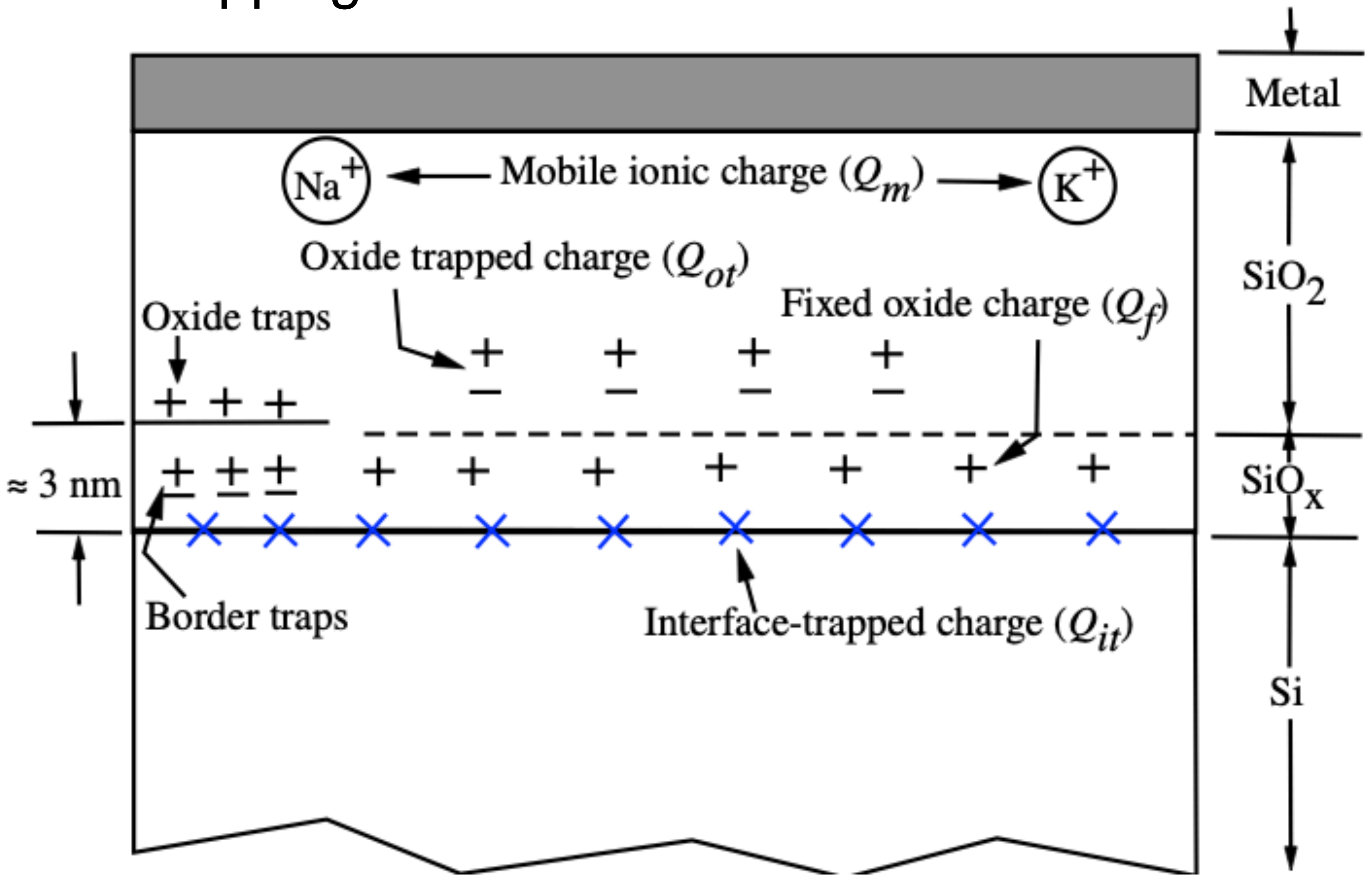
Radiation damage

From:
A new model for the TCAD simulation of the silicon damage by high fluence proton irradiation, J. Schwandt et. al

Surface damage modelling

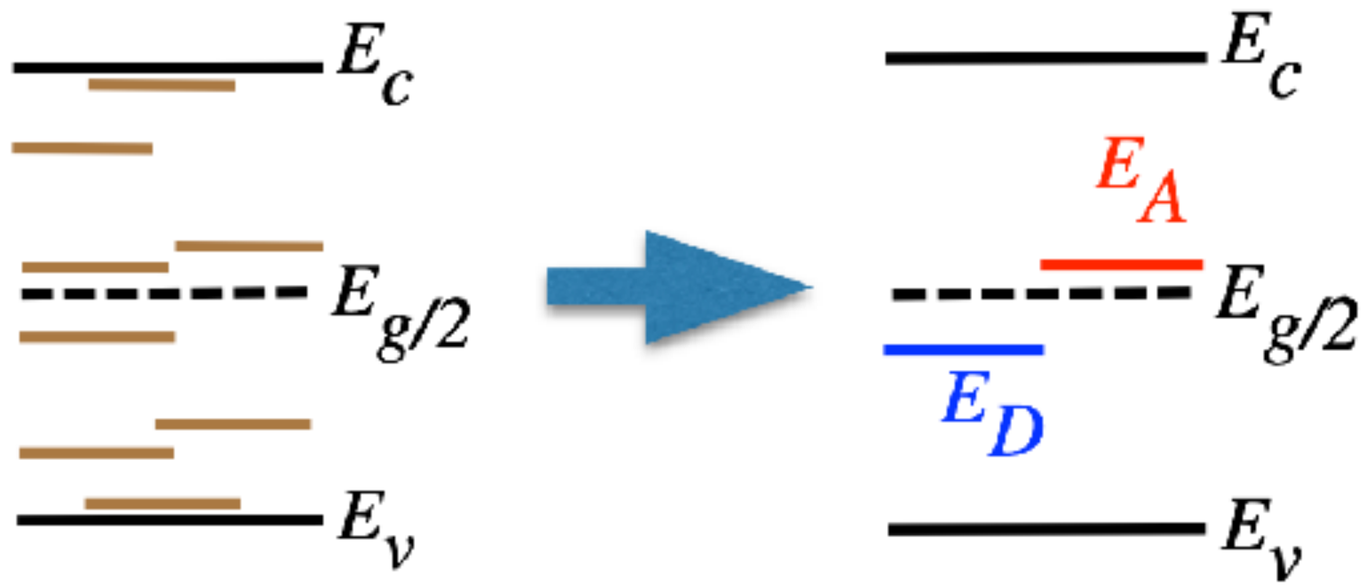
Oxide charges and interface traps build up at interface to silicon:

- Increasing surface current
- Electric field changes near silicon-oxide interface
- Trapping near to the silicon-oxide interface

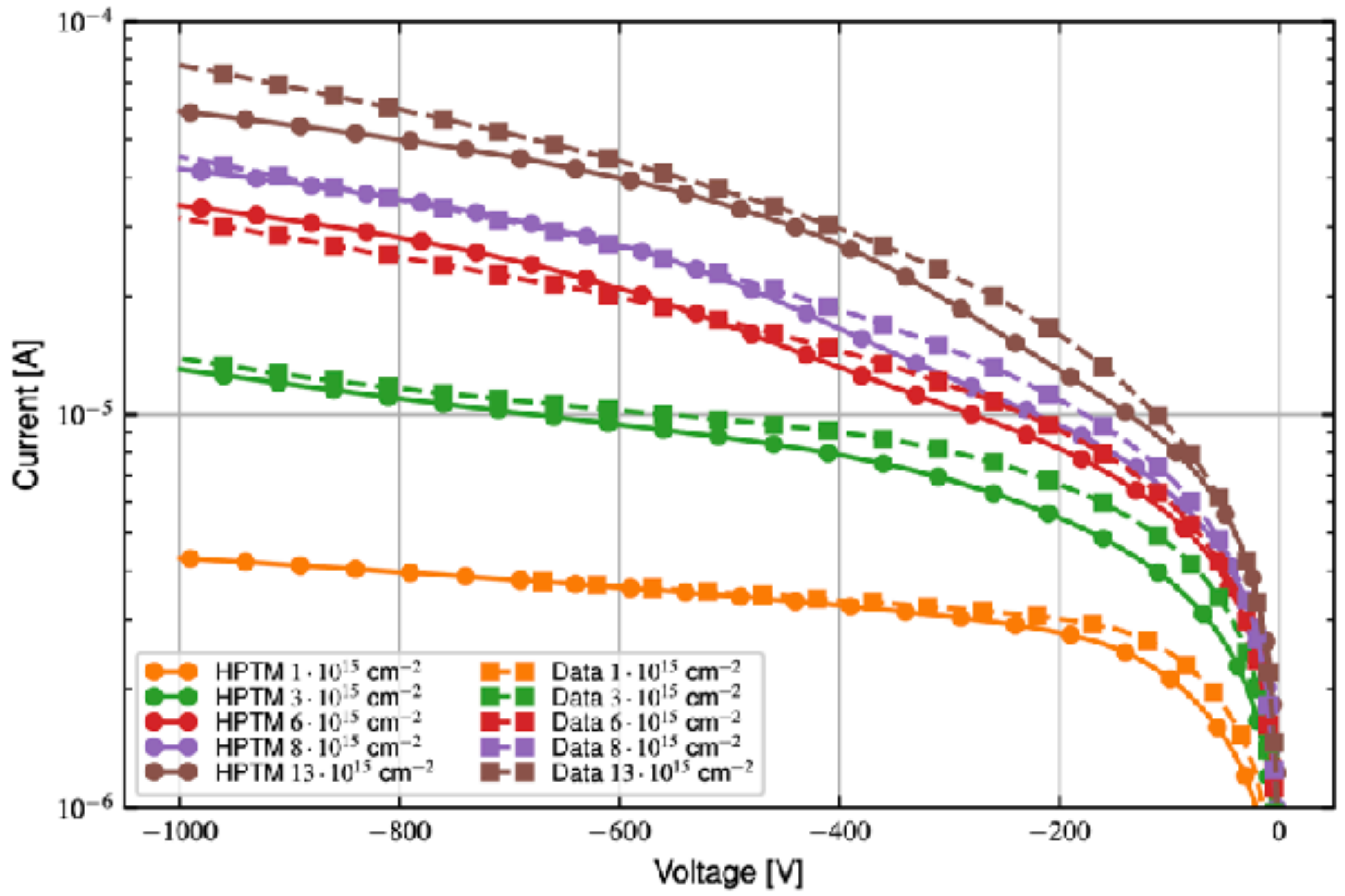


Bulk damage modelling:

Modelling of effective trap levels:



Example results - comparison TCAD/data:



→ Large effort for characterisation and modelling of radiation damage in silicon detectors within RD50 collaboration.

