Simulation tools for radiation detectors before and after irradiation

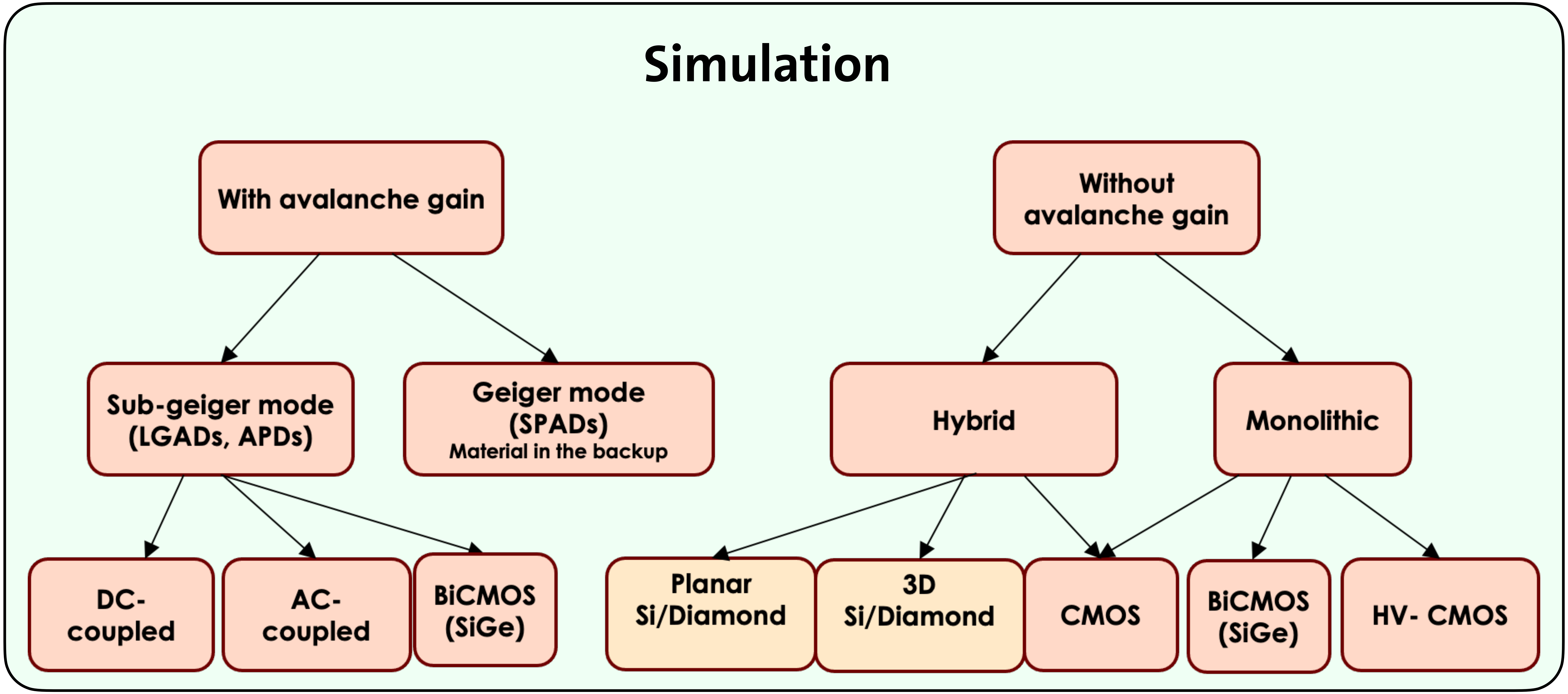
J. Schwandt

Institute for Experimental Physics
University of Hamburg

ECFA Detector R&D Roadmap Symposium of Task Force 3
Solid State Detectors
23rd April 2021

SOLID STATE DETECTORS FOR FUTURE (4D) TRACKERS

Simulation



With avalanche gain

Without avalanche gain

Sub-geiger mode (LGADs, APDs)

Geiger mode (SPADs)
Material in the backup

Hybrid

Monolithic

DC-coupled

AC-coupled

BiCMOS (SiGe)

Planar Si/Diamond

3D Si/Diamond

CMOS

BiCMOS (SiGe)

HV- CMOS

INTRODUCTION

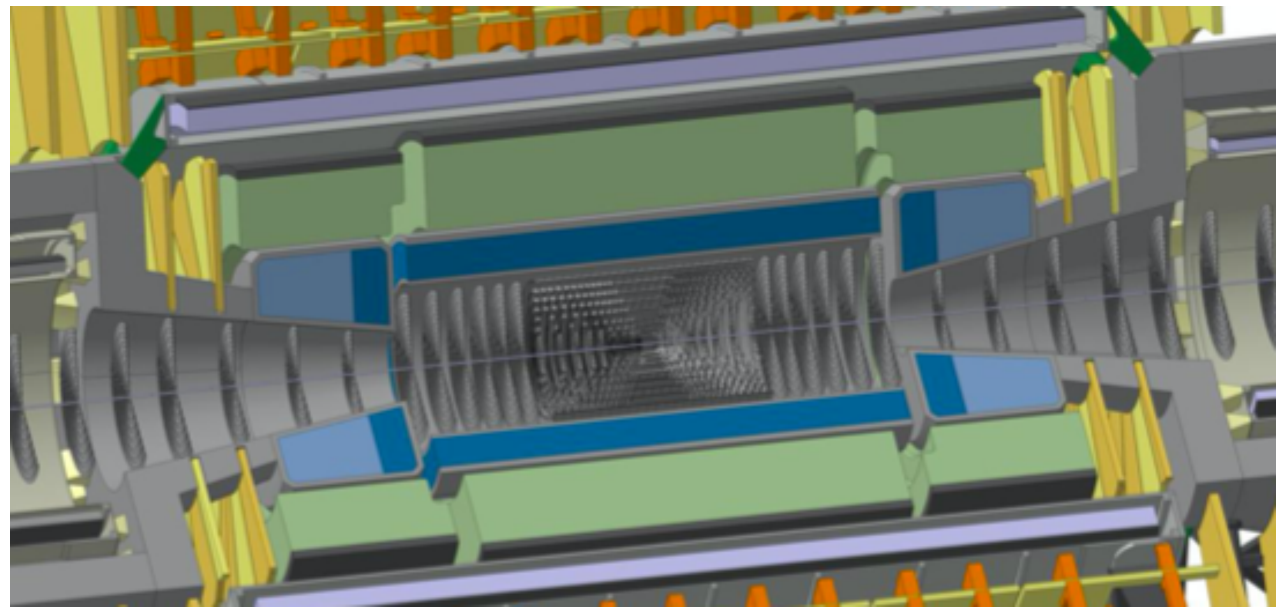
Future requirements for solid state detectors:

- **FCC-hh**
  - Up to $\Phi_{eq} \approx 1\mathrm{x}10^{18}\,\mathrm{cm}^{-2}$ 1 MeV neutron equivalent fluence , TID 300 MGy
  - Pixel size: 25x50 μm^2
  - Timing of tracks at the < 10 ps level
- **Future Linear High energy e^+e^- Machines**
  - Single point resolution: ≈ 3 µm
  - Lowest possible mass: ≈ 0.2% X_0 per layer
  - Pixel size: ≤ 25x25 μm^2
- **Strong Interaction Experiments**
  - DCA resolution: ≈ 25 µm at p_t = 100 MeV/c
  - Material budget: 0.1% X_0 per layer
  - Pixel size: ≤ 10x10 μm^2

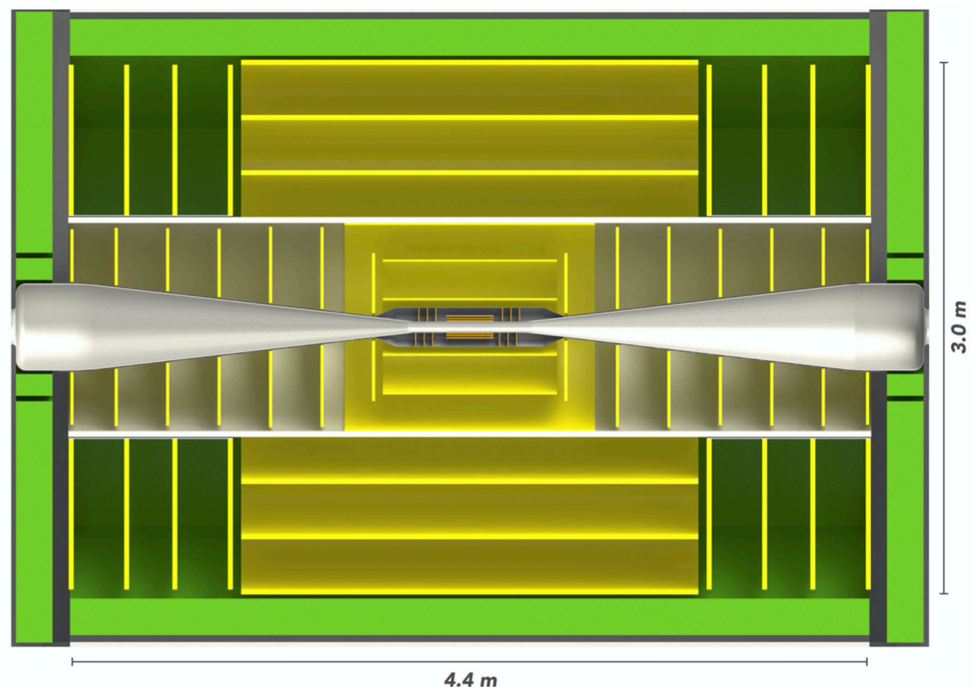
- Extreme radiation tolerance
- Very fast
- Very thin
- High granularity