Transient simulations

- SDEVICE simulations for HEP in Synopsys Sentaurus -

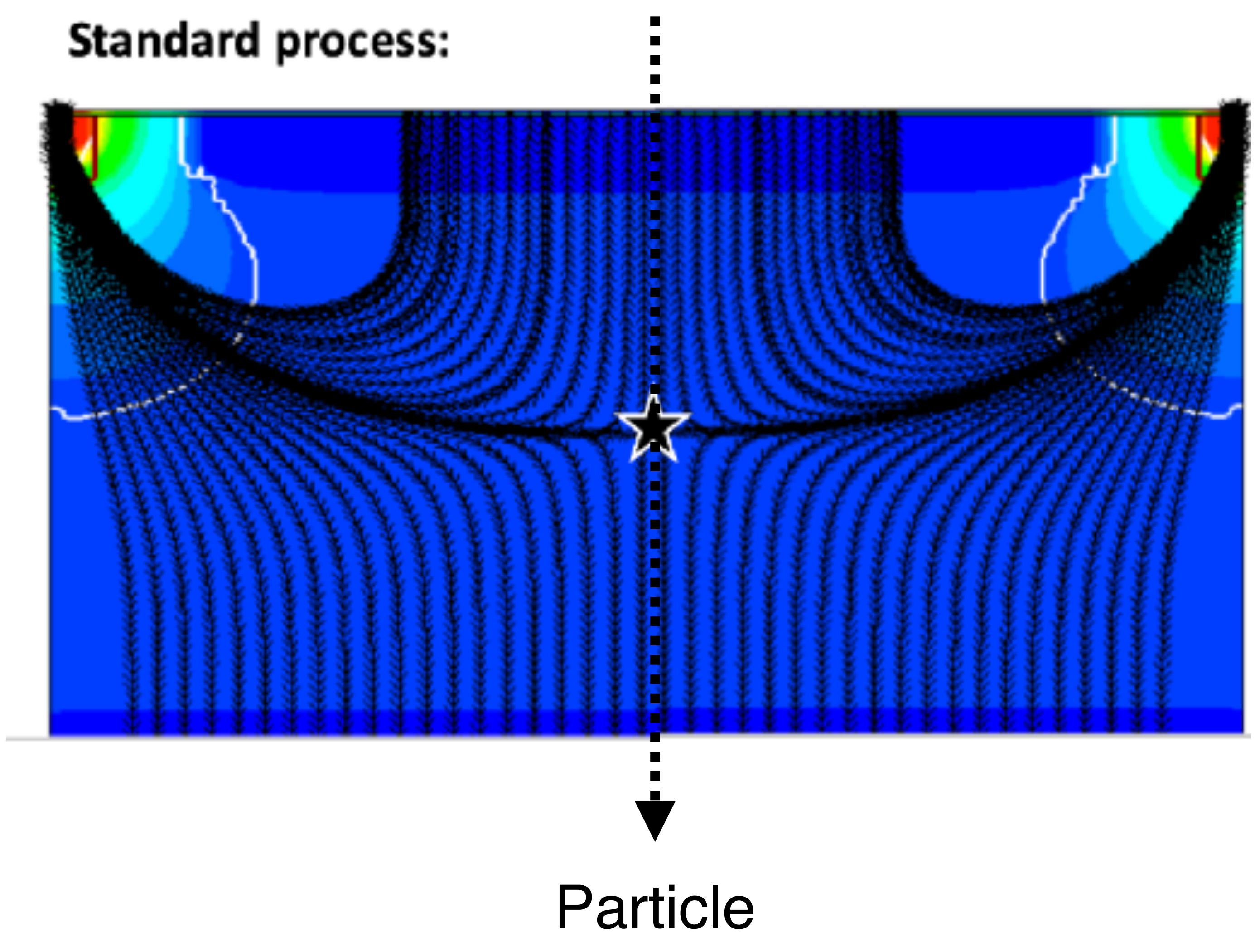
Aim:
Understand response of device to particle hits

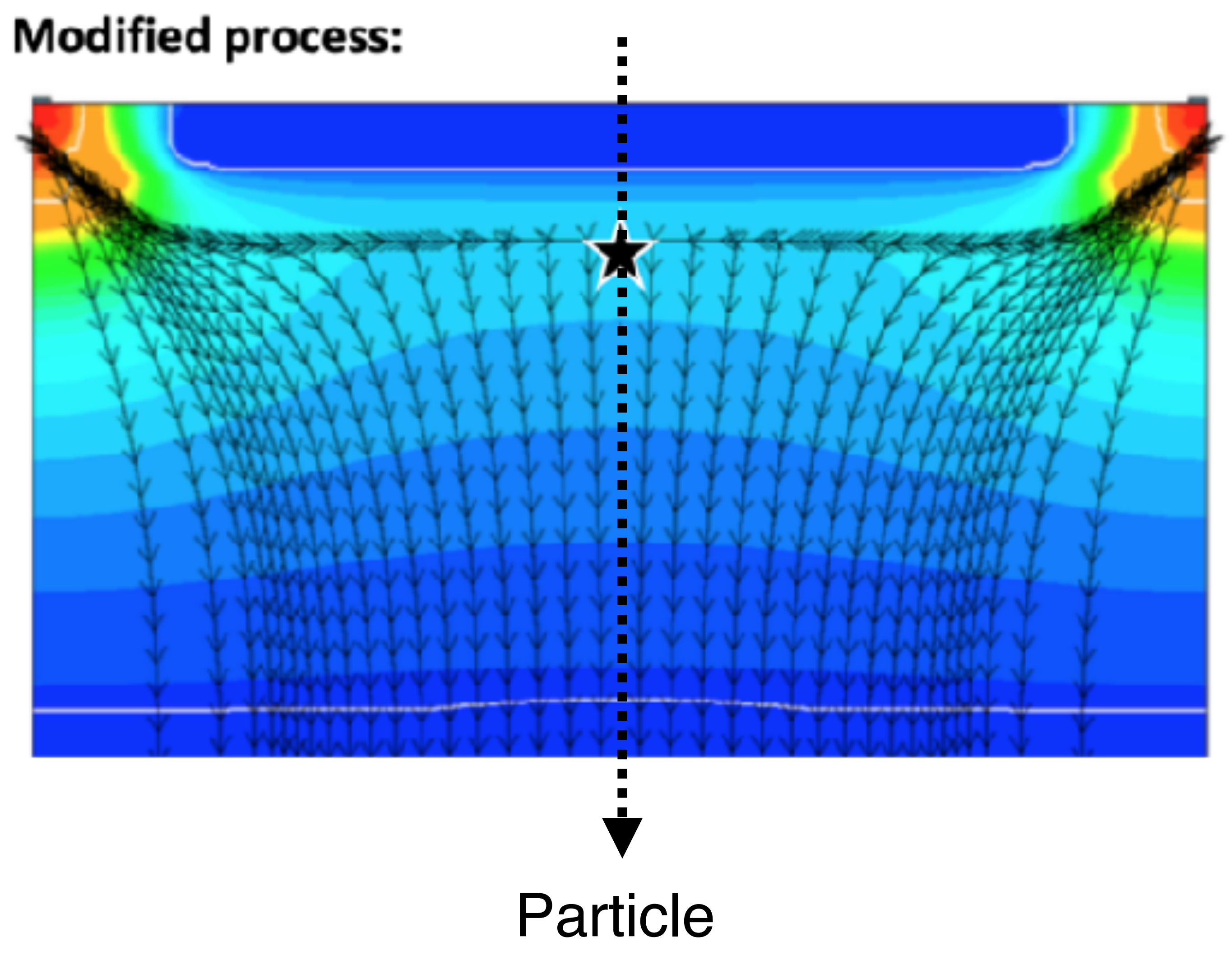
Increasing relevant in HEP due to advanced sensors needed to reach ambitious requirements of future silicon detectors in HEP

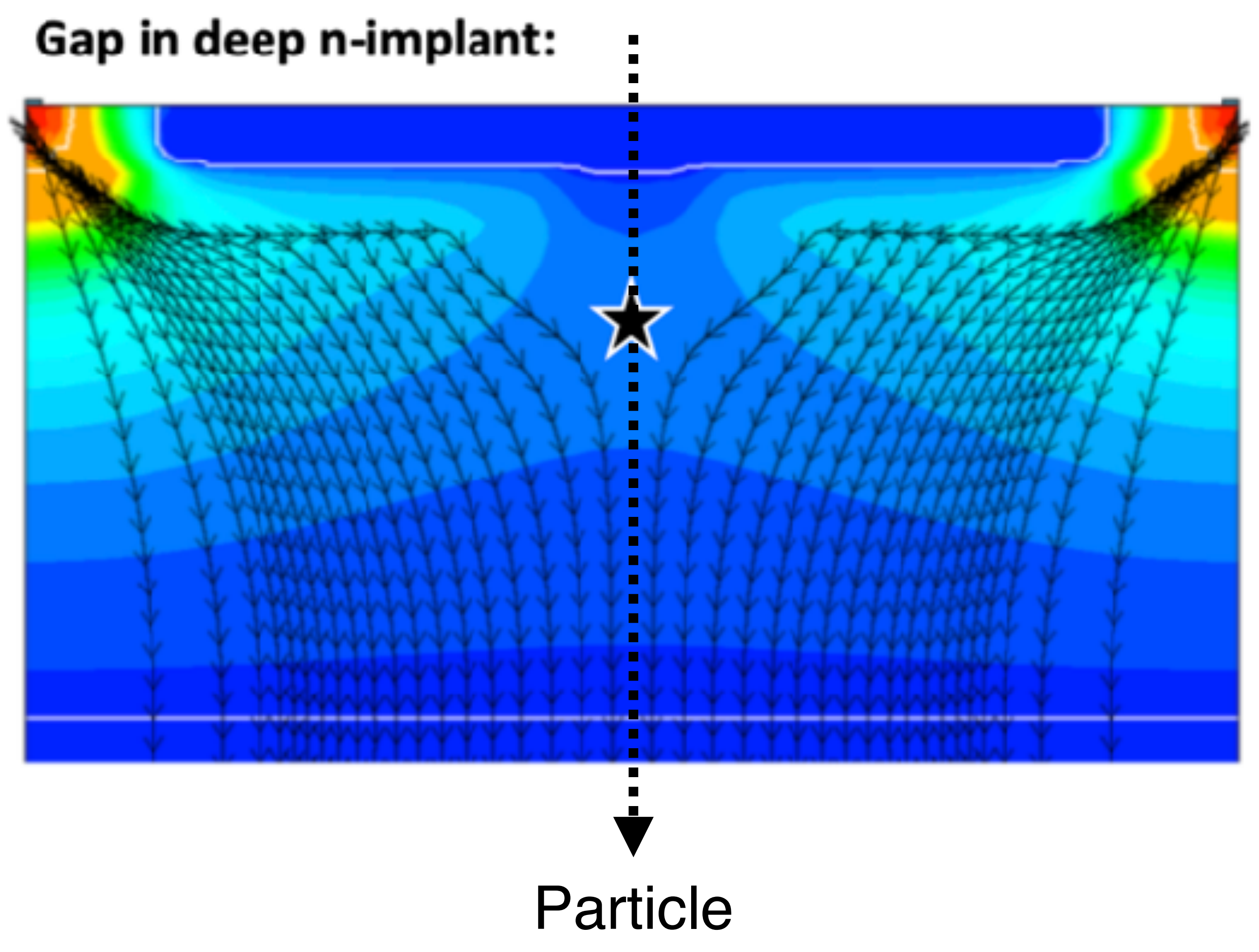
Small collection electrode CMOS

SDEVICE HeavyIon simulation in Synopsys Sentaurus

Electrostatic potential (color scale), depletion (white line), electric field streamlines (black arrows) and electric field minimum (star symbol):


Standard process:


Modified process:

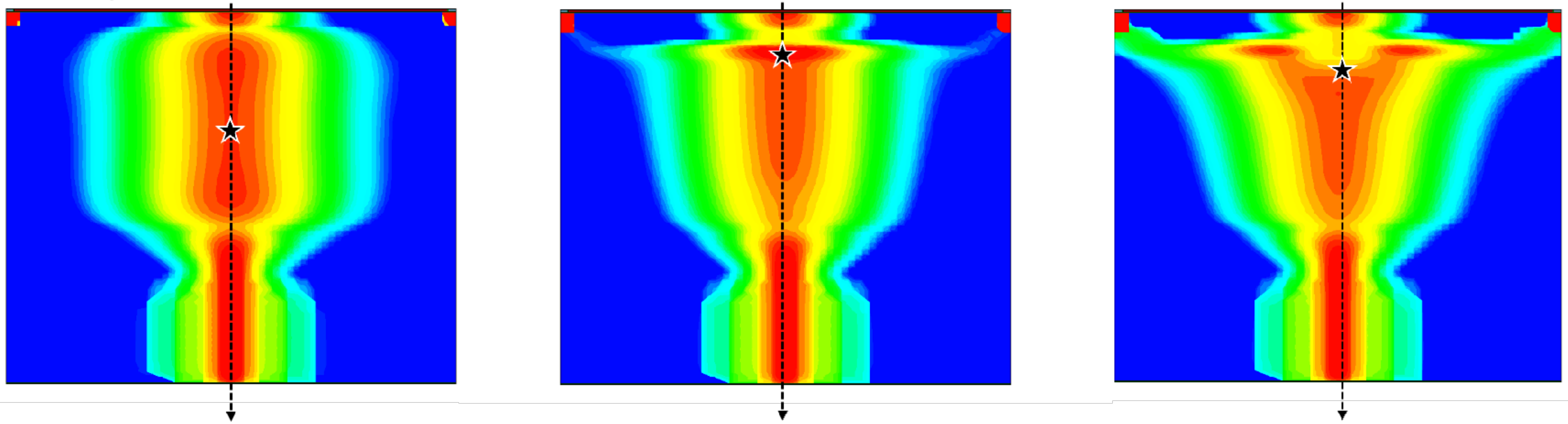

Gap in deep n-implant:

→ Simulation of particle traversing pixel corner.

Small collection electrode CMOS

Additional sensor optimization – mitigation of field minimum

Electron density **0.5ns after signal generation** for the different sensor designs:



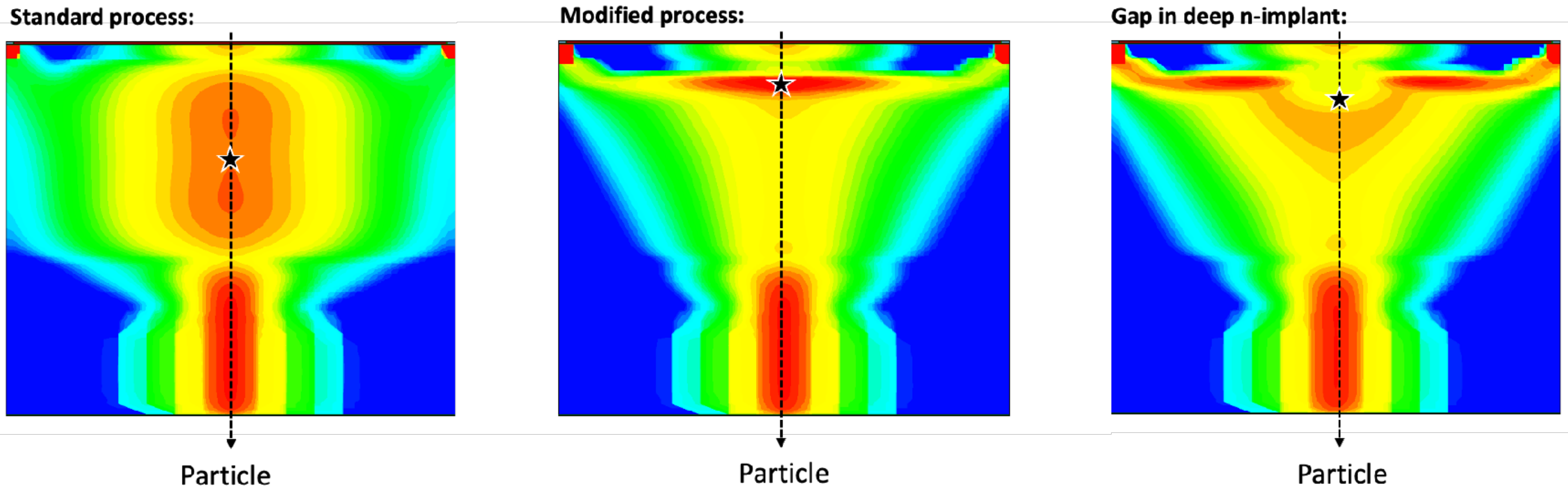
Standard process: **Modified process:** **Gap in deep n-implant:**

★ = electric field minimum

Small collection electrode CMOS

Additional sensor optimization – mitigation of field minimum

Electron density **1.5ns after signal generation** for the different sensor designs:

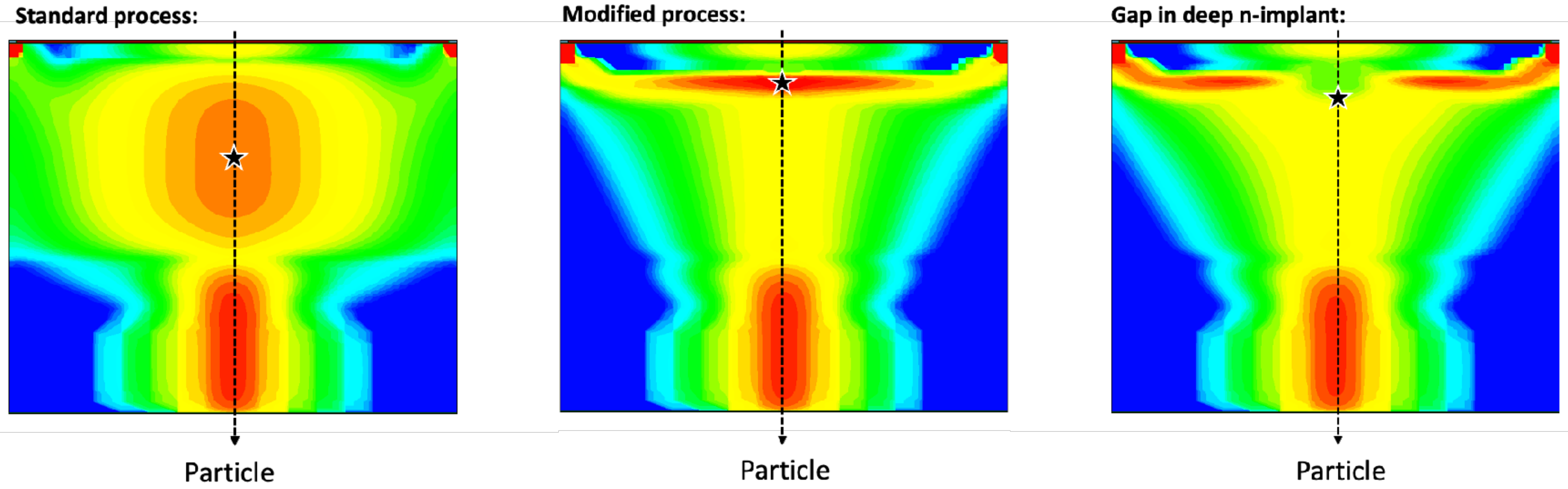


★ = electric field minimum

Small collection electrode CMOS

Additional sensor optimization – mitigation of field minimum

Electron density **2.5ns after signal generation** for the different sensor designs:

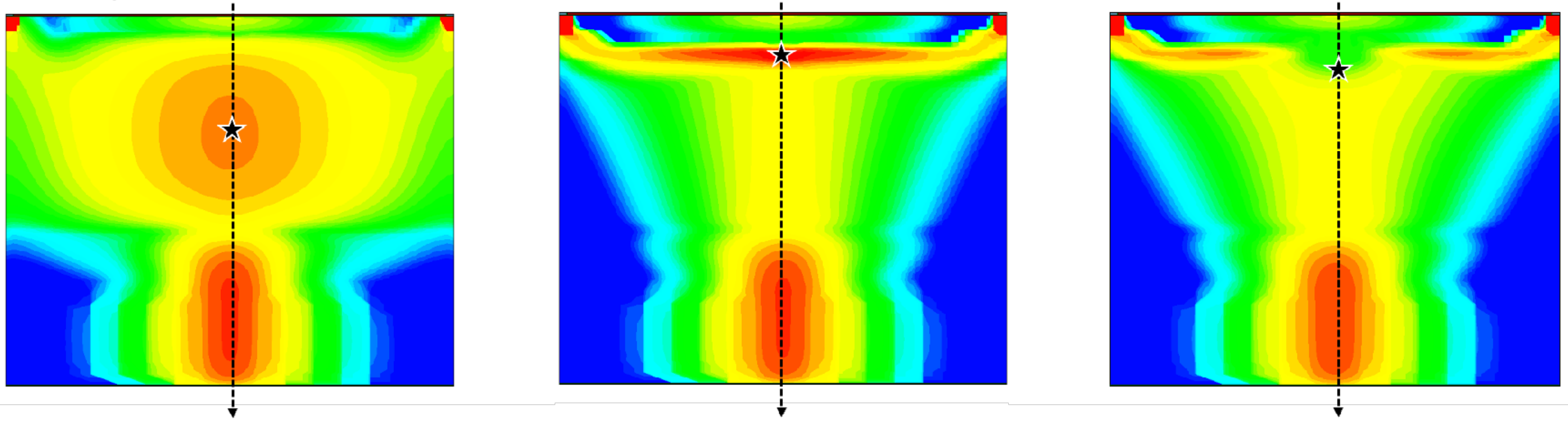


★ = electric field minimum

Small collection electrode CMOS

Additional sensor optimization – mitigation of field minimum

Electron density **3.5ns after signal generation** for the different sensor designs:



Standard process:

Modified process:

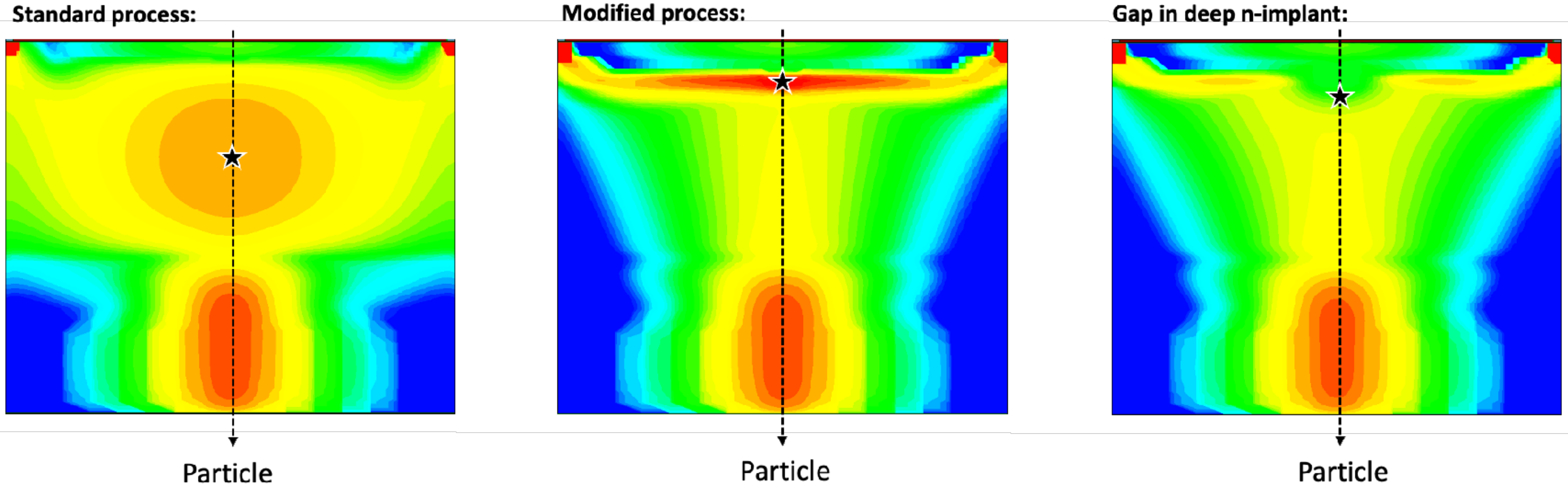
Gap in deep n-implant:

★ = electric field minimum

Small collection electrode CMOS

Additional sensor optimization – mitigation of field minimum

Electron density **4.5ns after signal generation** for the different sensor designs:

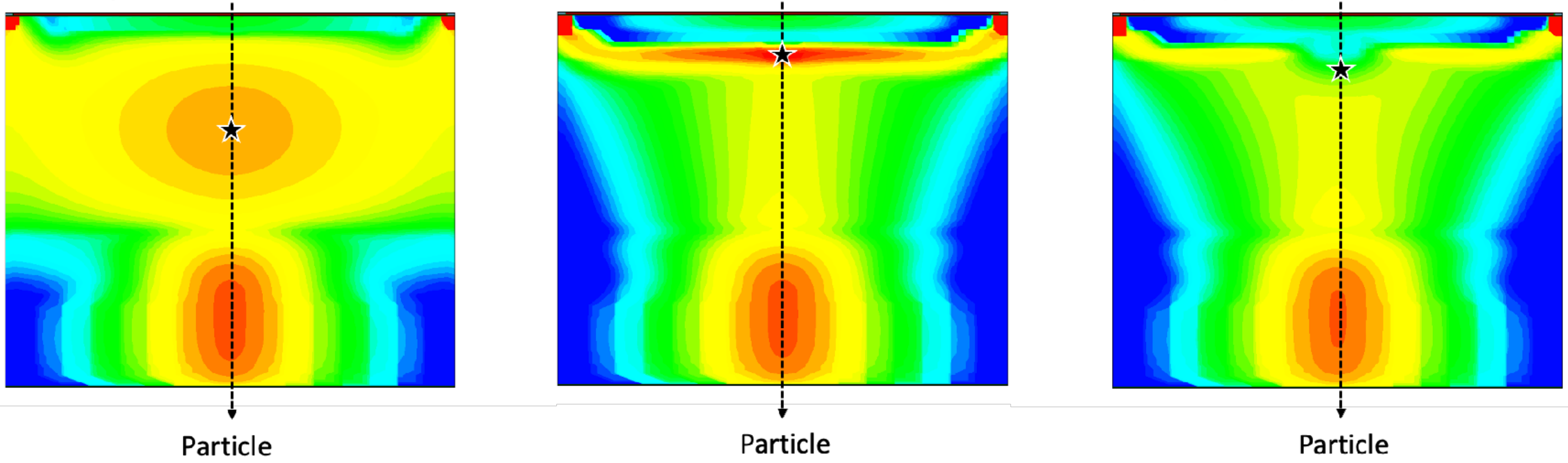


★ = electric field minimum

Small collection electrode CMOS

Additional sensor optimization – mitigation of field minimum

Electron density **6.5ns after signal generation** for the different sensor designs:



Standard process:

Modified process:

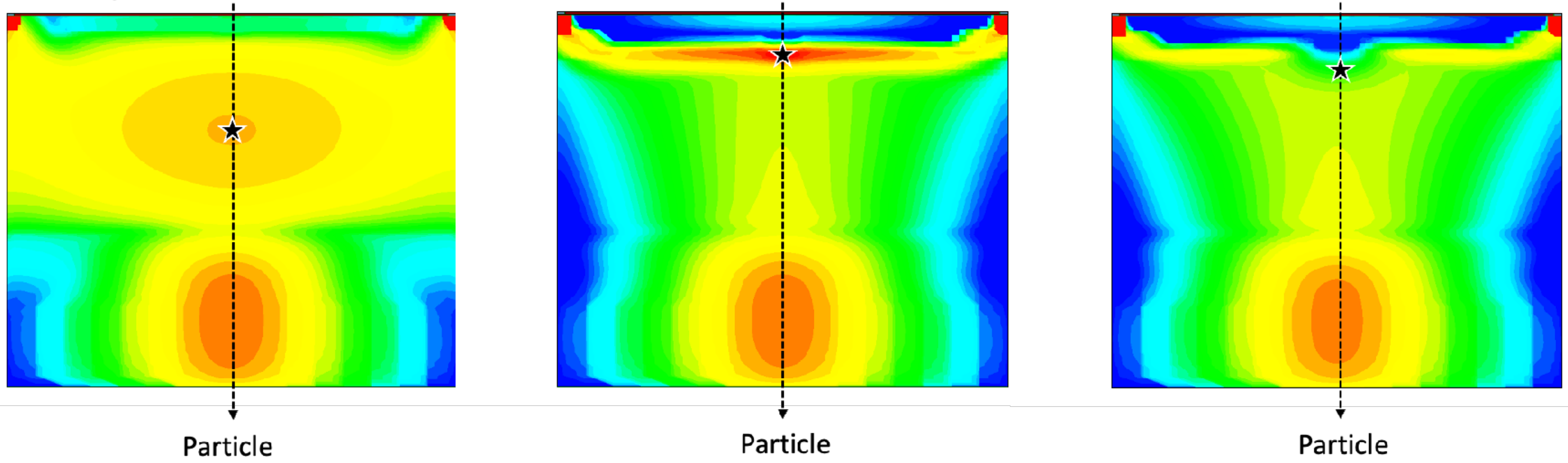
Gap in deep n-implant:

★ = electric field minimum

Small collection electrode CMOS

Additional sensor optimization – mitigation of field minimum

Electron density **9.5ns after signal generation** for the different sensor designs:



Standard process:

Modified process:

Gap in deep n-implant:

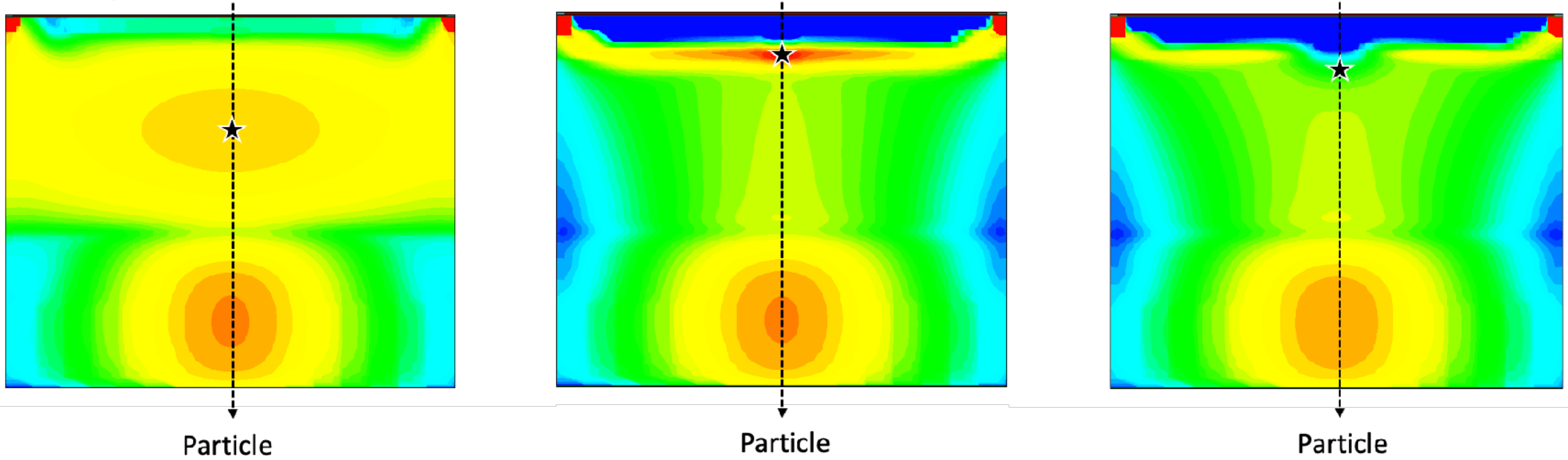
★ = electric field minimum

Small collection electrode CMOS

Additional sensor optimization – mitigation of field minimum

Electron density **14.5ns after signal generation** for the different sensor designs:

Standard process: **Modified process:** **Gap in deep n-implant:**



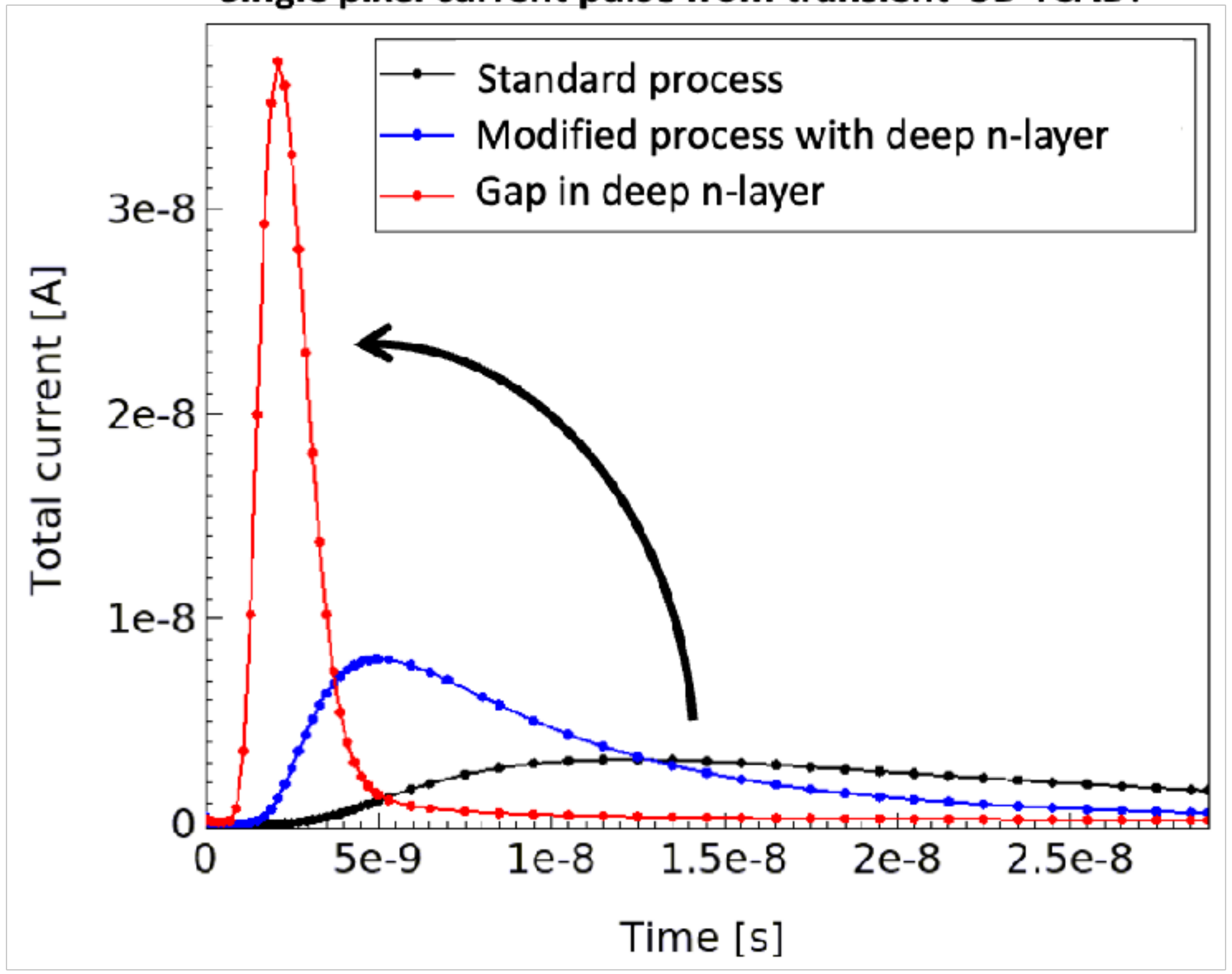
★ = electric field minimum

- The gap and the additional p-implant bent the streamlines away from the minimum to the collection electrodes
- Reduced drift path + charges do not get pushed and trapped in minimum
- Faster charge collection

Small collection electrode CMOS

Additional sensor optimization – mitigation of field minimum

Single pixel current pulse from transient 3D TCAD:



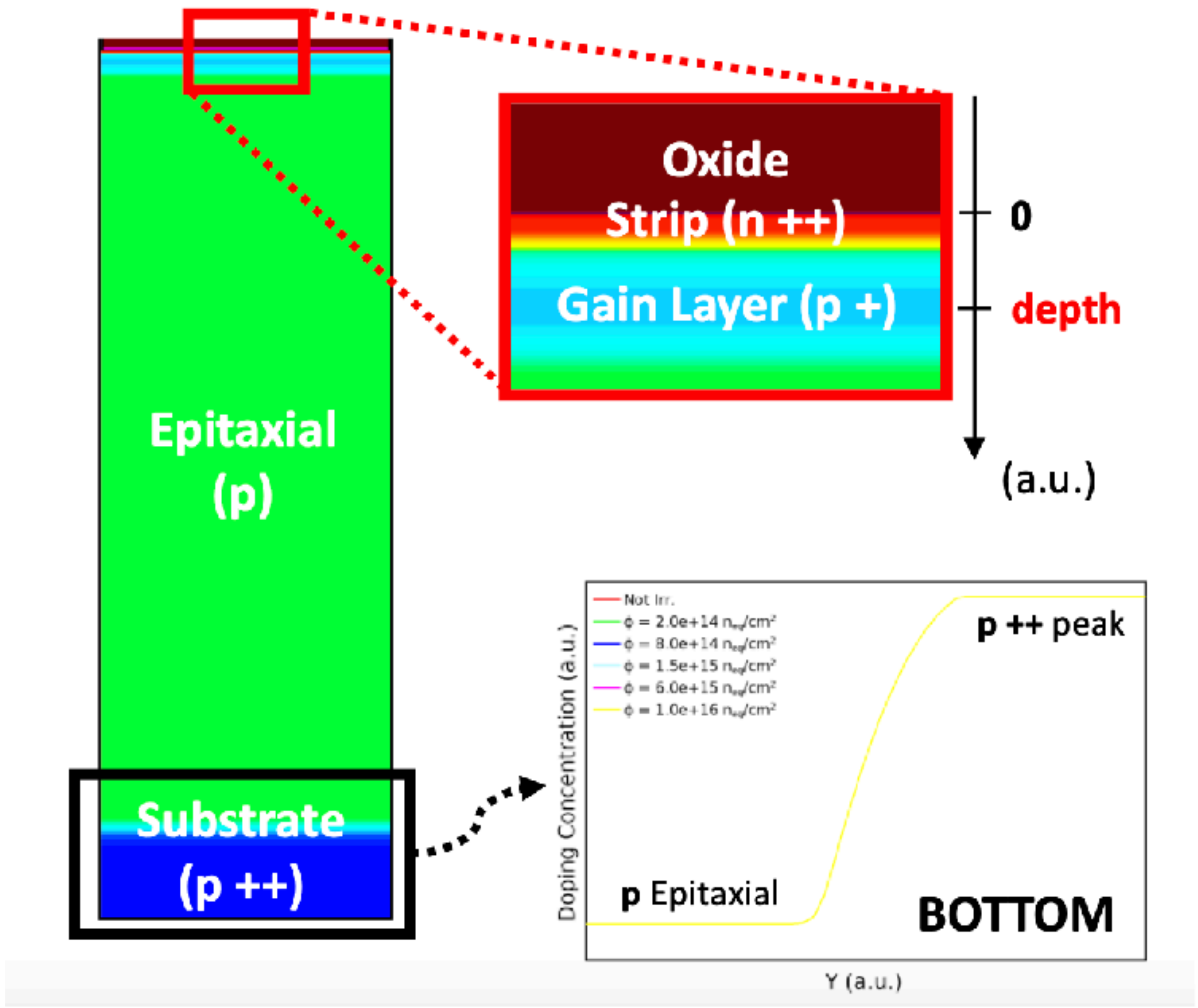
→ Mitigation of impact of electric field minimum on charge collection, order of magnitude improvement in charge collection speed

→ Significant improvement of time stamping capabilities, radiation hardness and efficiency for thin sensors