*) DCA = Distance of closest approach

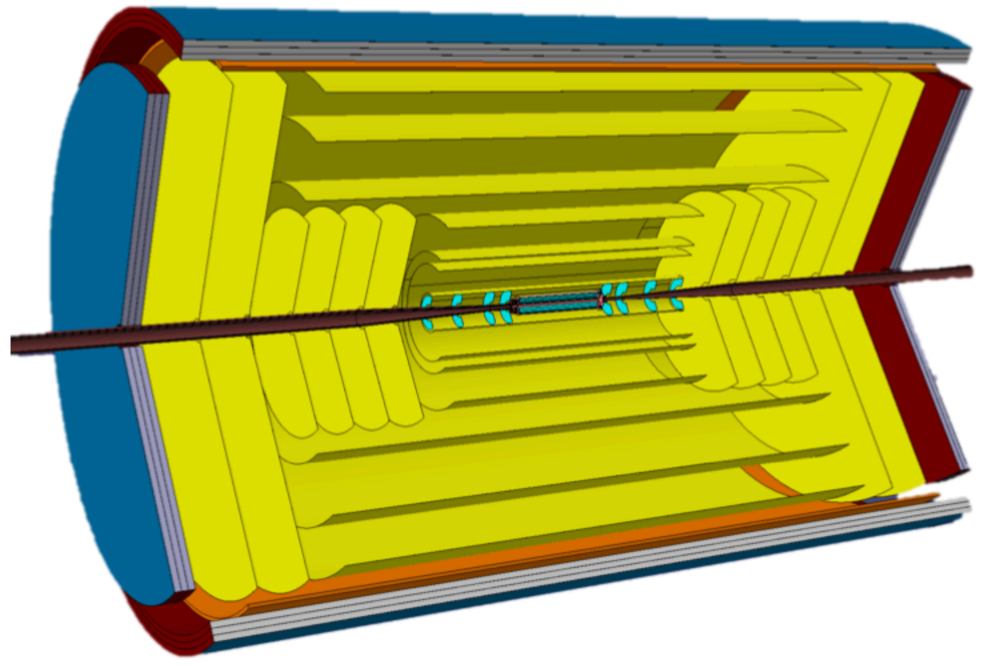
FCC-hh



CLIC



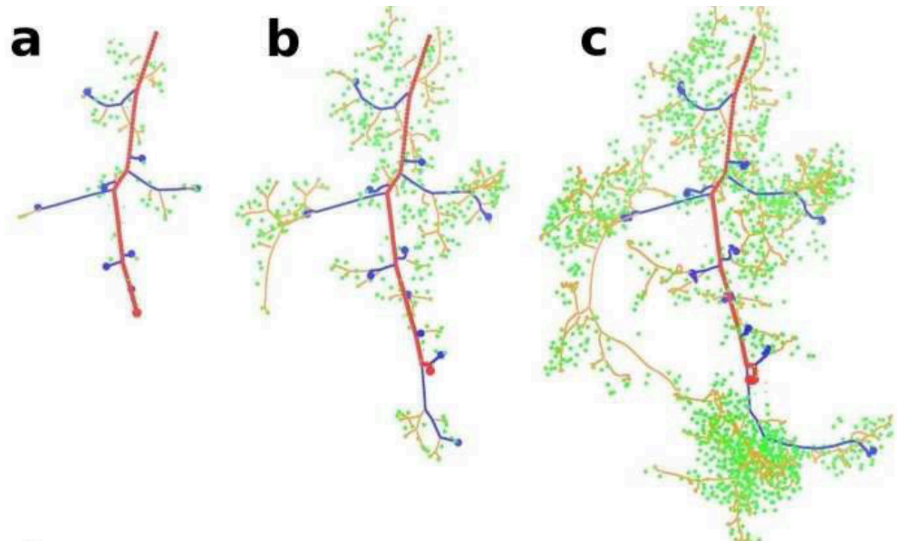
ALICE 3

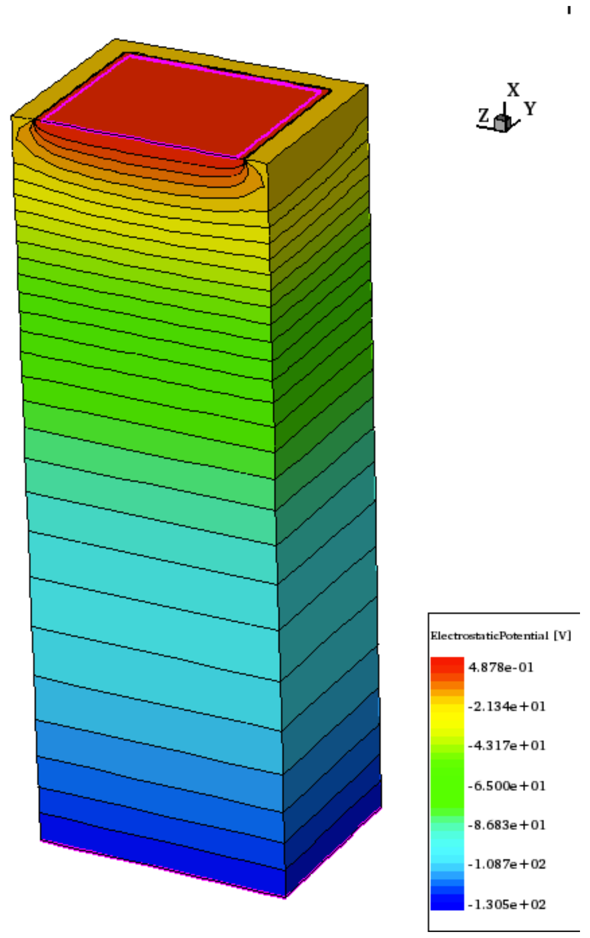


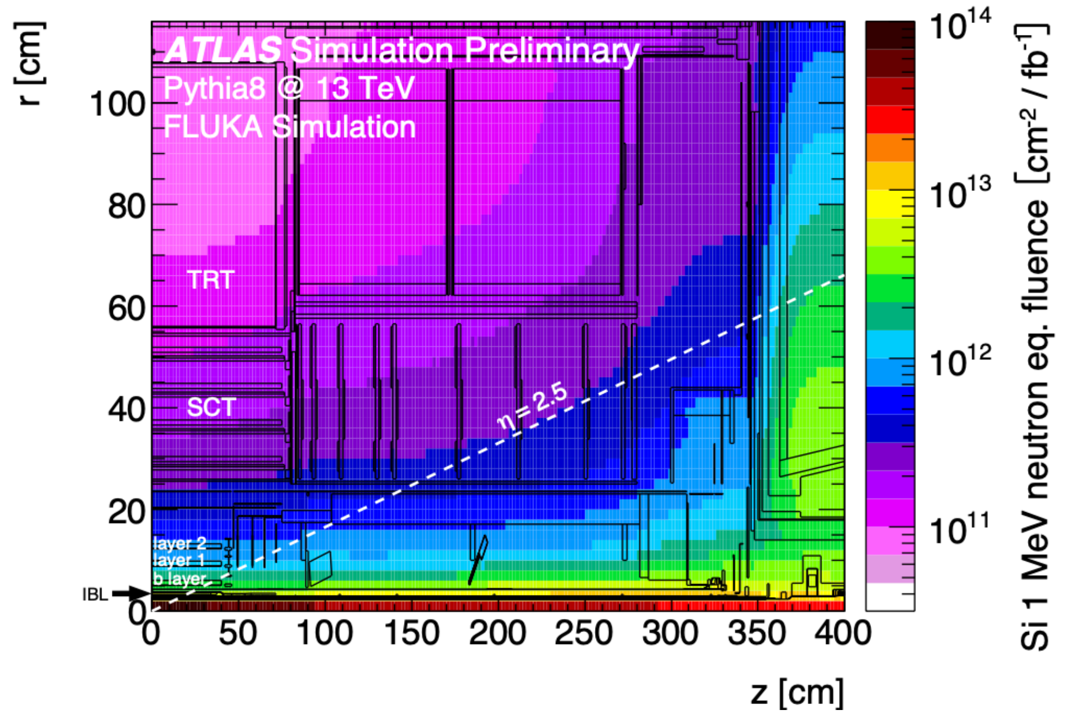
INTRODUCTION

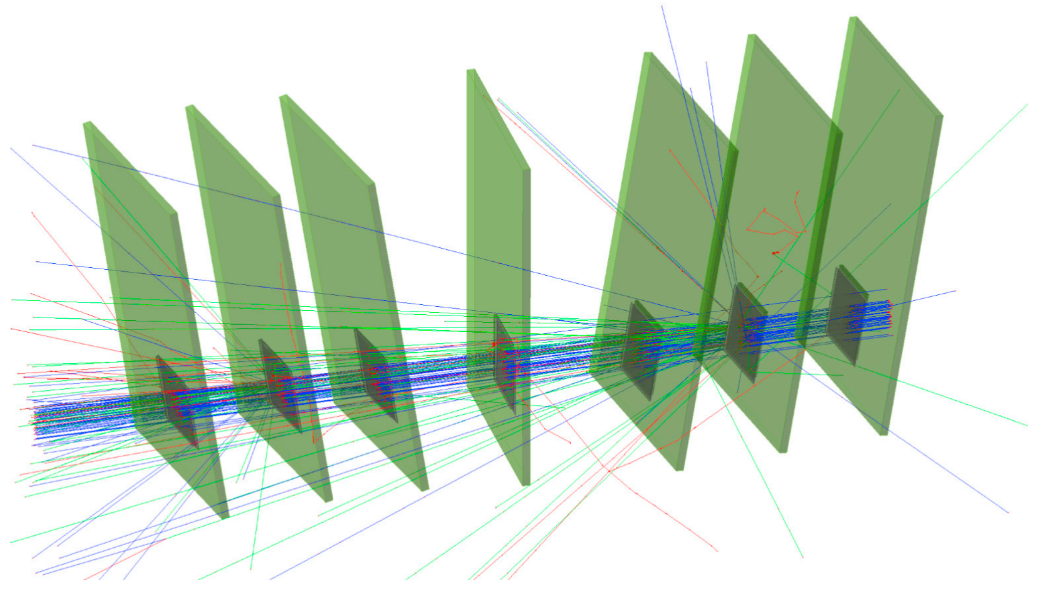
Types of simulations in the context of radiation detectors:

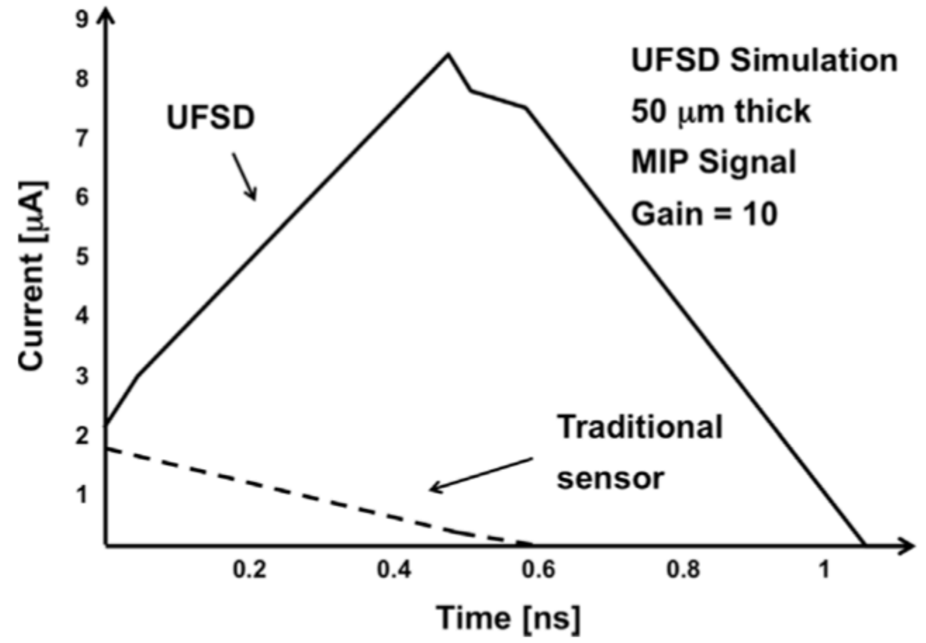
- **Displacement damage simulation**
  - Determine stable defect configurations and energy levels in the band gap
- **Technology Computer-Aided Design (TCAD)**
  - Understand and design sensors that meet specific requirements
- **Signal simulation**
  - Investigate the performance of sensor coupled to the readout, Monte Carlo studies
- **Experimental setup simulation**
  - Understand detector in complex environments, such as in a test beam setup
- **Full detector system simulation**
  - Predict and compare performance to running experiments











RADIATION DAMAGE

Surface damage (Ionizing Energy Loss):

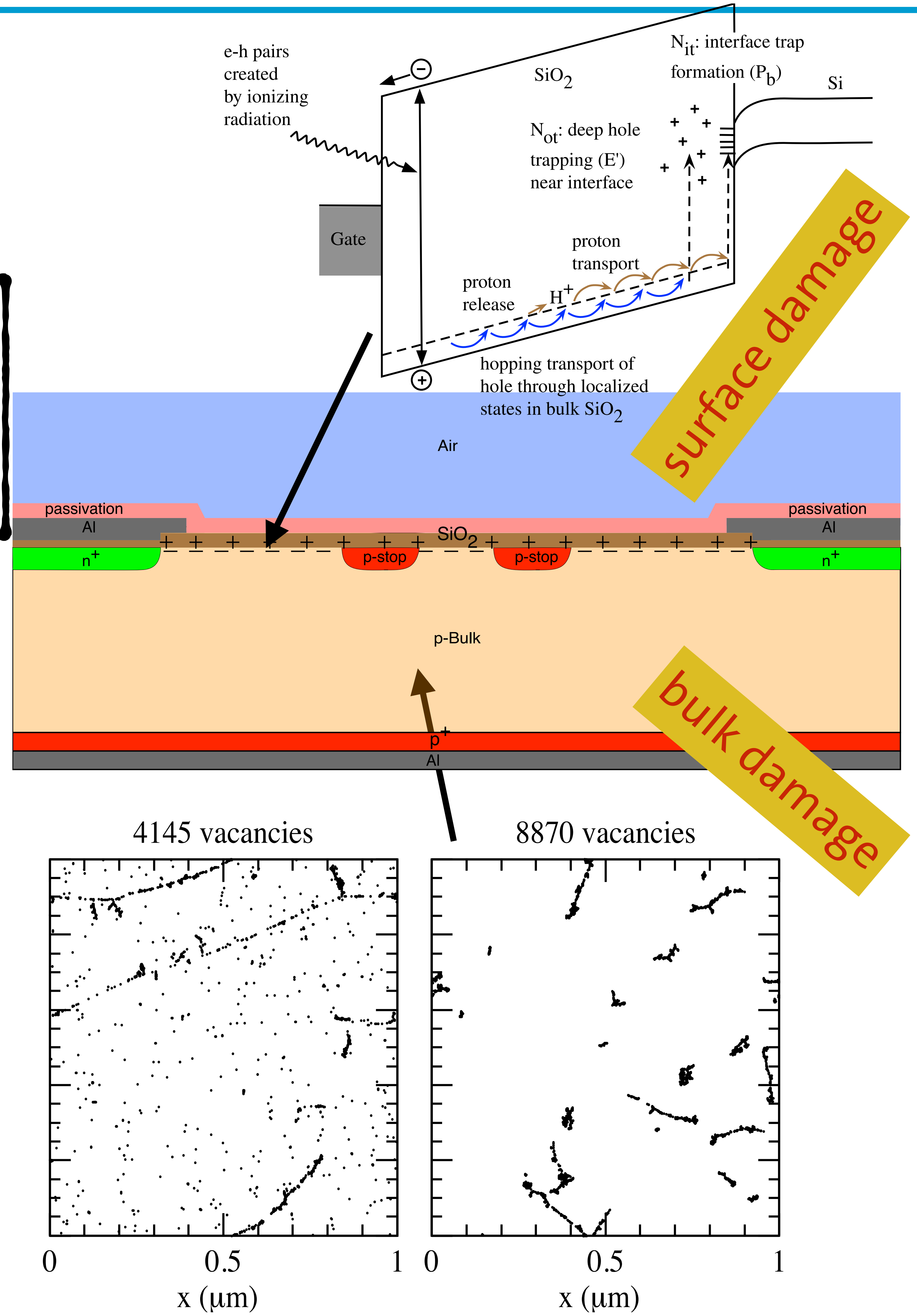
- Build up of **oxide charges, border** and **interface traps**
  - ➡Increase of surface current
  - ➡Change of electrical field near to the Si-SiO_2 interface
  - ➡Trapping near to the Si-SiO_2 interface

C-V/I-V on MOS capacitors, MOSFET and gate controlled diodes

Bulk damage (NIEL):

- **Point** and **cluster** defects in the silicon lattice
  - ➡Increase of leakage current
  - ➡Change of the space charge
  - ➡Trapping of drifting charge