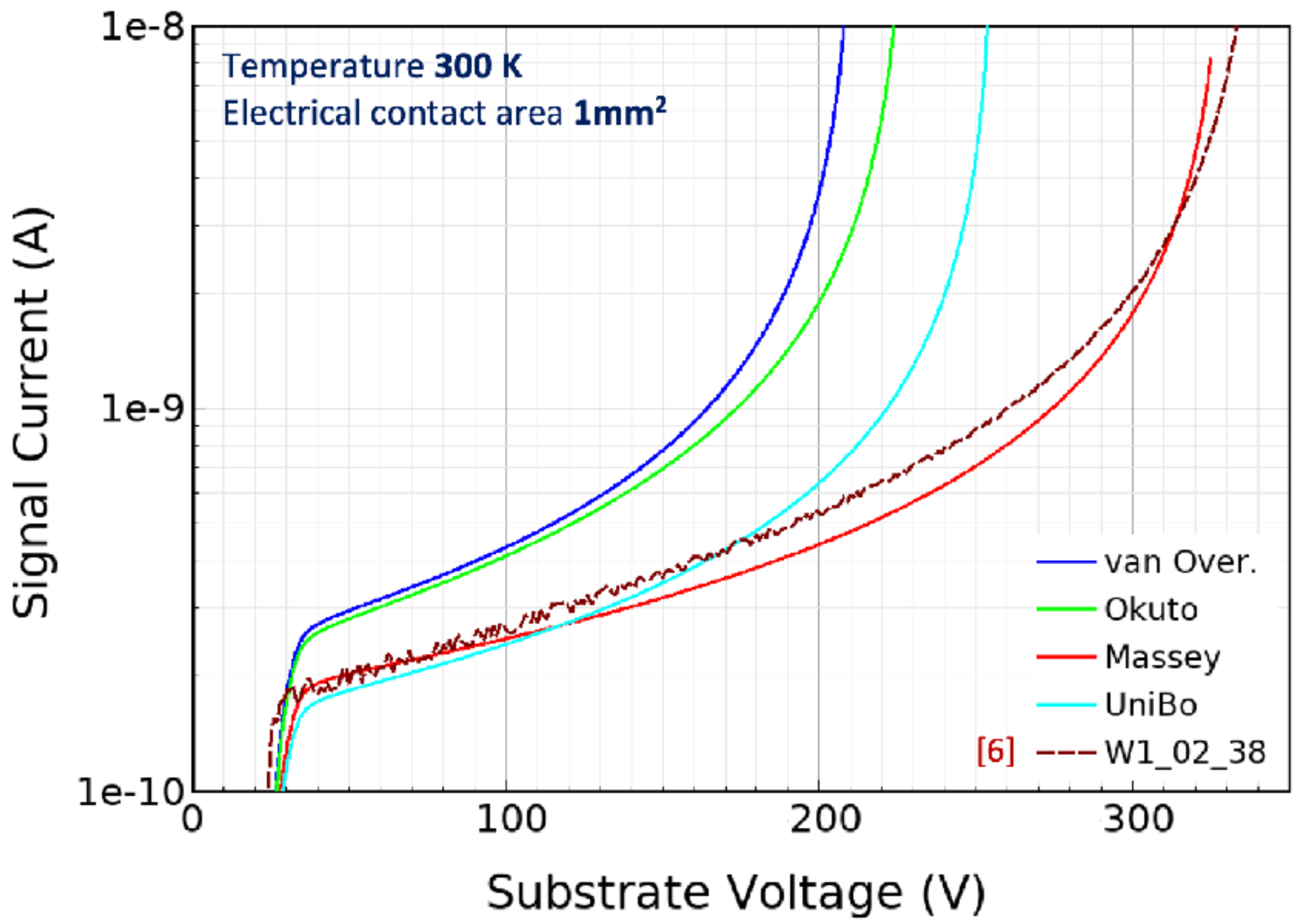
LGADs - model comparison

From:
TCAD numerical simulation of irradiated Low Gain Avalanche Diodes, T. Croci et. al

Simulated 2D structure:



Signal current simulated in TCAD with different models for the charge multiplication:



- Significant differences between different multiplication models

→ Important to select correct model for use case and tune parameter in parameter file sdevice.par against data

Space charge effects

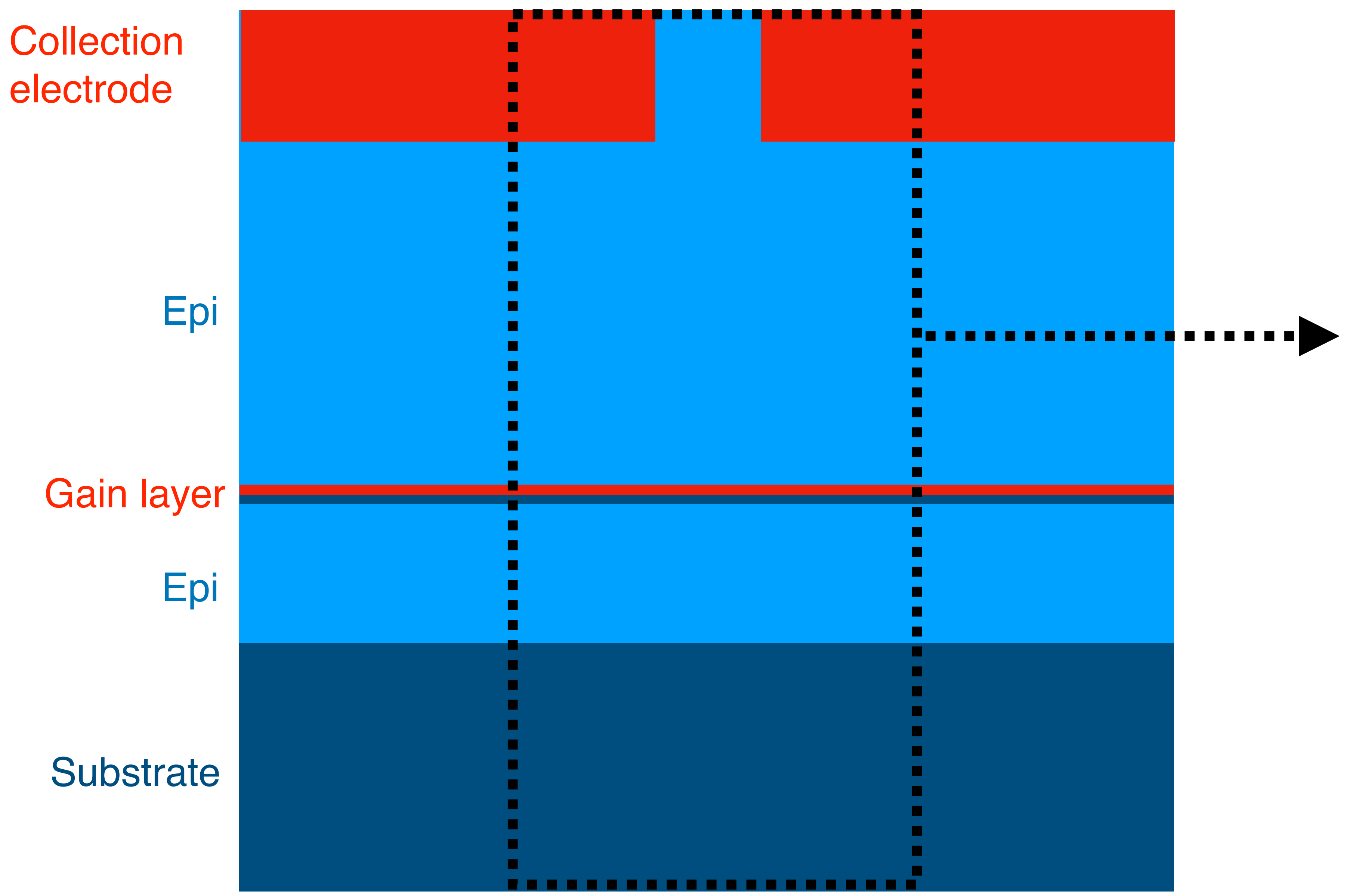
What are space charge effects?:

Transient high local charge densities that deform the electrostatic field

→ Deformation of field also changes drift behaviour (speed and direction) of signal charges

→ Impact on detector performance

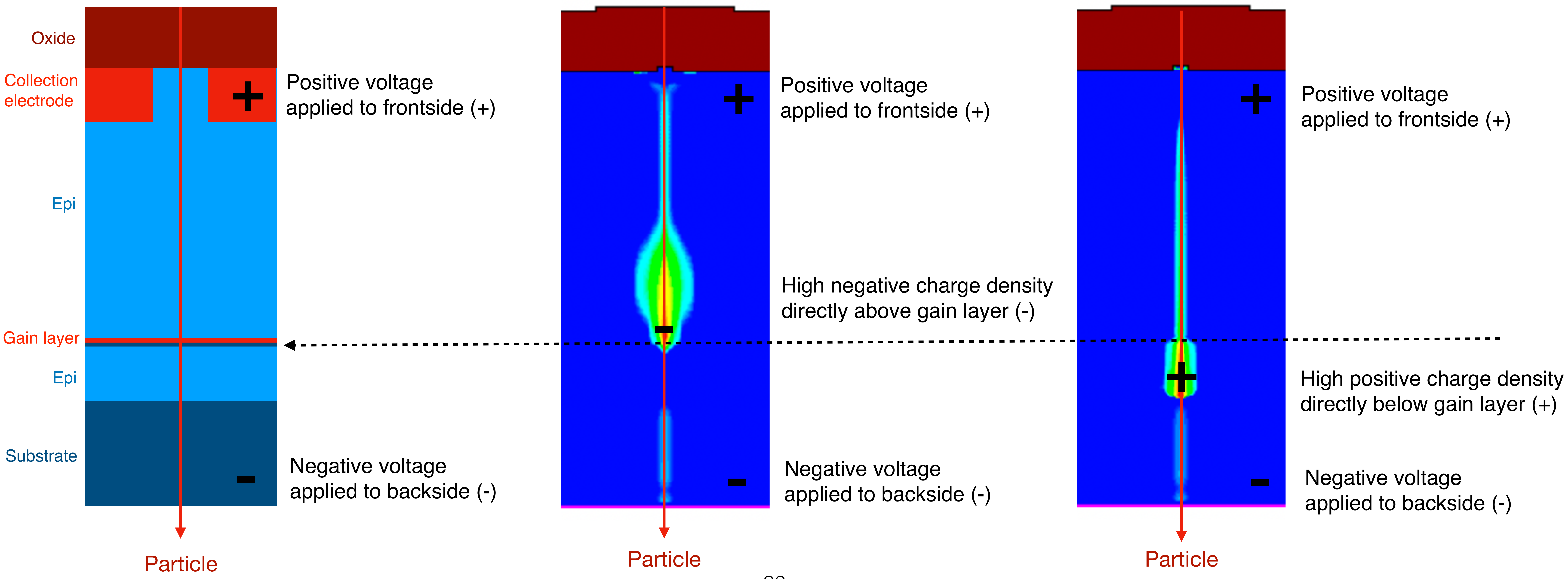
Example picosecond Avalanche Detector picoAD:



Section shown in next slides

Space charge effects in sensors with gain layer

Example - picosecond Avalanche Detector picoAD:



Process cross section:

E-density (before charge generation) -
E-density (10ps after charge generation):

H-density (before charge generation) -
H-density (10ps after charge generation):

Positive voltage applied to frontside (+)

Negative voltage applied to backside (-)

Positive voltage applied to frontside (+)

High negative charge density directly above gain layer (-)

Negative voltage applied to backside (-)

Positive voltage applied to frontside (+)

High positive charge density directly below gain layer (+)

Negative voltage applied to backside (-)