I-V, C-V and CCE on pad diodes



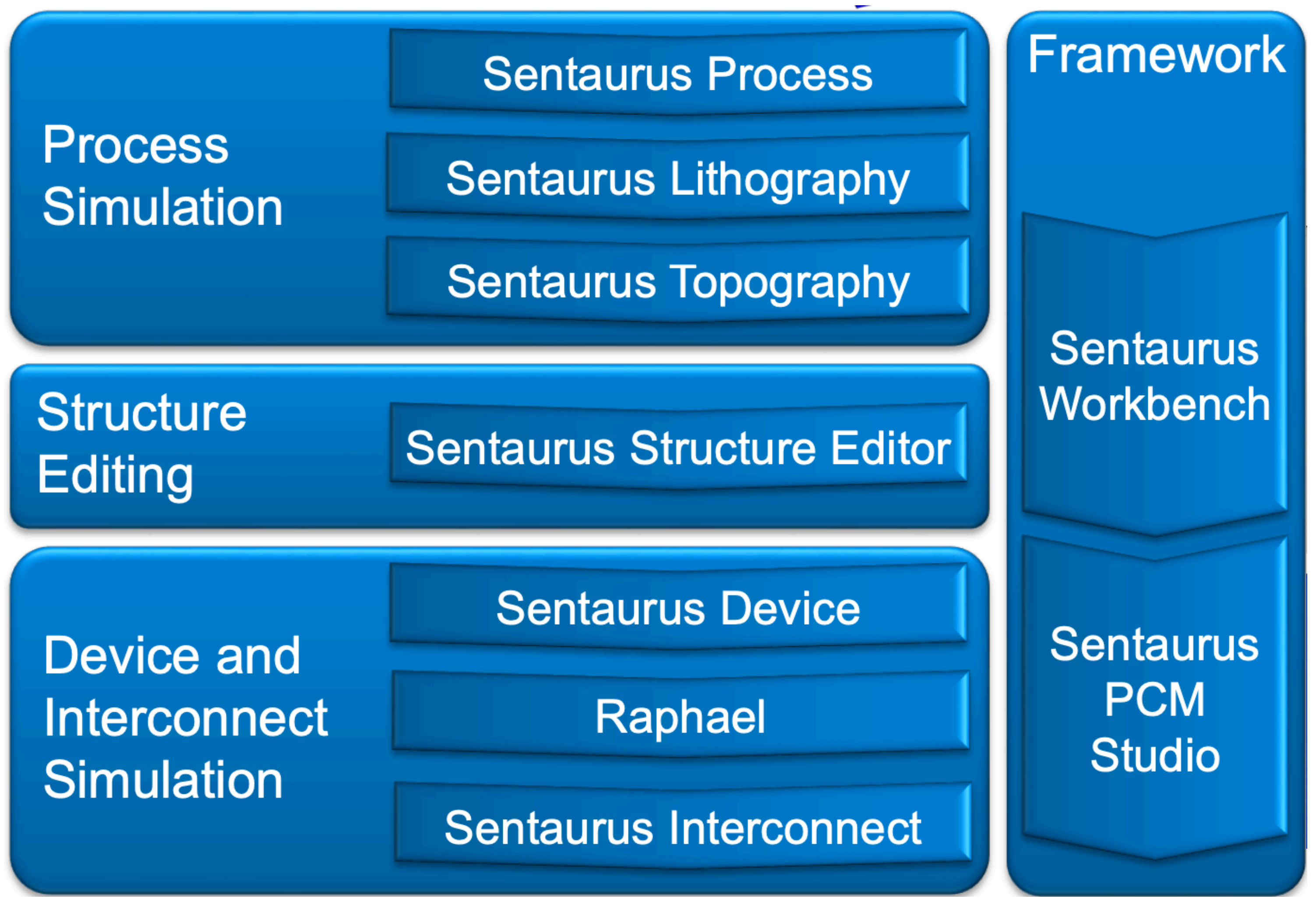
24 GeV/c protons 1 MeV neutrons

TCAD OVERVIEW

Technology Computer-Aided Design (TCAD):

- Is a brach of electronic design automation (EDA)
- In HEP, essentially only software suites from two **commercial** providers are used

SYNOPSYS®
Silicon to Software™
https://www.synopsys.com

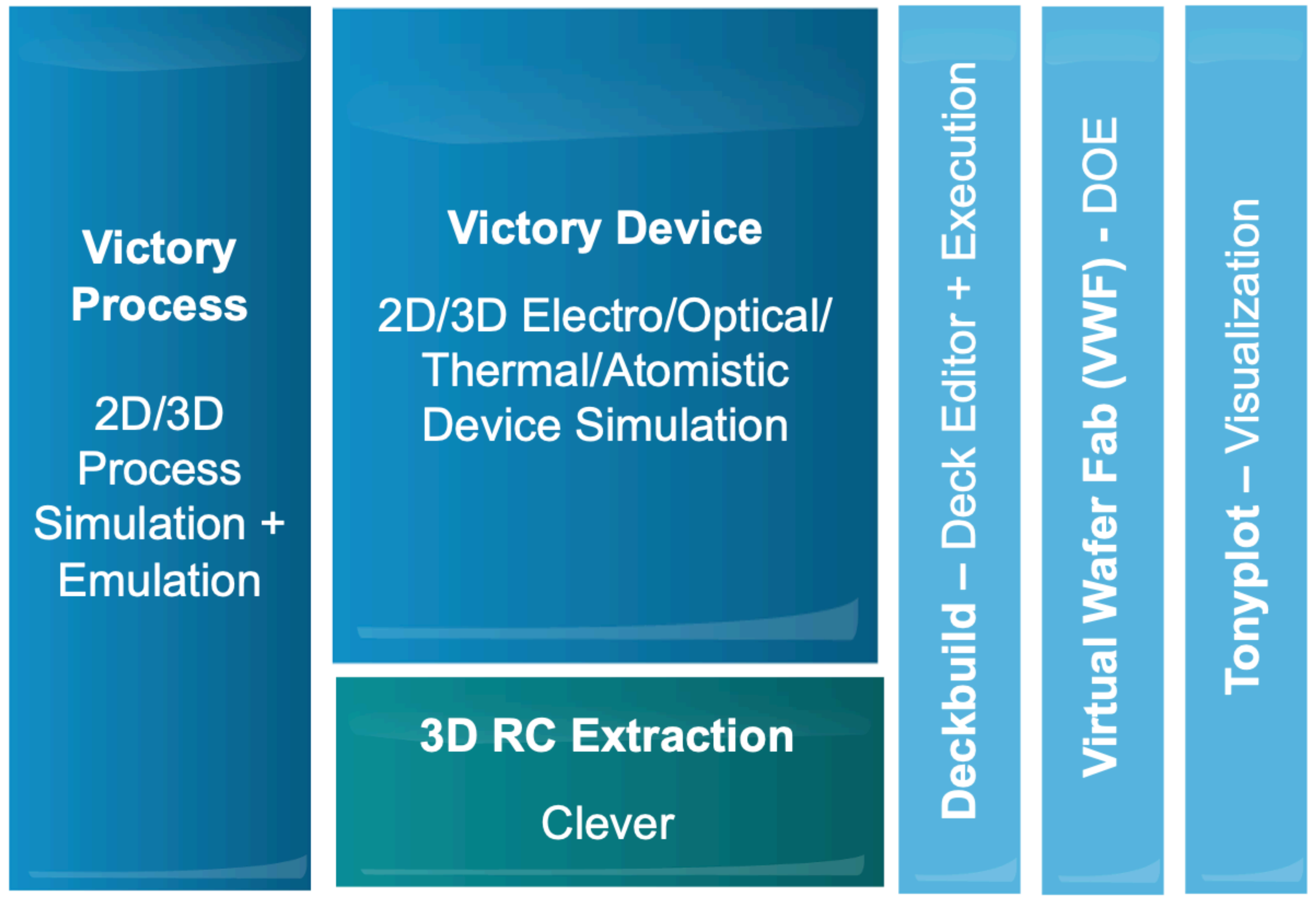

Process Simulation
Sentaurus Process
Sentaurus Lithography
Sentaurus Topography

Structure Editing
Sentaurus Structure Editor

Device and Interconnect Simulation
Sentaurus Device
Raphael
Sentaurus Interconnect

Framework
Sentaurus Workbench
Sentaurus PCM Studio

SILVACO
https://silvaco.com


Victory Process
2D/3D Process Simulation + Emulation

Victory Device
2D/3D Electro/Optical/ Thermal/Atomistic Device Simulation

3D RC Extraction
Clever

Deckbuild – Deck Editor + Execution

Virtual Wafer Fab (VWF) - DOE

Tonyplot – Visualization

- Licences for Synopsys via EUROPRACTICE ➡Majority of users in HEP

Most important tools are the device simulators and partially also the process simulators

PROCESS SIMULATION I

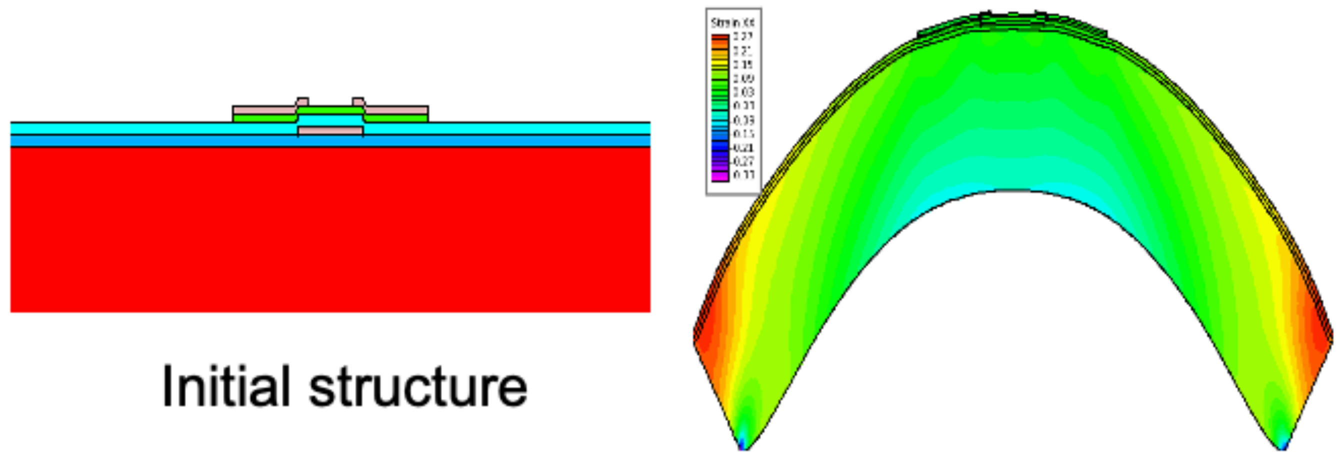
Aim of process simulation:

- Realistic doping profiles and structures

Sentaurus / Silvaco process simulators:

- General purpose multidimensional (2D/3D) process simulator
- Integrated 3D geometric modeling engine (depo/etch/pattern)
- Analytic and Monte Carlo implantation
- Diffusion: laser/flash annealing, kinetic Monte Carlo
- Mechanical stress, Oxidation/Silicidation etc.

Devices on flexible substrate



Initial structure

strain profile
(50 degree bending)

Non-Si materials process simulation:

- SiGe, Ge, 4H-,6H-SiC, III-V

Process simulations are essential for vendors, but our community has the problem that:

- **Process details** are usually **not available** from vendor due to competitions
- And if the they are, they are **strictly limited by NDA's**

→

- Cooperate with vendor and sign NDA
- Optimise your design and search for vendor who can process it

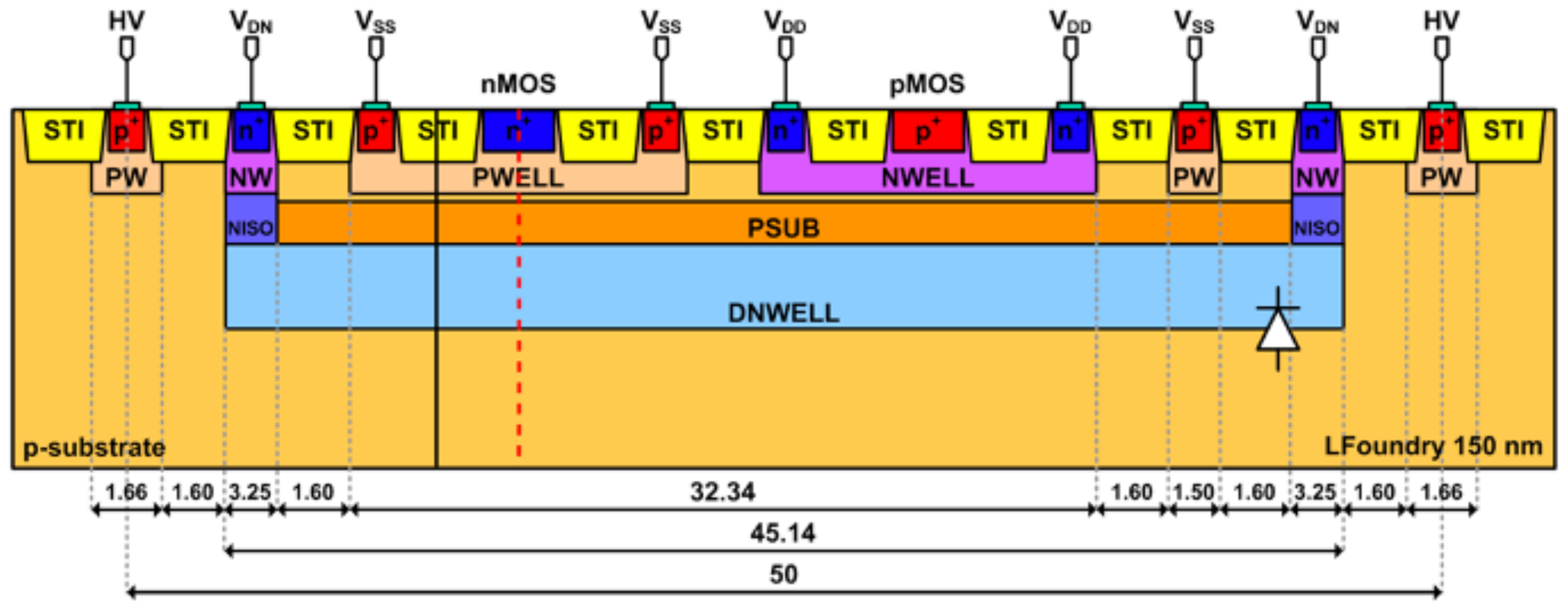
*) NDA = non-disclosure agreement

PROCESS SIMULATION II

Examples of process simulations:

1.CMOS Process simulation

L. Meng, CERN-THESIS-2018-153



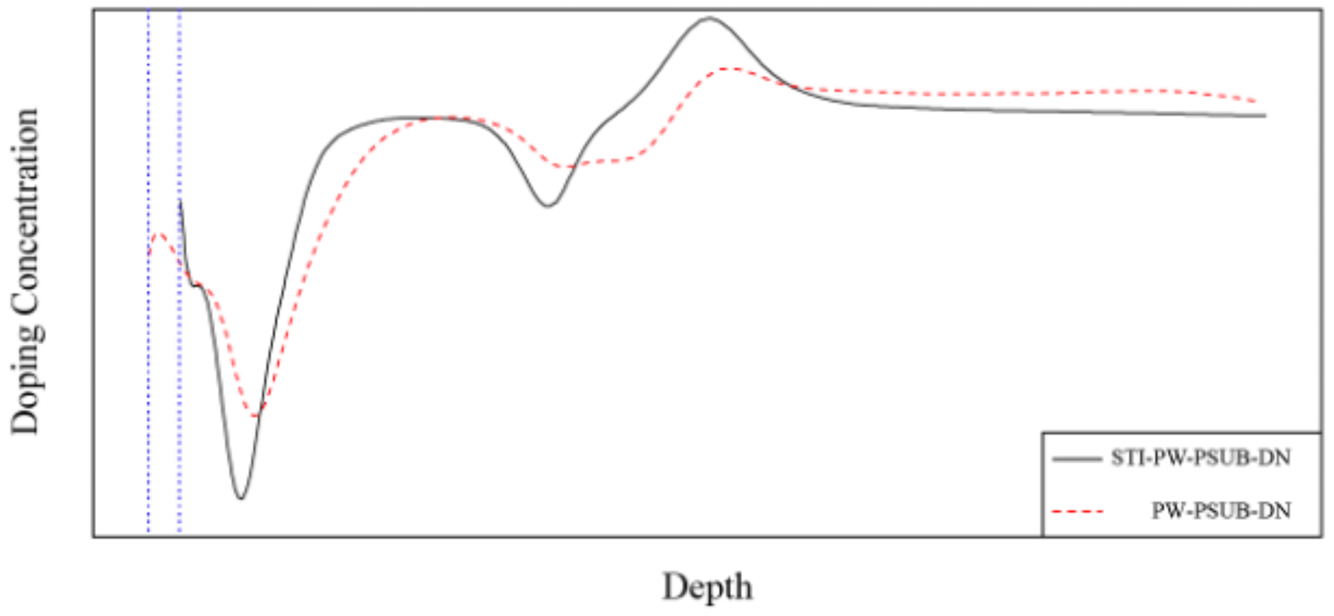
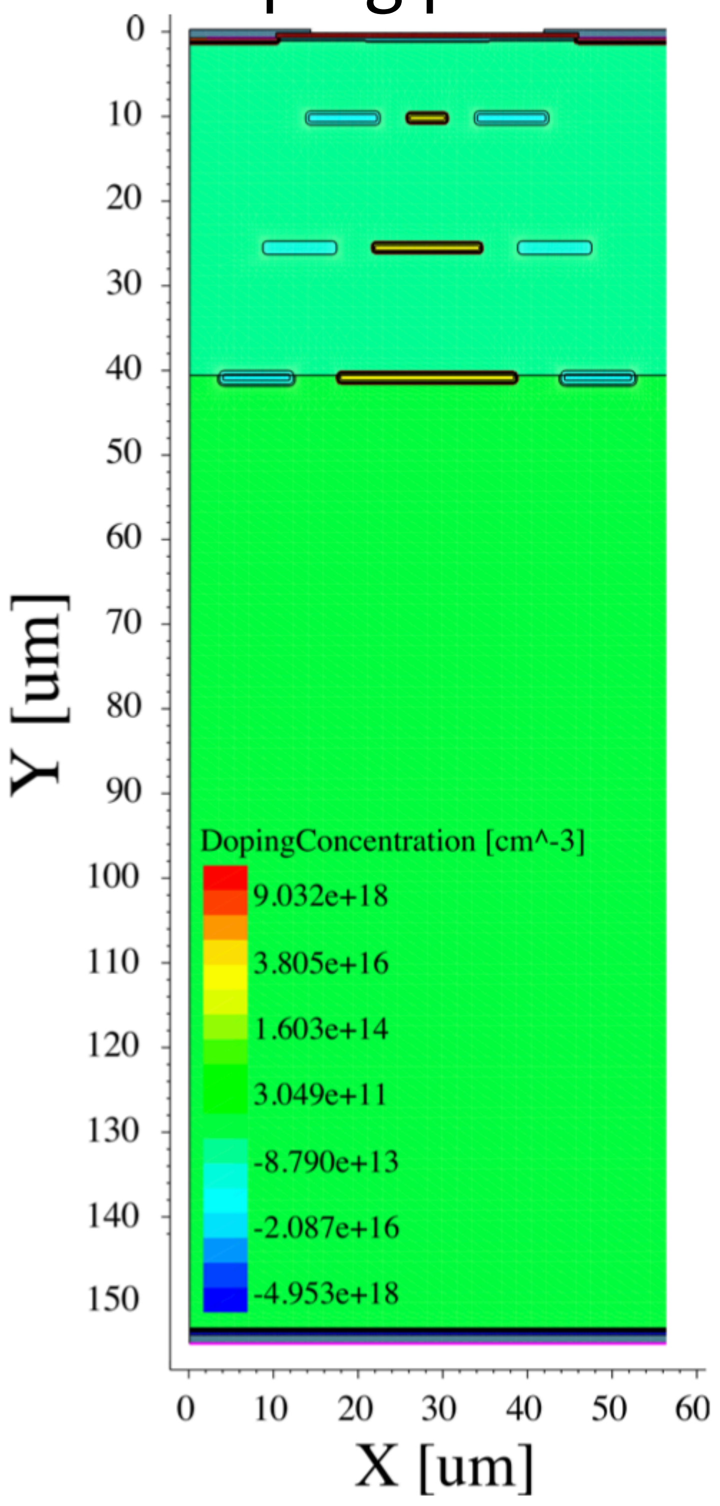


Figure 5.36: Comparison of doping profiles extracted from process simulation. Black solid line represents the doping profile of a region under an STI and red dashed line is the profile in regions without STI for the same implants PW-PSUB-DN, corresponding to the cut lines in Fig. 5.35 without the n^+ doping. No scales are shown due to confidentiality.

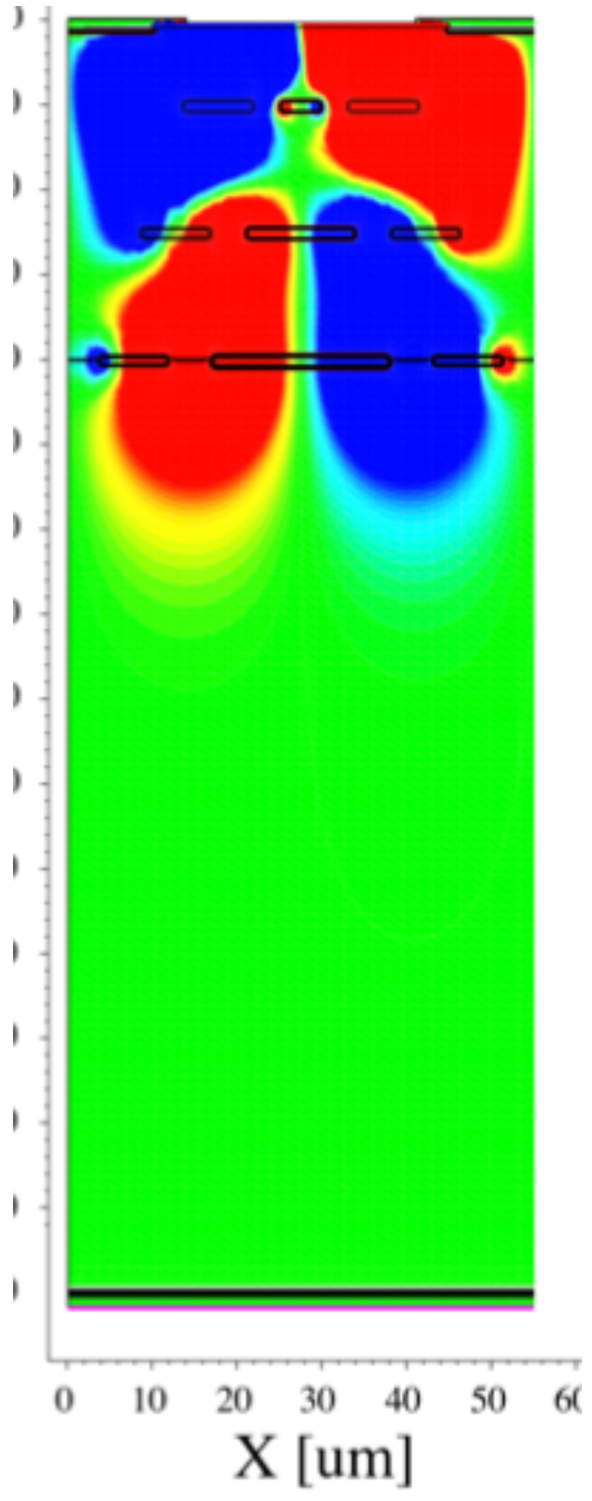
2.Enhanced Lateral Drift Sensor(ELAD)

A. Velyka, DESY-THESIS-2020-014

Doping profile



E-field



- Realistic profiles for device simulations
- Essential in the development of new sensor concepts

DEVICE SIMULATION I

Device simulations:

- Works by modelling electrostatic potential (Poisson's equation) and carrier continuity equations
- Applies semiconductor equations + boundary conditions on mesh and solves them in a self-consistent way

$$\left.\begin{array}{llll}
\textbf{Poisson} & \nabla\cdot\epsilon\nabla\phi = -\rho_{eff} & \text{with} & \rho_{eff} = q[p-n+N_D-N_A]-\rho_{traps} \\
\textbf{Electron continuity} & \dfrac{\partial n}{\partial t} = \dfrac{1}{q}\nabla\cdot\mathbf{J}_n + R_{net} & \text{where} & \mathbf{J}_n = qn\mu_n\mathbf{E} + qD_n\nabla n \\
\textbf{Hole continuity} & \dfrac{\partial p}{\partial t} = -\dfrac{1}{q}\nabla\cdot\mathbf{J}_p + R_{net} & \text{where} & \mathbf{J}_p = qp\mu_p\mathbf{E} - qD_p\nabla p
\end{array}\right\}\ \boxed{\text{drift-diffusion}}$$

- Different versions of **physics models** are available (**mobility**, **impact-ionisation**, **tunnelling** etc)
- Radiation damage will change the net **recombination rate** R_{net} and the **charge density** due to ρ_{traps}

- More complex transport models such as **hydrodynamic**, **thermodynamic**, and **full band Monte Carlo** transport are already available

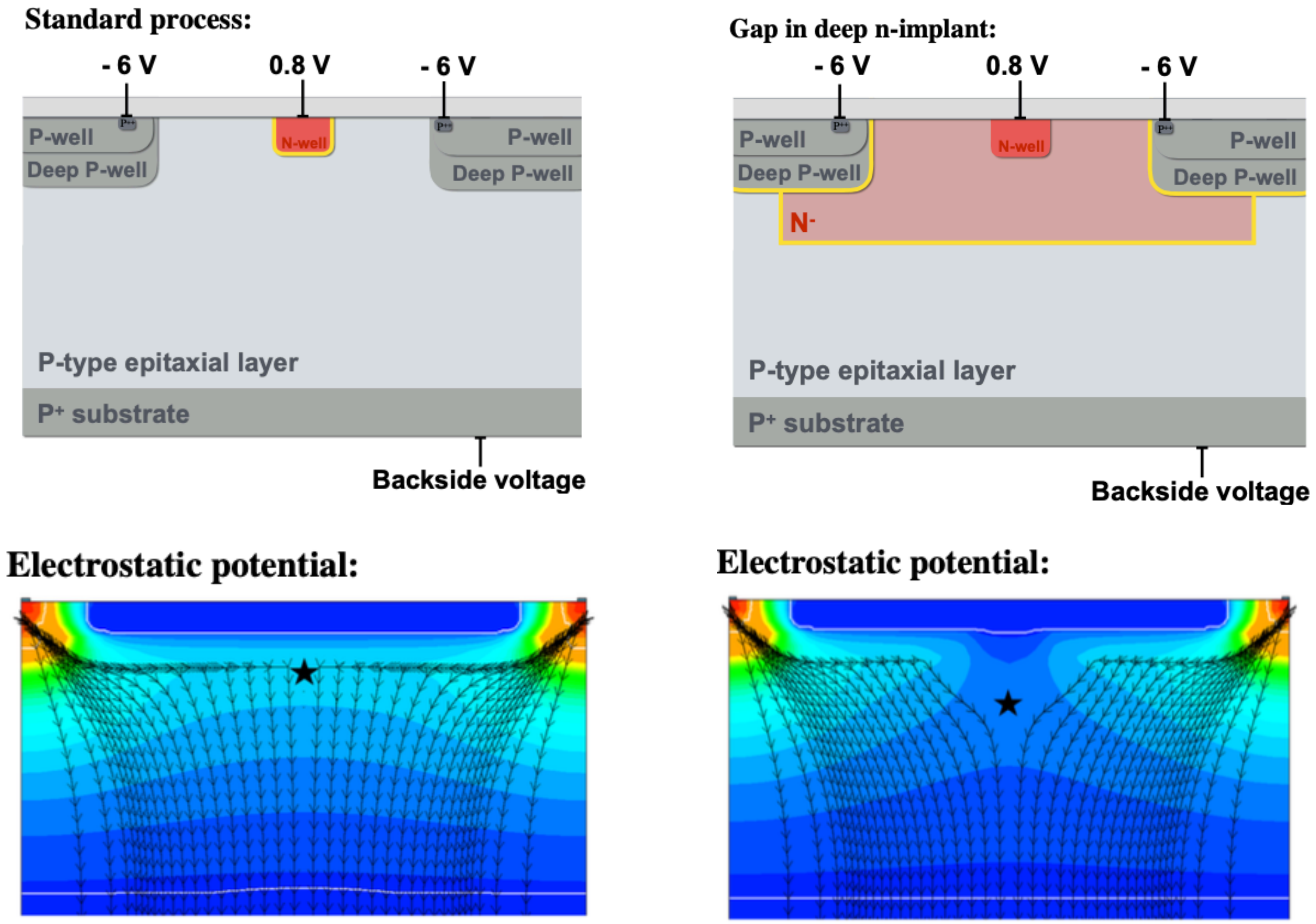
→ Monolithic sensors based on 28 nm and even below could be simulated with the current device simulators