Space charge effects in sensors with gain layer

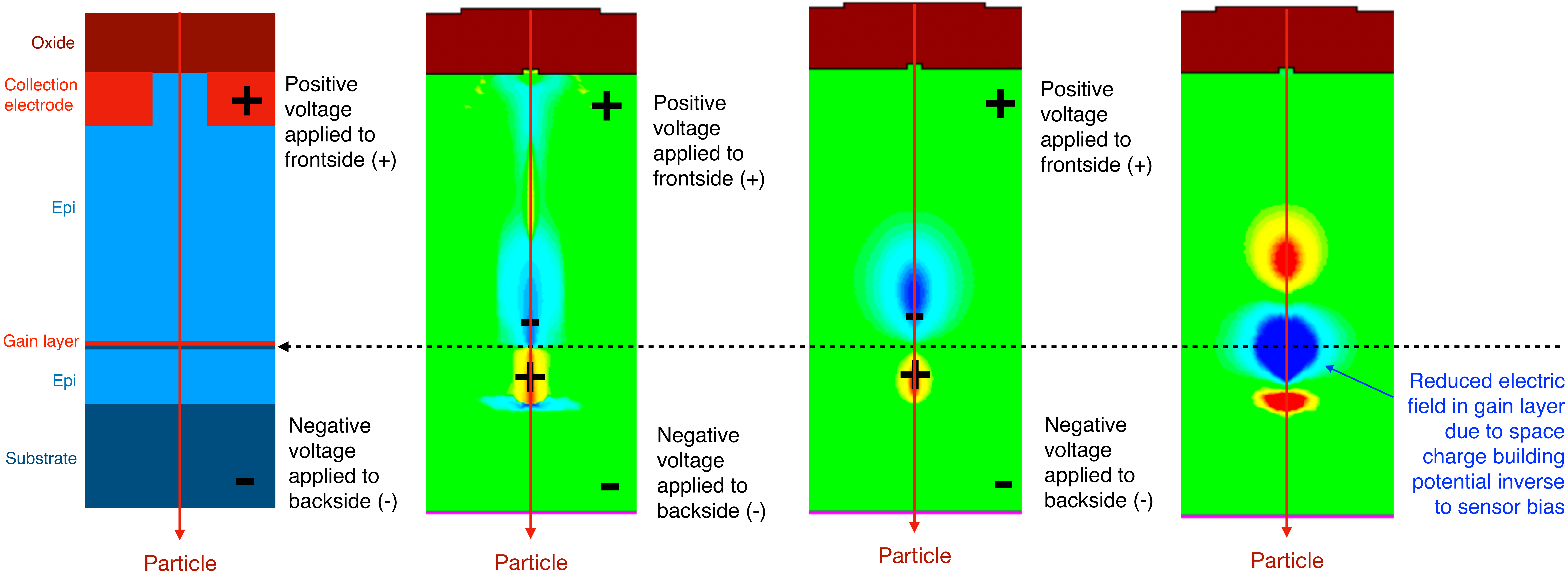
Example - picosecond Avalanche Detector picoAD:

Process cross section:

Space charge (before charge generation) - Space charge (10ps after charge generation):

E-potential (before charge generation) - E-potential (10ps after charge generation):

E-field (before charge generation) - E-field (10ps after charge generation):



Positive voltage applied to frontside (+)

Negative voltage applied to backside (-)

Positive voltage applied to frontside (+)

Negative voltage applied to backside (-)

Positive voltage applied to frontside (+)

Negative voltage applied to backside (-)

Reduced electric field in gain layer due to space charge building potential inverse to sensor bias

→ Transient field simulations necessary.

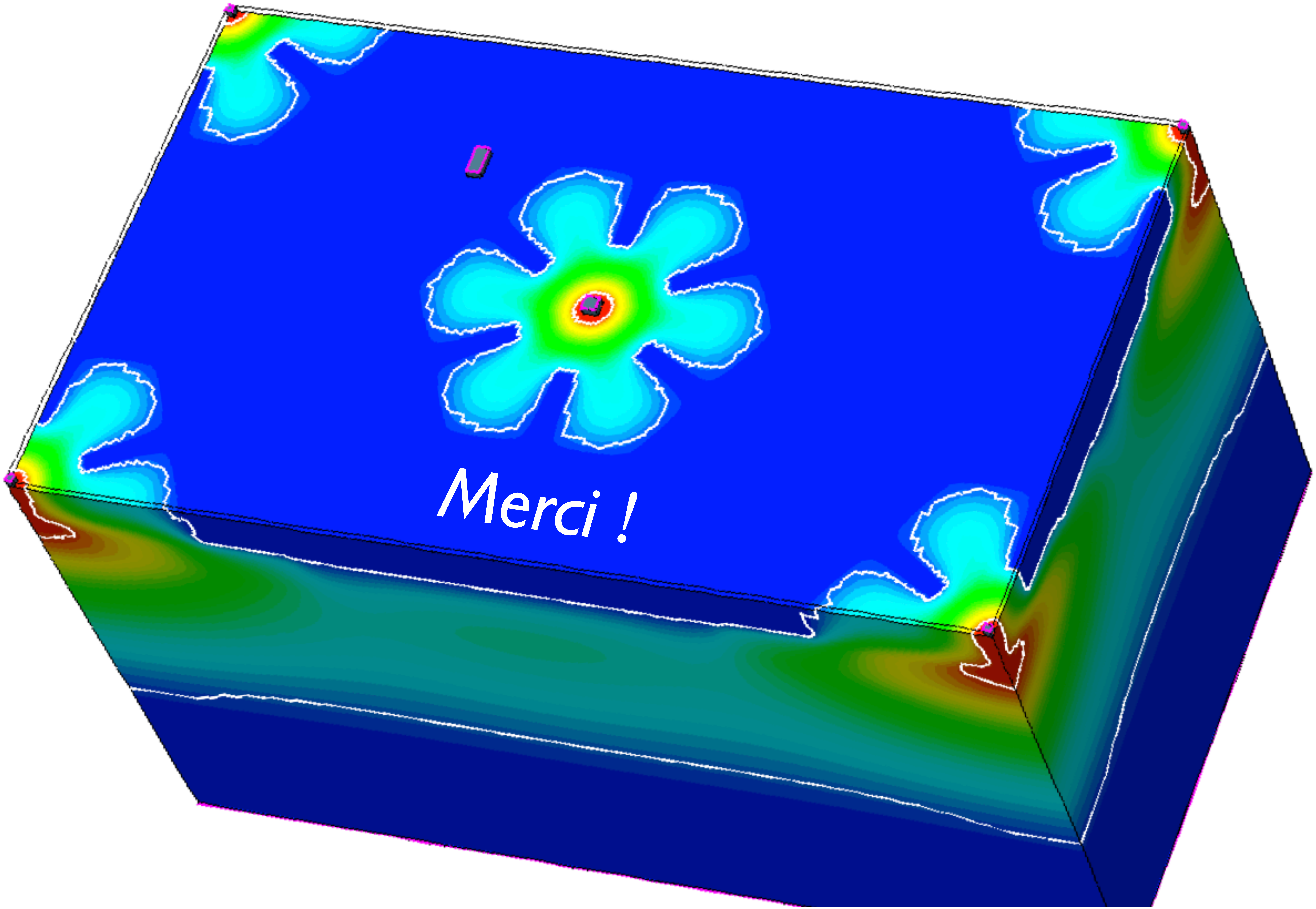
Summary

- 3D TCAD simulations with Synopsys Sentaurus are a powerful tool to develop and explore new silicon detector technologies
- Due to the stringent requirements of silicon detectors at future HEP experiments, more advanced silicon sensor concepts are explored:

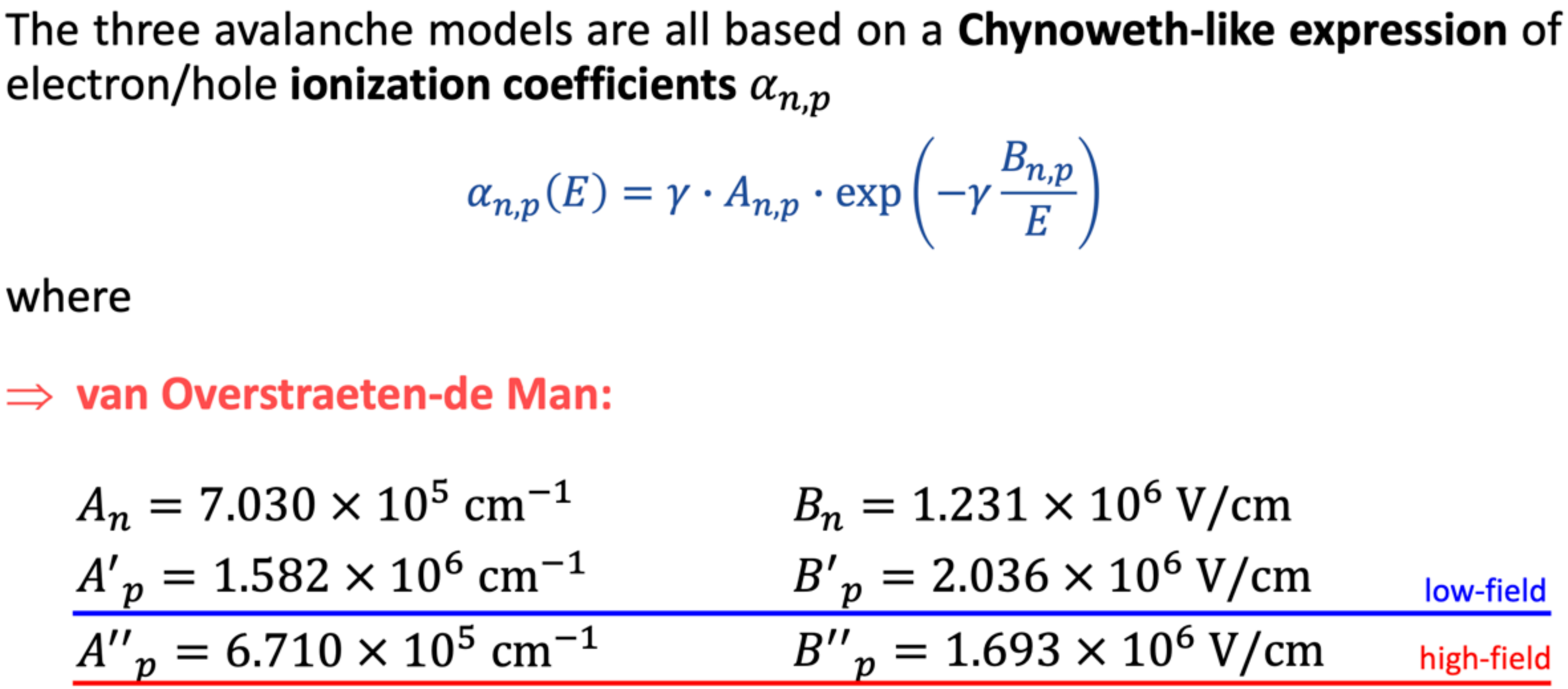
  → Need of 3D TCAD simulations and for understanding and optimisations
  → Speed up of R&D cycle

My personal point of view:

Tools like Synopsys Sentaurus together with close collaborations between microelectronic designers, physicists and foundries are key for the development of silicon detectors in future HEP experiments. This will allow us to find innovative solutions and implement them in realistic prototypes



Merci !