DEVICE SIMULATION II

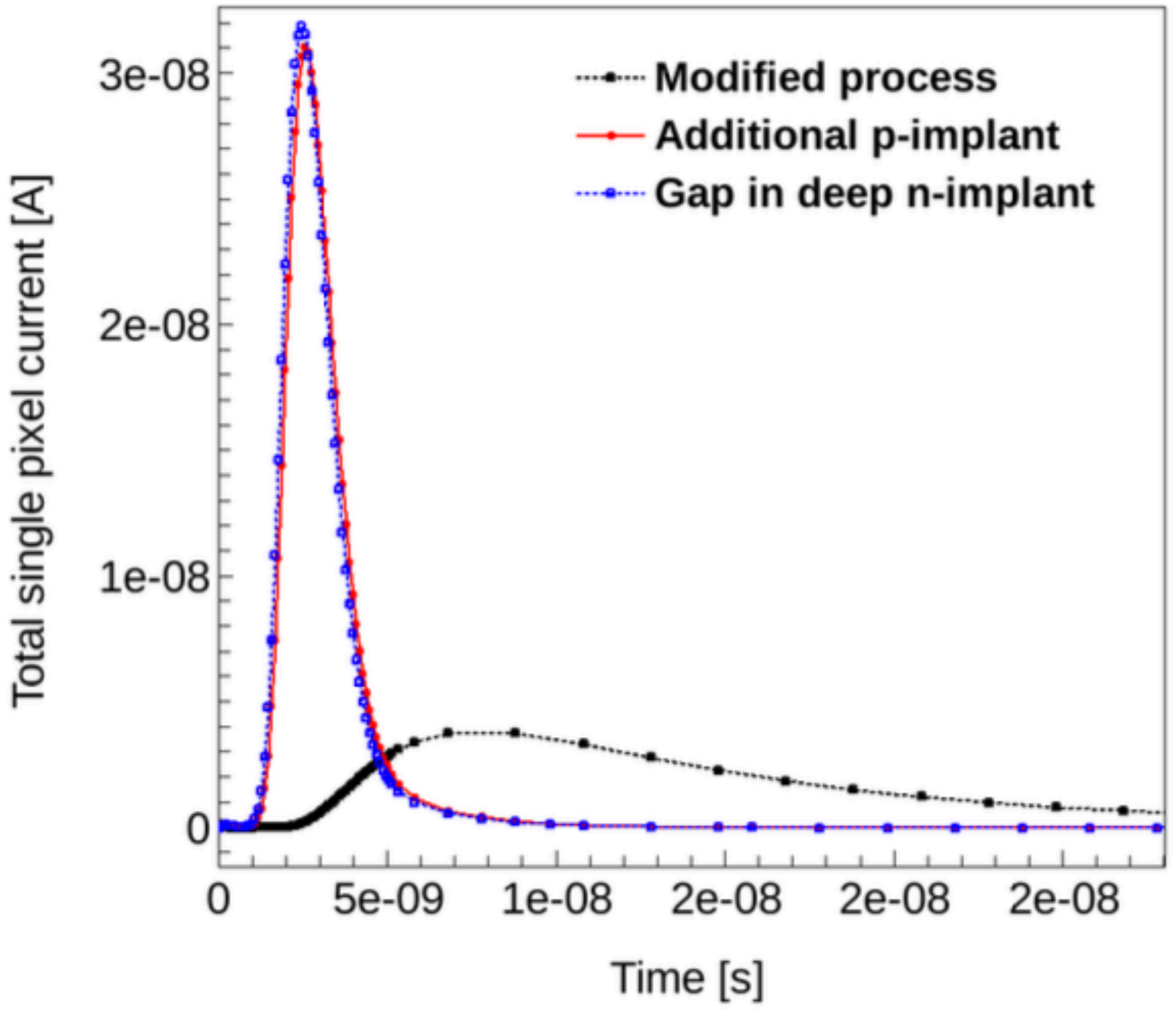
All kinds of silicon radiation sensors (strip, pixel, 3D pixel, DMAPS, LGAD etc) have been simulated successfully with TCAD

Examples of device simulations:

- Improving CMOS pixel sensor for faster charge collection



M. Munker et al 2019 JINST 14 C05013



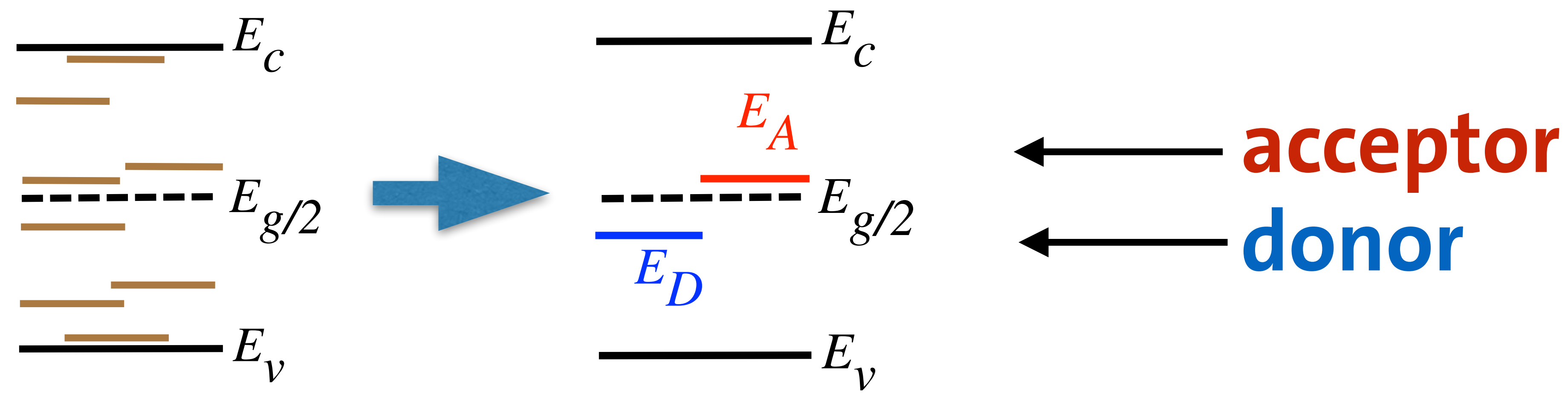
- 3D TCAD simulations are challenging in terms of runtime and memory
- Automatic minimization of parameters is generally possible

Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

RADIATION DAMAGE MODELLING I

Bulk damage modelling:

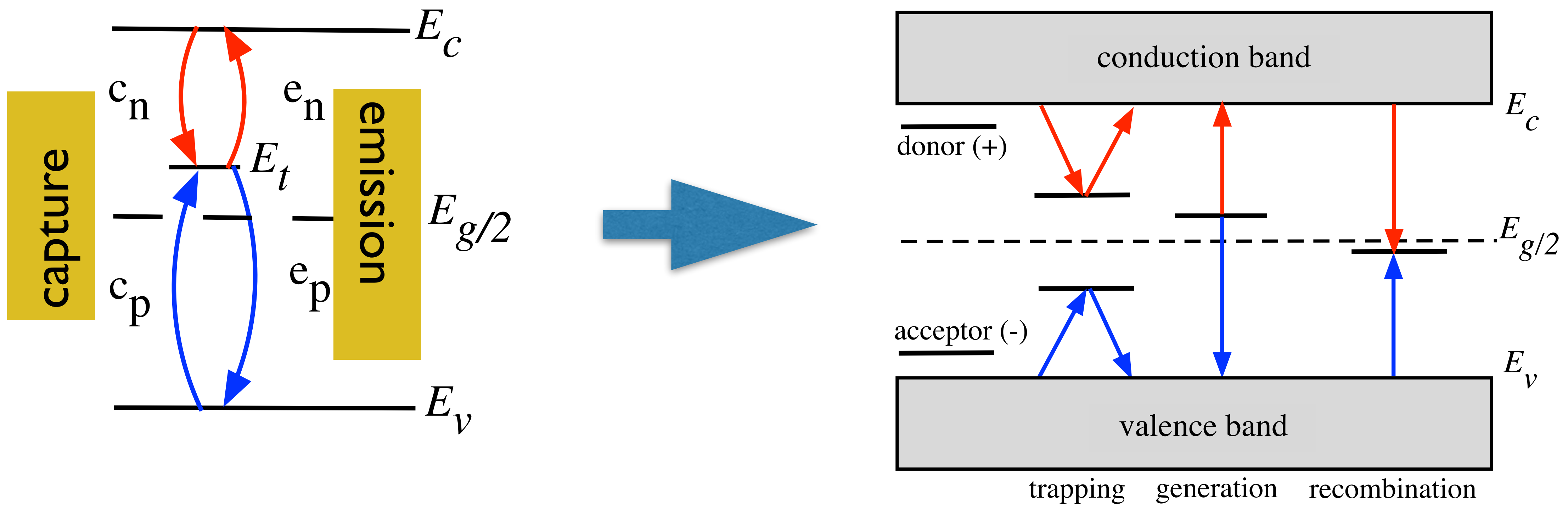
- Usually **effective** trap levels modelling the measured identified point and cluster defects
- It is assumed that the traps obey **SRH** statistics



Example: 2 trap model → 6 free parameter

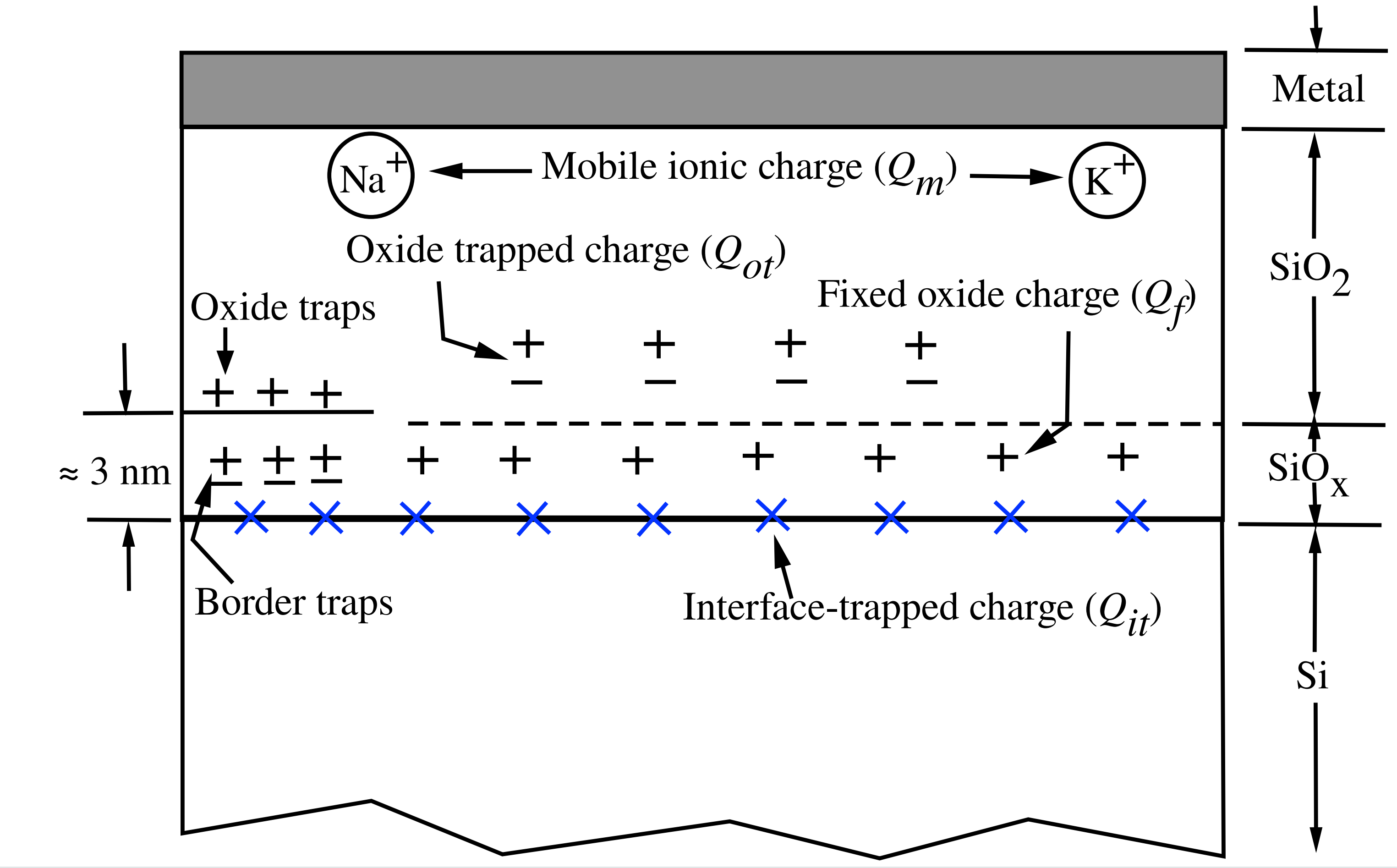
1. **Energy levels + type**: E_A , E_D fixed
2. **Concentrations**: N_A , N_D
3. **Cross sections:** $\sigma^A{}_e$, $\sigma^A{}_h$, $\sigma^D{}_e$, $\sigma^D{}_h$

➡$\rho_{trap} = q[N_D f_D - N_A f_A], f_D, f_A, R_{net}$



Surface damage modelling:

- **Fixed** oxide charge + surface recombination **velocity**
- Or **fixed** oxide charge + **interface trap** state distribution