The three avalanche models are all based on a **Chynoweth-like expression** of electron/hole **ionization coefficients** $\alpha_{n,p}$

$$\alpha_{n,p}(E) = \gamma \cdot A_{n,p} \cdot \exp\left(-\gamma \frac{B_{n,p}}{E}\right)$$

where

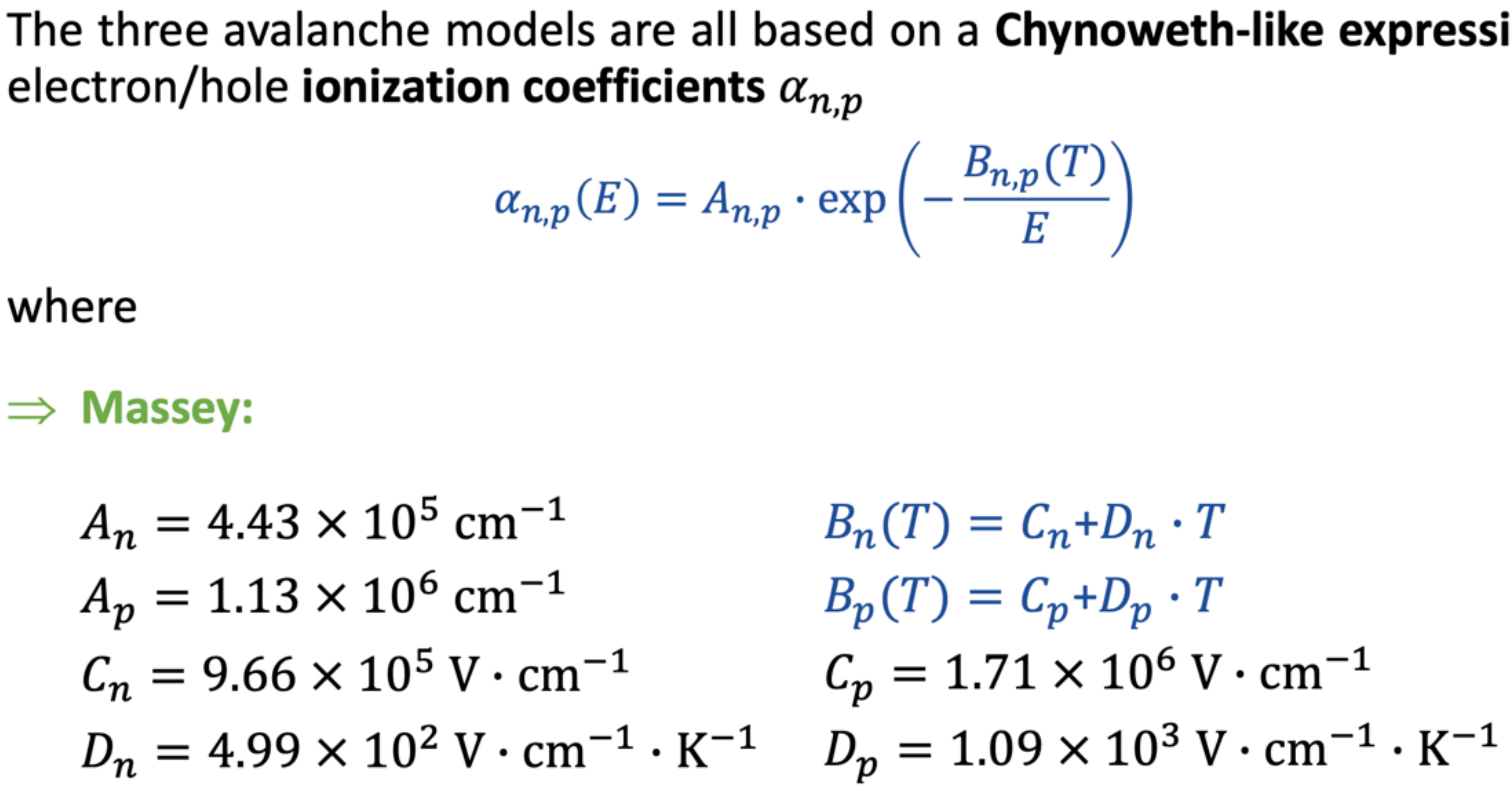
⇒ van Overstraeten-de Man:

$A_n = 7.030 \times 10^5 \text{ cm}^{-1}$ $\quad$ $B_n = 1.231 \times 10^6 \text{ V/cm}$

$A'_p = 1.582 \times 10^6 \text{ cm}^{-1}$ $\quad$ $B'_p = 2.036 \times 10^6 \text{ V/cm}$ $\quad$ low-field

$A''_p = 6.710 \times 10^5 \text{ cm}^{-1}$ $\quad$ $B''_p = 1.693 \times 10^6 \text{ V/cm}$ $\quad$ high-field

From:
https://indico.cern.ch/event/637212/contributions/2608617/attachments/1470689/2275558/5MarcoMandurrino_30thRD50.pdf



The three avalanche models are all based on a **Chynoweth-like expression** of electron/hole **ionization coefficients** $\alpha_{n,p}$

$$\alpha_{n,p}(E) = A_{n,p} \cdot \exp\left(-\frac{B_{n,p}(T)}{E}\right)$$

where

⇒ **Massey:**

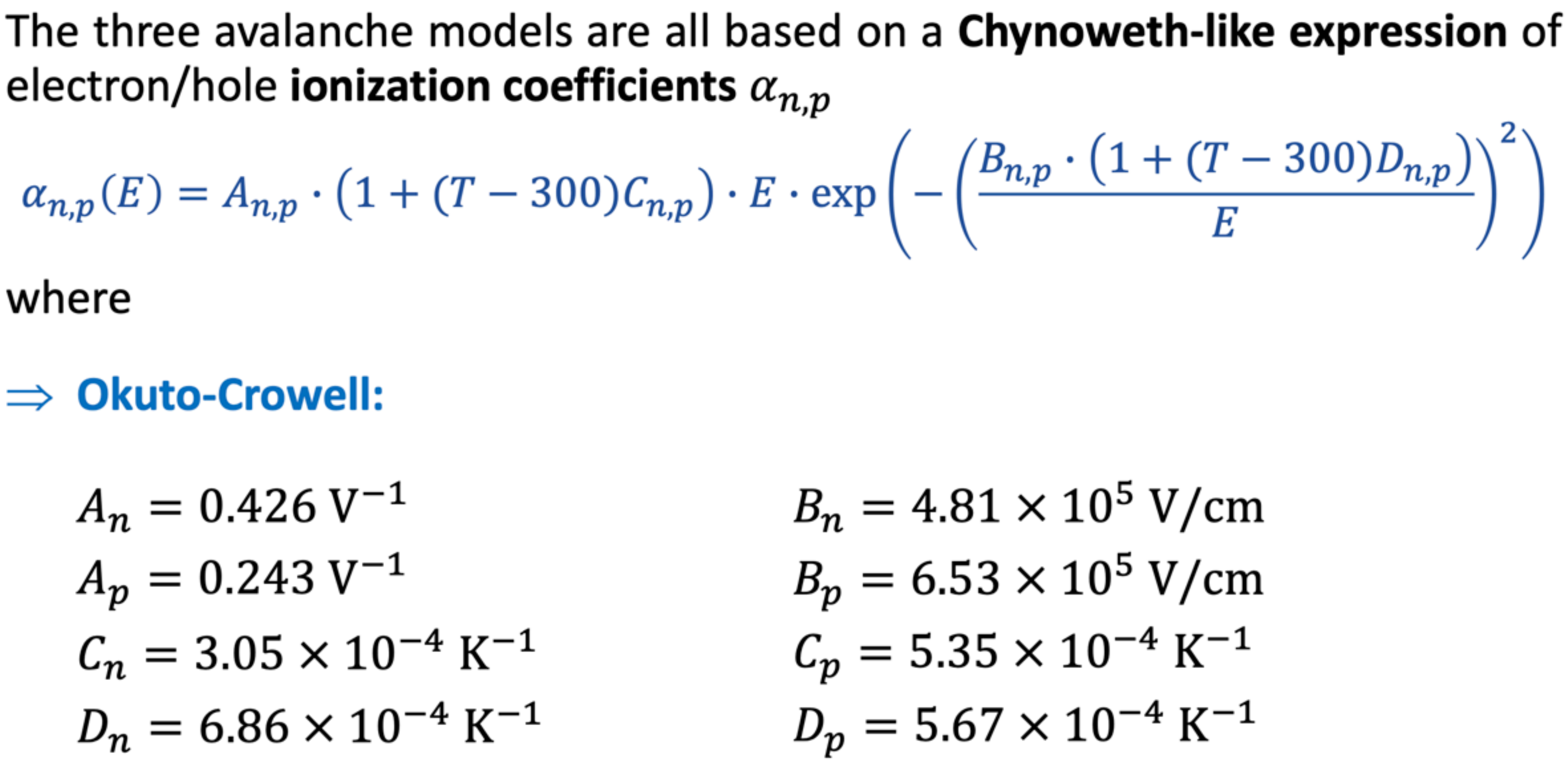
$$A_n = 4.43 \times 10^5 \text{ cm}^{-1} \qquad B_n(T) = C_n + D_n \cdot T$$

$$A_p = 1.13 \times 10^6 \text{ cm}^{-1} \qquad B_p(T) = C_p + D_p \cdot T$$

$$C_n = 9.66 \times 10^5 \text{ V} \cdot \text{cm}^{-1} \qquad C_p = 1.71 \times 10^6 \text{ V} \cdot \text{cm}^{-1}$$

$$D_n = 4.99 \times 10^2 \text{ V} \cdot \text{cm}^{-1} \cdot \text{K}^{-1} \qquad D_p = 1.09 \times 10^3 \text{ V} \cdot \text{cm}^{-1} \cdot \text{K}^{-1}$$

From:
https://indico.cern.ch/event/637212/contributions/2608617/attachments/1470689/2275558/5MarcoMandurrino_30thRD50.pdf



The three avalanche models are all based on a **Chynoweth-like expression** of electron/hole **ionization coefficients** $\alpha_{n,p}$

$$\alpha_{n,p}(E) = A_{n,p} \cdot \left(1 + (T - 300)C_{n,p}\right) \cdot E \cdot \exp\left(-\left(\frac{B_{n,p} \cdot \left(1 + (T - 300)D_{n,p}\right)}{E}\right)^2\right)$$

where

$\Rightarrow$ **Okuto-Crowell:**

$A_n = 0.426\ \mathrm{V}^{-1}$

$A_p = 0.243\ \mathrm{V}^{-1}$

$C_n = 3.05 \times 10^{-4}\ \mathrm{K}^{-1}$

$D_n = 6.86 \times 10^{-4}\ \mathrm{K}^{-1}$

$B_n = 4.81 \times 10^{5}\ \mathrm{V/cm}$

$B_p = 6.53 \times 10^{5}\ \mathrm{V/cm}$

$C_p = 5.35 \times 10^{-4}\ \mathrm{K}^{-1}$

$D_p = 5.67 \times 10^{-4}\ \mathrm{K}^{-1}$

From:
https://indico.cern.ch/event/637212/contributions/2608617/attachments/1470689/2275558/5MarcoMandurrino_30thRD50.pdf