*) SRH = Shockley-Reed-Hall

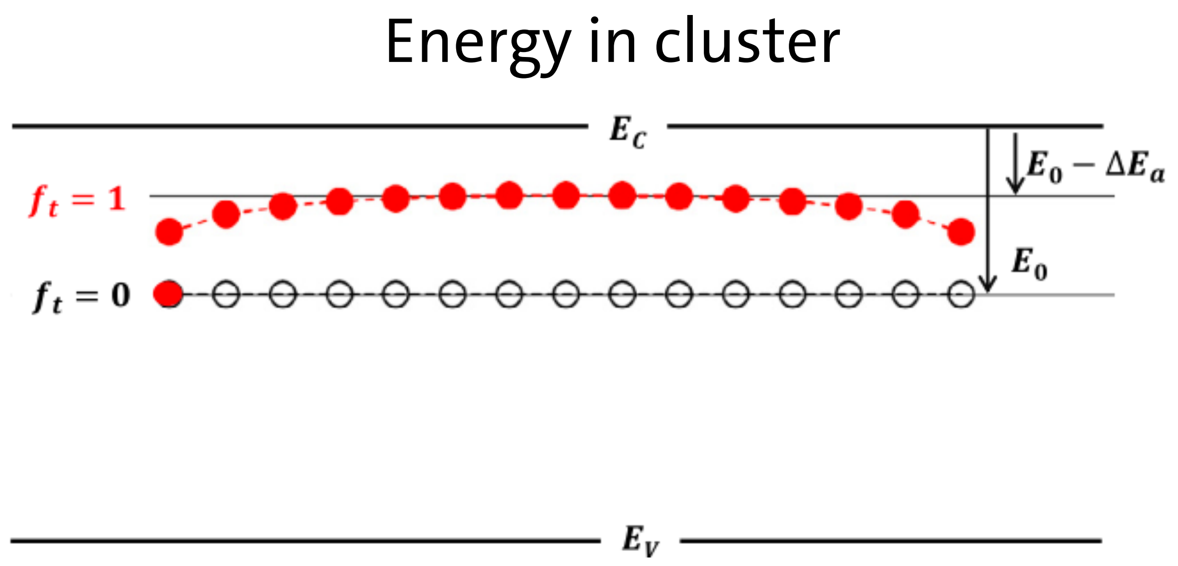
RADIATION DAMAGE MODELLING II

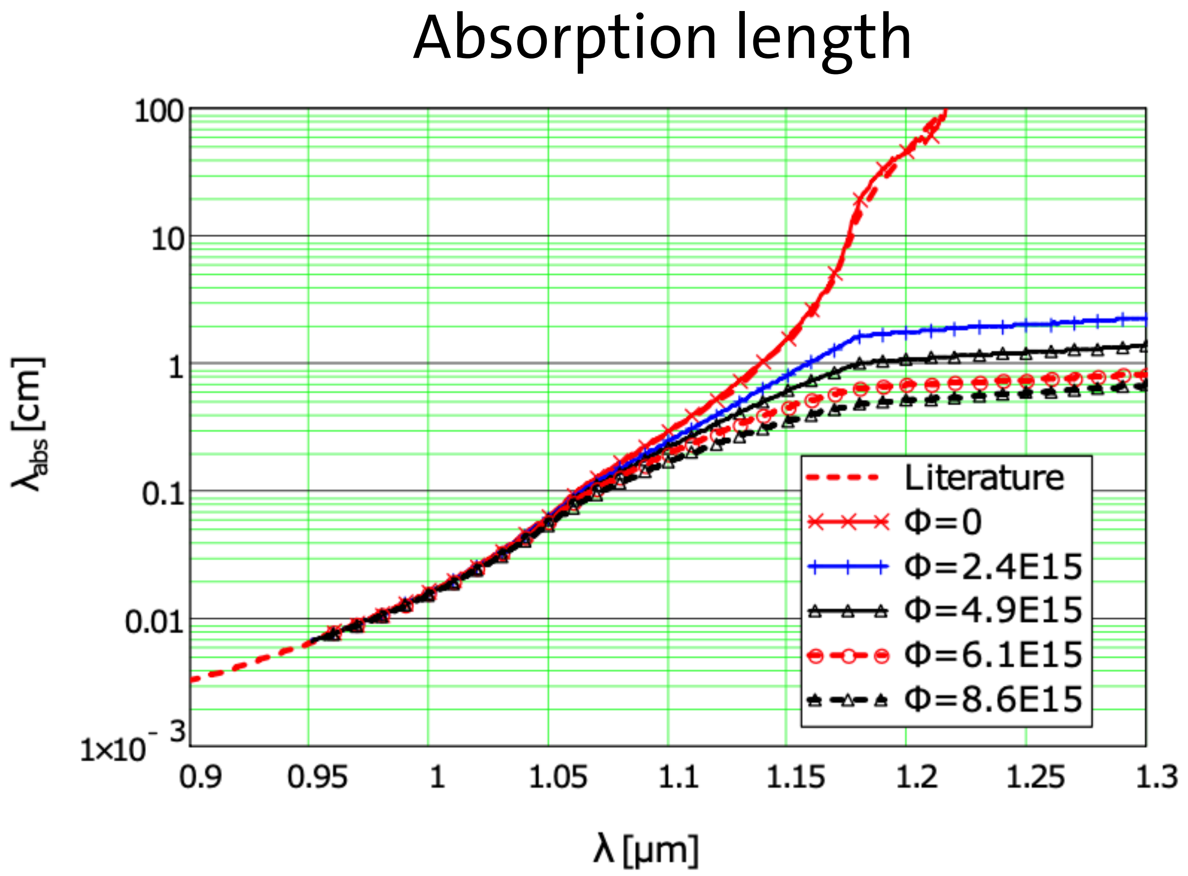
Radiation damage models up to 2×10^{16} n_{eq}/cm^2:

- New “University of Perugia”: 3 level for bulk damage + surface damage
- Hamburg Penta Trap Model (HPTM): 5 levels
- Many more models for lower fluences in the backup

Challenges of radiation damage modelling for fluences up to 1×10^{18} n_{eq}/cm^2:

1. Parametrisation of cluster defects
   - One possibility is an occupation-dependent ionization energy
2. Mobility reduction due to scattering by ionised defects (*I. Mandić et al.*)
3. Possible impact-ionisation via local-level (*V. Vaitkus et al.*)
4. Changes of the absorption of near-infrared light
5. Modelling of acceptor removal
   - First attempts using “analytical” model (*T. Croci et al.*)
   - Can possibly also be modelled as modified incomplete ionisation


Energy in cluster


Absorption length

E. Donegani et al., doi:10.1016/j.nima.2018.04.051

C. Scharf et al., doi:10.1016/j.nima.2020.163955

New physical models required to build in TCAD. Partially this is possible with the “Physical Model Interface” for users. Other things require cooperation with the providers.

ALTERNATIVE MATERIALS

Numerical modelling of diamond in TCAD:

- Diamond is not part of the material library of Synopsys TCAD
- With in the *TimeSpot* project poly-CVD diamond devices with 3D graphite columns have been designed for timing applications (*A. Morozzi et al.*)
- Models for scCVD and pcCVD have been adapted
- Radiation damage not yet included

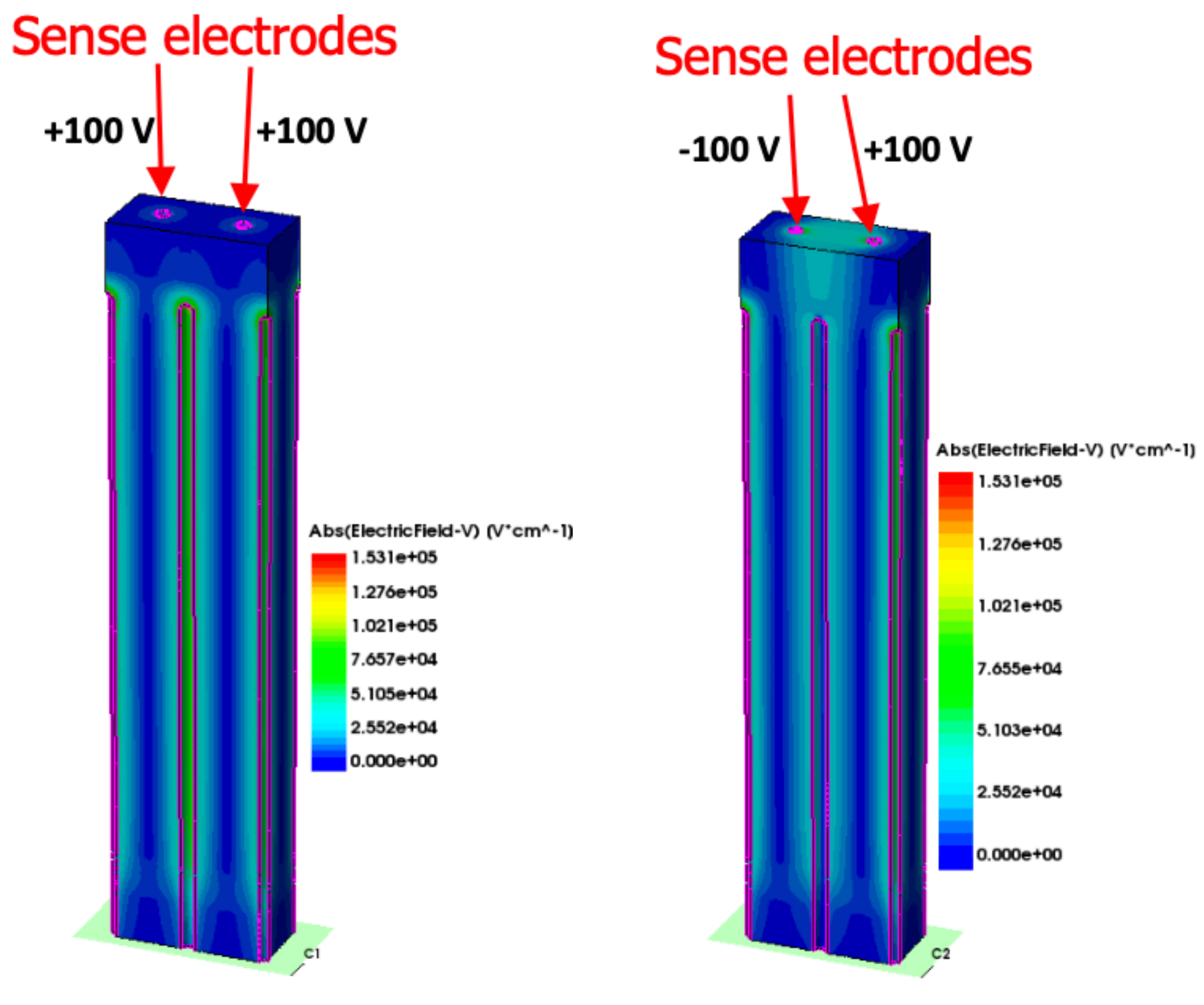
Gallium Nitride (GaN):

- GaN is in the material library of TCAD
- Physical models not as accurate as for silicon
- Investigation of radiation hardness and development of reliable TCAD models within a new RD50 project

Silicon-Germanium (SiGe):

- SiGe is in the material library of TCAD

Comparison between two polarization strategies



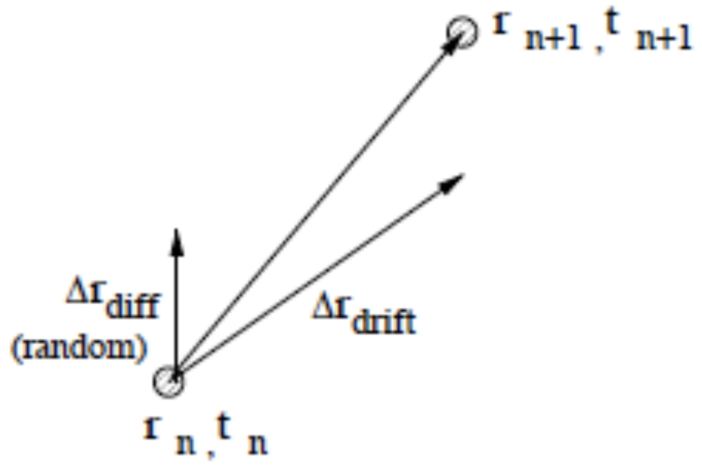
A. Morozzi et al 2020 JINST 15 C01048

→ Radiation damage models for alternative materials need to be developed and incorporated in TCAD

SIGNAL SIMULATION TOOLS I

Main features:

- 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 faster and allows minimization
- The induced current is calculated by Shockley-Ramo's theorem directly



These tools are in many ways complementary to TCAD:

- They 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, resolution, B-field)
- Are often open source code →new materials can easily incorporated
- Are fast and therefore allow for modelling and fitting of the field parameters to the measurements
- Allow TCAD fields to be imported for Monte-Carlo studies

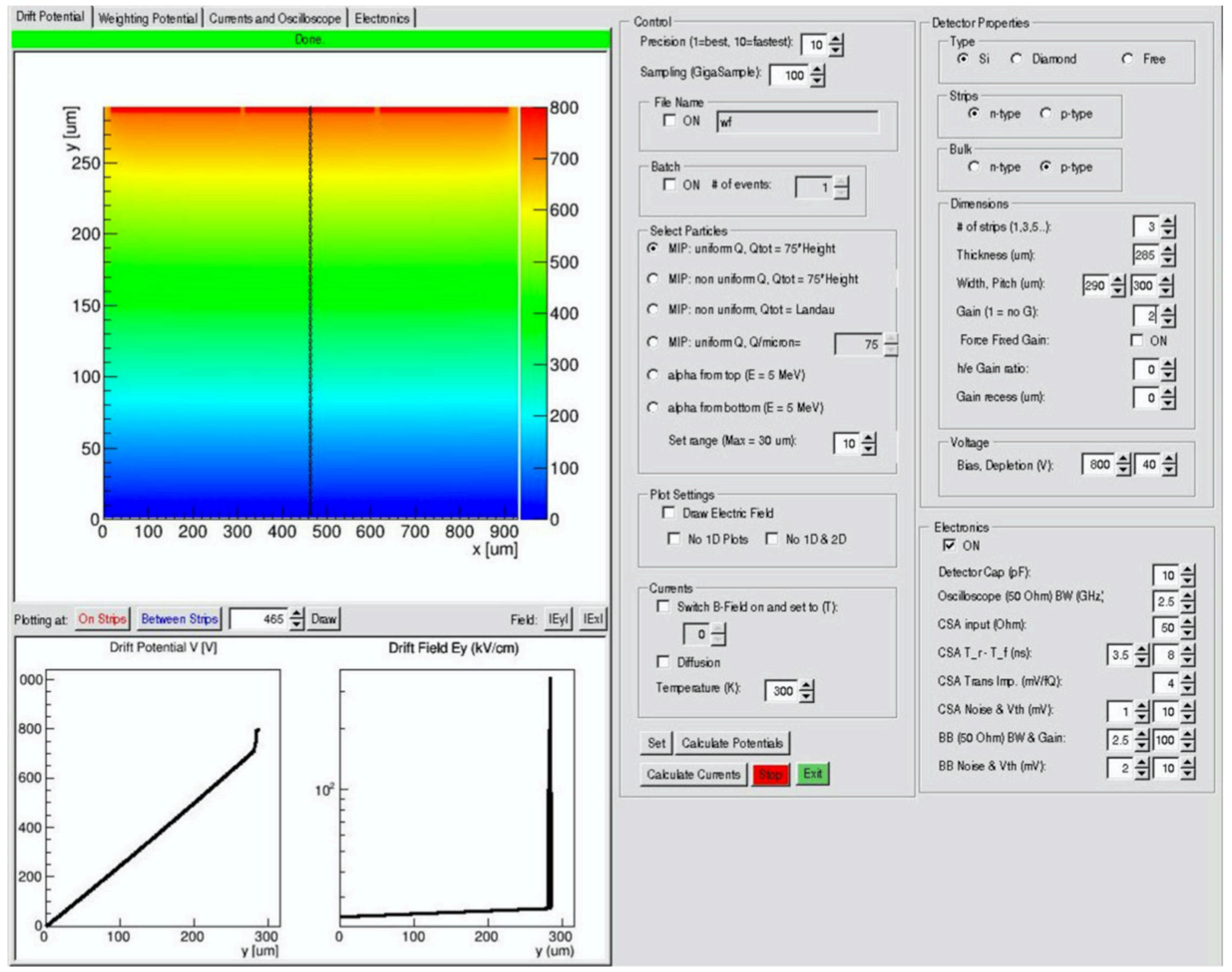
SIGNAL SIMULATION TOOLS II

Many available:

- Weightfield2, KDetSim, PixelAV, TRACS, TCODE, GARFIELD++, Allpix², etc.

Examples:

Weightfield2



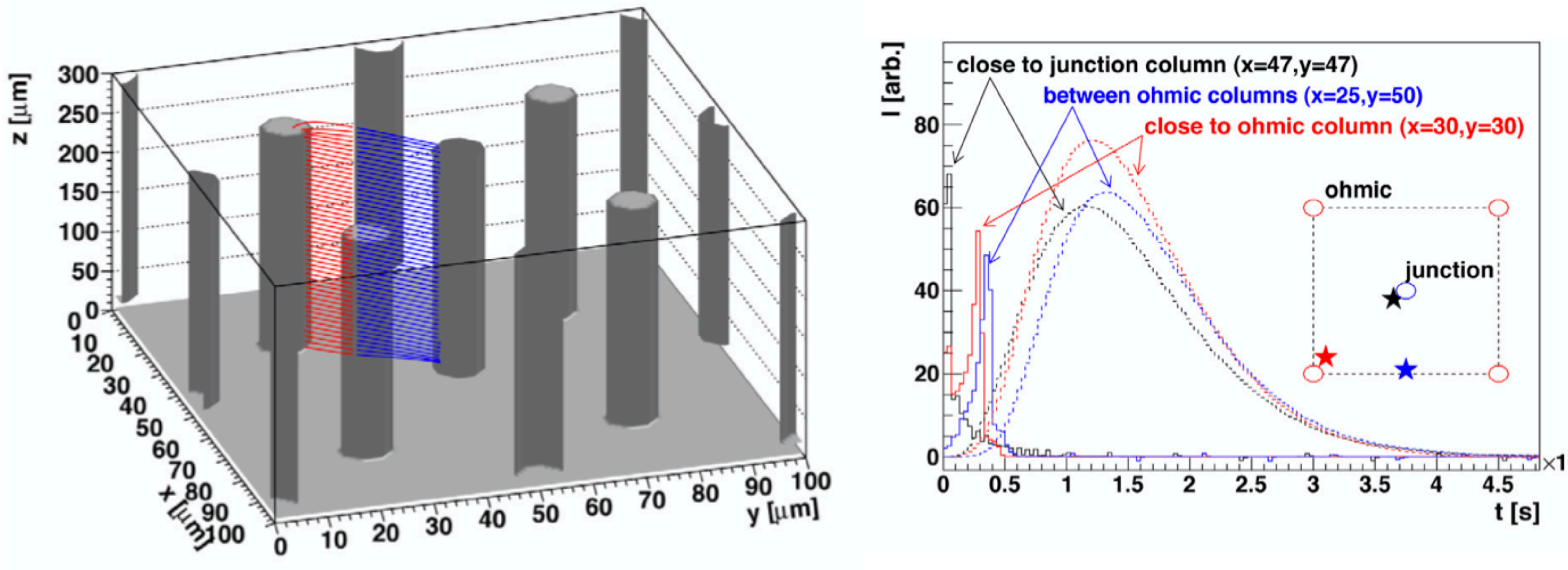
Control
Precision (1=best, 10=fastest): 10
Sampling (GigaSample): 100
File Name
☐ ON wf
Batch
☐ ON # of events: 1
Select Particles
● MIP: uniform Q, Qtot = 75*Height
○ MIP: non uniform Q, Qtot = 75*Height
○ MIP: non uniform, Qtot = Landau
○ MIP: uniform Q, Q/micron= 75
○ alpha from top (E = 5 MeV)
○ alpha from bottom (E = 5 MeV)
Set range (Max = 30 um): 10
Plot Settings
☐ Draw Electric Field
☐ No 1D Plots ☐ No 1D & 2D
Currents
☐ Switch B-Field on and set to (T): 0
☐ Diffusion
Temperature (K): 300

Plotting at: 465

Detector Properties
Type
● Si ○ Diamond ○ Free
Strips
● n-type ○ p-type
Bulk
○ n-type ● p-type
Dimensions
# of strips (1,3,5..): 3
Thickness (um): 285
Width, Pitch (um): 290 300
Gain (1 = no G): 2
Force Fixed Gain: ☐ ON
h/e Gain ratio: 0
Gain recess (um): 0
Voltage
Bias, Depletion (V): 800 40
Electronics
☑ ON
Detector Cap (pF): 10
Oscilloscope (50 Ohm) BW (GHz): 2.5
CSA input (Ohm): 50
CSA T_r - T_f (ns): 3.5 8
CSA Trans Imp. (mV/fQ): 4
CSA Noise & Vth (mV): 1 10
BB (50 Ohm) BW & Gain: 2.5 100
BB Noise & Vth (mV): 2 10

F. Cenna et al., doi:10.1016/j.nima.2015.04.015

KSetSim



G. Kramberger et al., doi:10.1016/j.nima.2019.04.088

Main challenges:

- Radiation damage simulation based on TCAD

➡Electrical field and trapping rates for electron and holes from TCAD (often trapping rates are taken independently from TCAD → inconsistency)

$$\boxed{\begin{aligned} \frac{1}{\tau_e} &= \sum_{defects} v_e^{th}\sigma_{t,n}(1-f_t)N_t \\ \frac{1}{\tau_h} &= \sum_{defects} v_h^{th}\sigma_{t,p}f_tN_t \end{aligned}}$$

EXPERIMENTAL SETUP SIMULATION

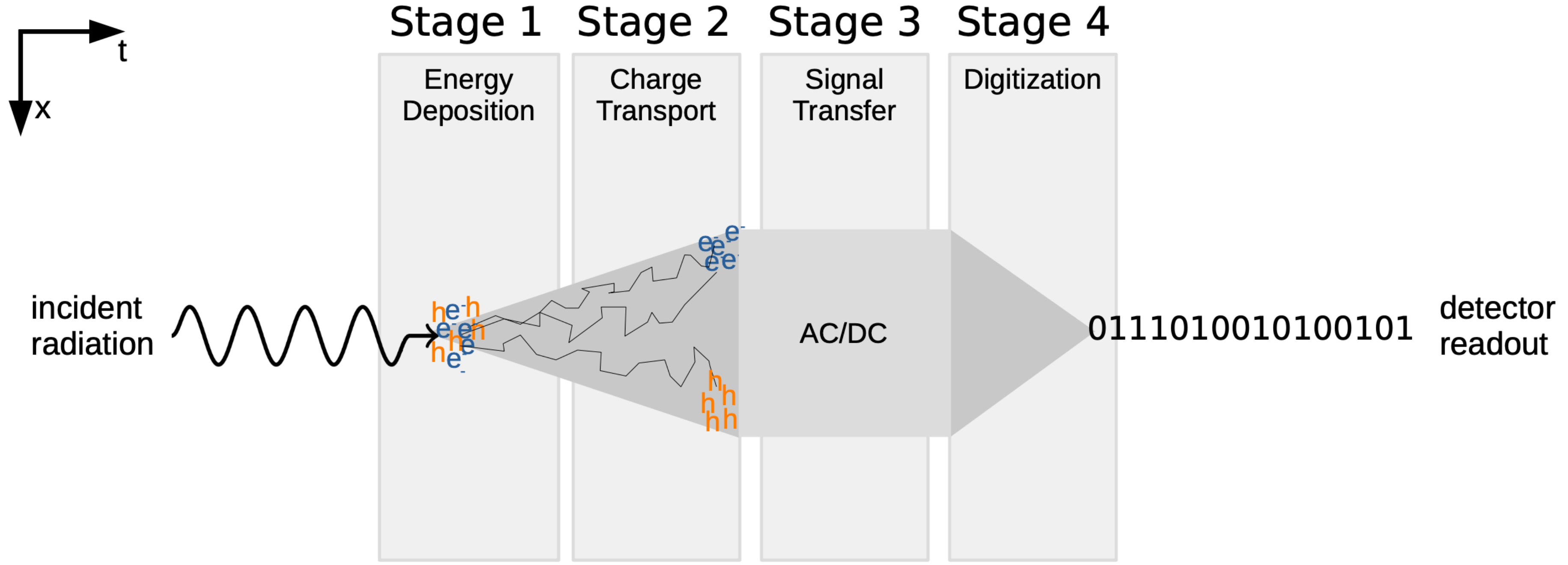
S. Spannagel et al., doi:10.1016/j.nima.2018.06.020

Allpix² Framework:

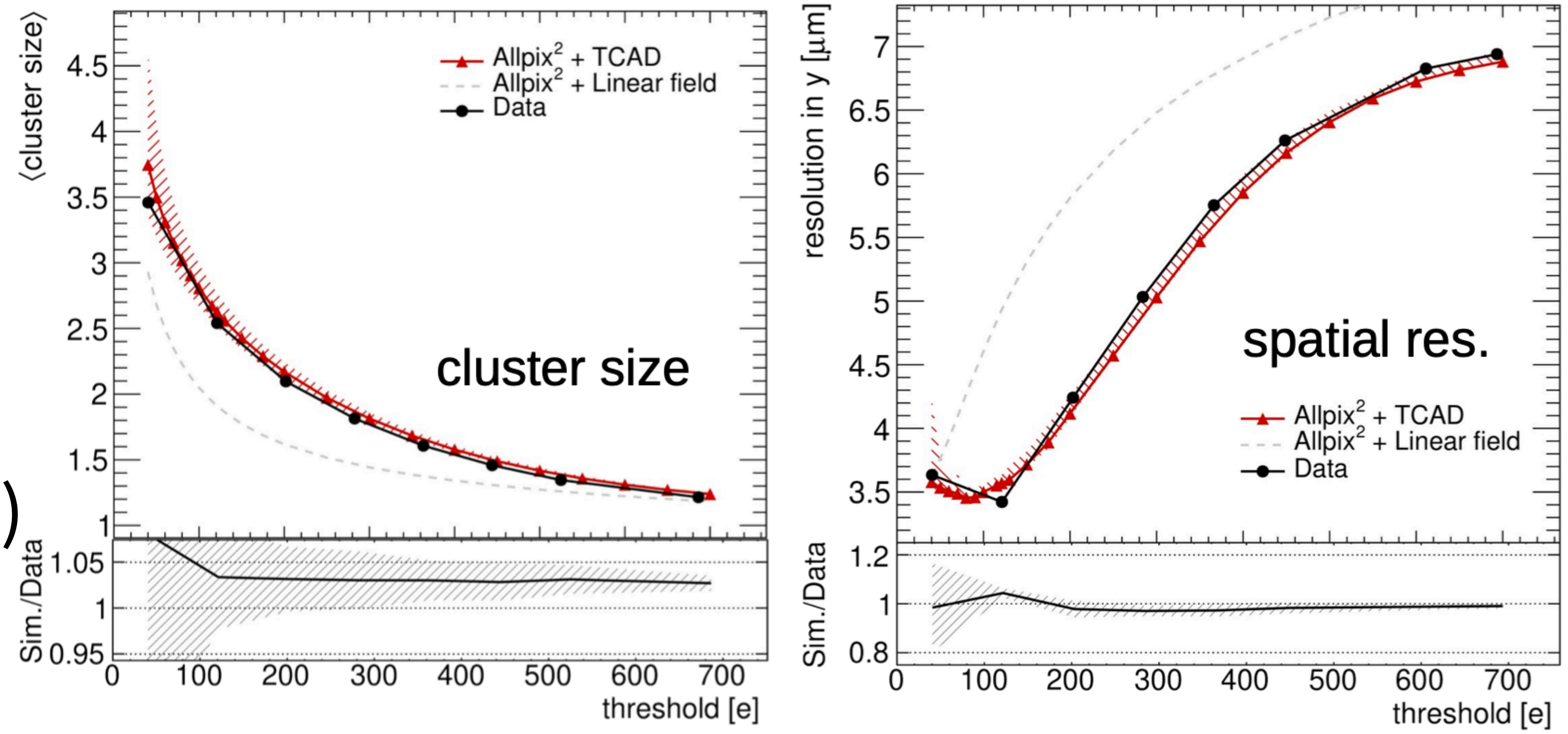
- Simulate full chain: energy deposition, signal formation, transfer and digitisation
- Include stochastic effects, fluctuations, secondaries
- Requires simplifications:
  - No self-interaction, static electric field, empirical models for different stages, …
- Allows to derive performance parameters:
  - Position resolution, timing, efficiency
  - Combine with results from TCAD to increase accuracy

Further developments/challenges:

- Charge carrier lifetime modelling (effects from epi layer)
- Charge carrier multiplication
- 3D sensors, hexagonal pixels
- Radiation damage modelling of sensor + electronics



Validation



D. Dannheim et al., doi:10.1016/j.nima.2020.163784

FULL DETECTOR SYSTEM SIMULATION

I. Dawson (Ed.), CERN-2021-001


CERN Yellow Reports:
Monographs

CERN-2021-001

Radiation effects
in the LHC experiments

Impact on detector performance and operation

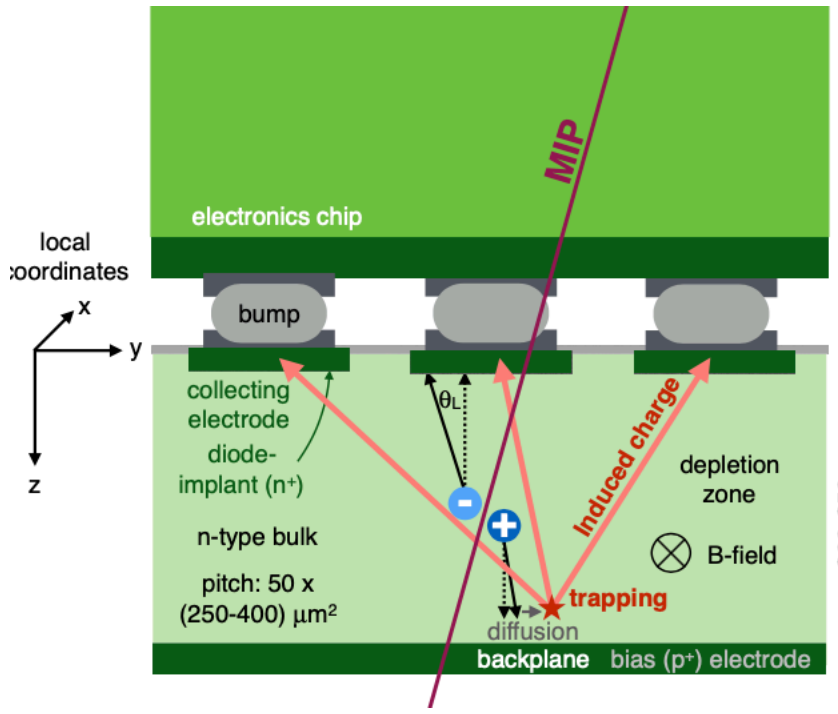
Editor:
I. Dawson

Aim:

- Understand the impact of radiation effects on detector performance and operation

Requires:

- Simulation of radiation environments
  - Event generation (e.g. PHYTHIA8),
  - particle transport (e.g. FLUKA, Geant4)
  - Radiation damage estimators (1 MeV neutron equivalent fluence, TID)
- Measurements of radiation damage on silicon sensors
  - Leakage current, depletion voltage, hit/cluster efficiency, collected charge etc.
- Simulations radiation effects and signal response in silicon sensors
  - Examples are the ATLAS pixel digitizer or PixelAV in case of CMS. Both require electrical field maps from TCAD.



Some challenges:

- Radiation damage estimators
- Sensor temperatures in running experiments often not known precisely
- Predictive radiation damage models from TCAD

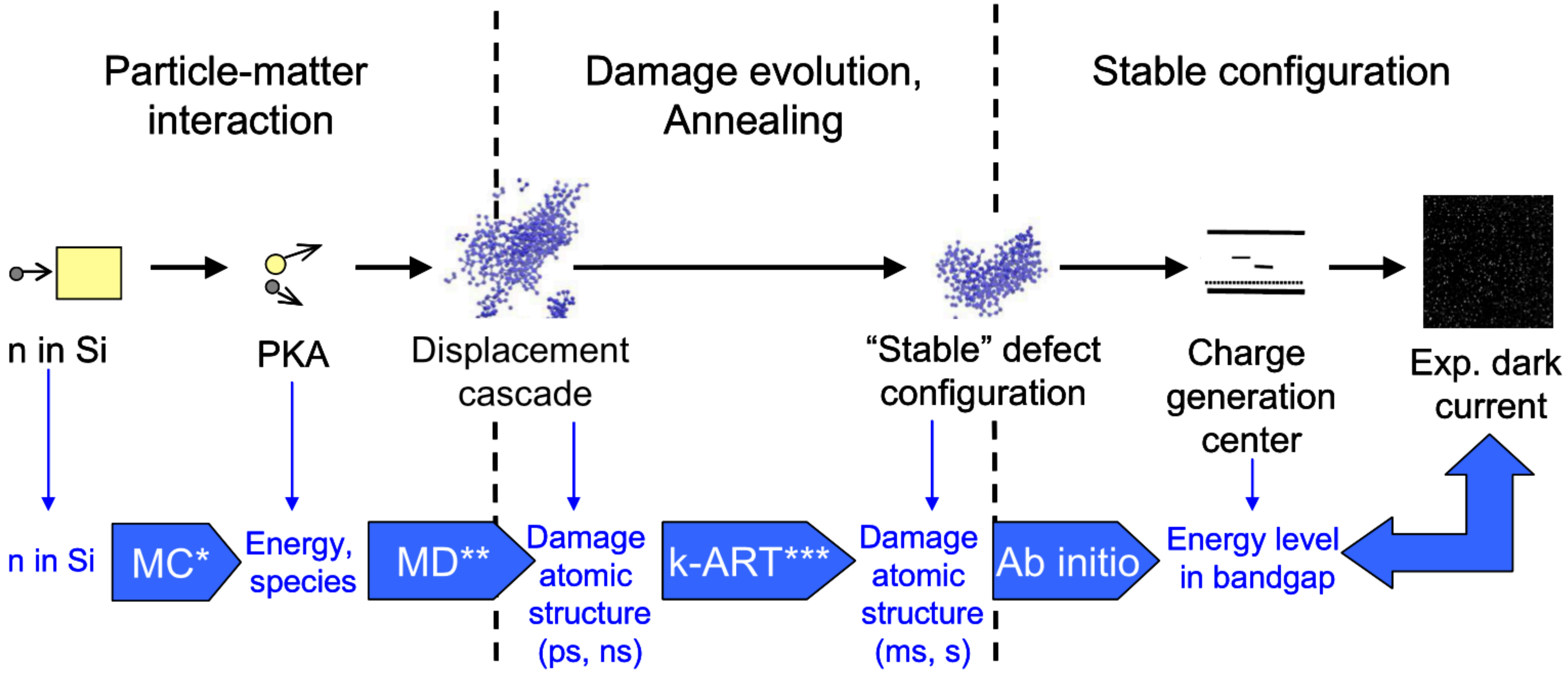
DISPLACEMENT DAMAGE SIMULATION

Simulation of the full damage process:

- Primary interaction and distribution of PKA energies (Geant4)
- Spatial distribution of displaced atoms and vacancies (Geant4/Trim)
- Recombination of primary damage (MD, KMC)
- Point defect formation (KMC)
- Ab initio simulation for the determination of energy levels

TCAD device simulation

M. Raine et al., doi:10.1109/TNS.2016.2615133



Particle-matter interaction | Damage evolution, Annealing | Stable configuration

n in Si → PKA → Displacement cascade → "Stable" defect configuration → Charge generation center → Exp. dark current

n in Si → MC* → Energy, species → MD** → Damage atomic structure (ps, ns) → k-ART*** → Damage atomic structure (ms, s) → Ab initio → Energy level in bandgap

*MC = Monte Carlo (Binary Collision Approximation)
**MD = Molecular Dynamics
***k-ART = Kinetic Activation-Relaxation Technique

Possible application:

- Improved NIEL scaling, describe observed macroscopic "NIEL violation"
- Single TCAD model describing damage from protons, neutrons and electrons

CONCLUSIONS

TCAD:

- TCAD is an essential tool for the development of new detectors. The long term access to TCAD (in this case Synopsys) tools through Europractice or similar frames is essential (similar for TF7)
- Cooperation with software providers needed to add certain new features in TCAD
- Community wide data availability for the development and validation of radiation damage models.
  - Data from test structures to disentangle different effects

Signal simulation tools:

- Large number of individually maintained tools. The community could benefit from fewer but well maintained and supported detector simulation packages.
- Implement empirical models which are accurate but does not degrade the runtime
- Validation data and reference data for new algorithms (beam tests, data preservation)

Displacement damage simulation:

- Simulation chain can be build with open-source code
- Requires good set of reliable experimental data

Thank you for your attention!

BACKUP

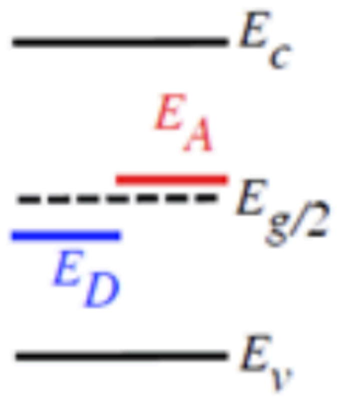
SIMULATION TOOLS

Synopsys TCAD	https://www.synopsys.com/silicon/tcad.html
Silvaco TCAD	https://silvaco.com/tcad/
COGENDA TCAD	https://cogenda.com
Weightfield2	http://personalpages.to.infn.it/~cartigli/Weightfield2
KDetSim	http://kdetsim.org
PixelAV	https://physics-astronomy.jhu.edu/directory/morris-swartz/
TRACS	https://github.com/IFCA-HEP/TRACS
TCODE	https://github.com/MultithreadCorner/TCode
GARFIELD++	https://garfieldpp.web.cern.ch/garfieldpp/
Allpix^2	https://project-allpix-squared.web.cern.ch/project-allpix-squared/
Geant4	https://geant4.web.cern.ch/
FLUKA	http://www.fluka.org/

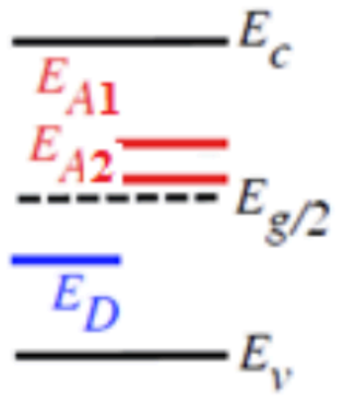
RADIATION DAMAGE MODELS

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



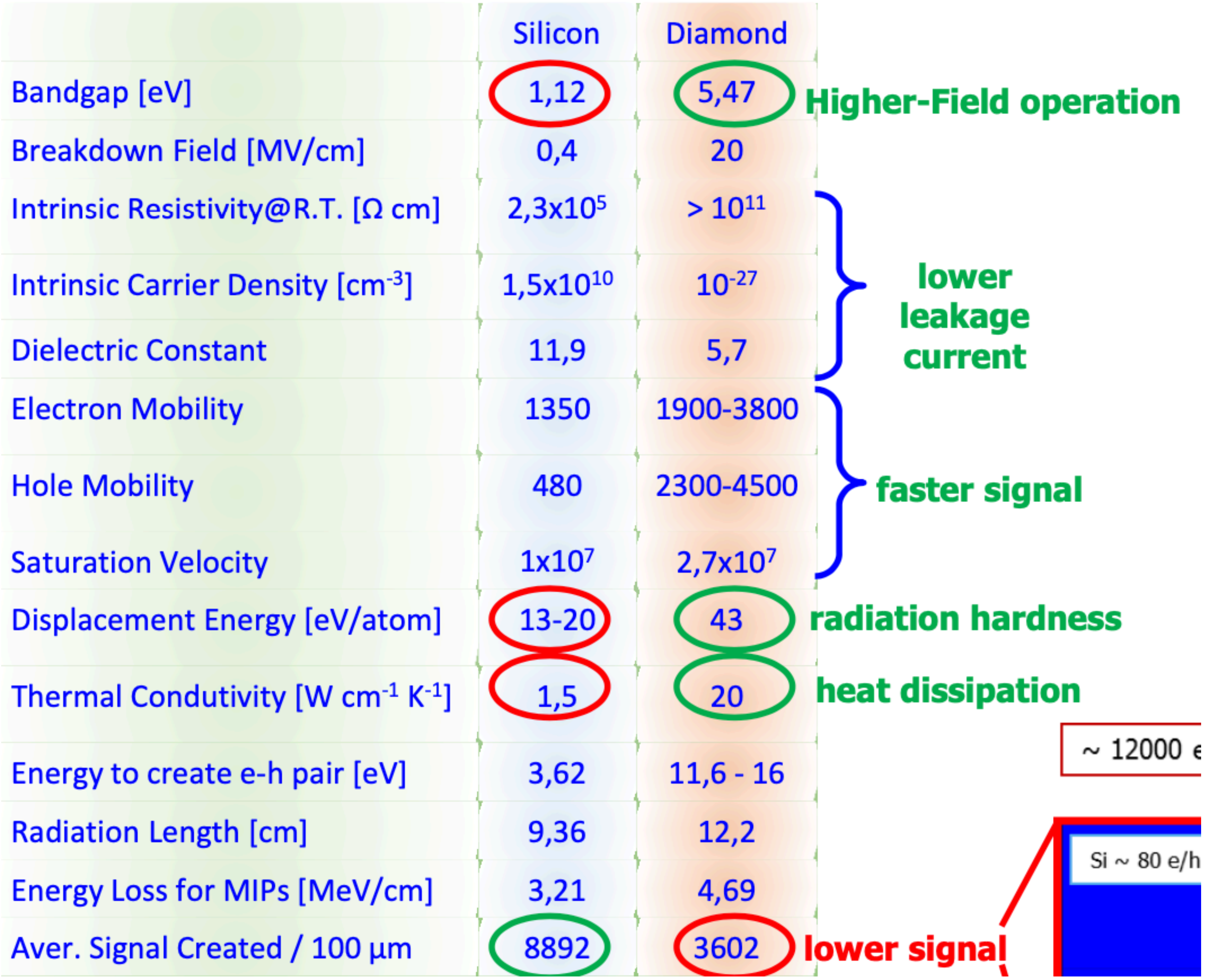
Perugia model
Three levels associated to donor CiOi, 1st acceptor to V_2 and 2nd acceptor to V_3



Model	E [eV]	g_{int} [cm^1]	$\sigma_{e[}$[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]	$\sigma_{e[}$[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

SILICON - DIAMOND



	Silicon	Diamond
Bandgap [eV]	1,12	5,47
Breakdown Field [MV/cm]	0,4	20
Intrinsic Resistivity@R.T. [Ω cm]	$2,3\times10^{5}$	$> 10^{11}$
Intrinsic Carrier Density [cm^{-3}]	$1,5\times10^{10}$	10^{-27}
Dielectric Constant	11,9	5,7
Electron Mobility	1350	1900-3800
Hole Mobility	480	2300-4500
Saturation Velocity	1×10^{7}	$2,7\times10^{7}$
Displacement Energy [eV/atom]	13-20	43
Thermal Condutivity [W cm^{-1} K^{-1}]	1,5	20
Energy to create e-h pair [eV]	3,62	11,6 - 16
Radiation Length [cm]	9,36	12,2
Energy Loss for MIPs [MeV/cm]	3,21	4,69
Aver. Signal Created / 100 µm	8892	3602

Higher-Field operation

lower leakage current

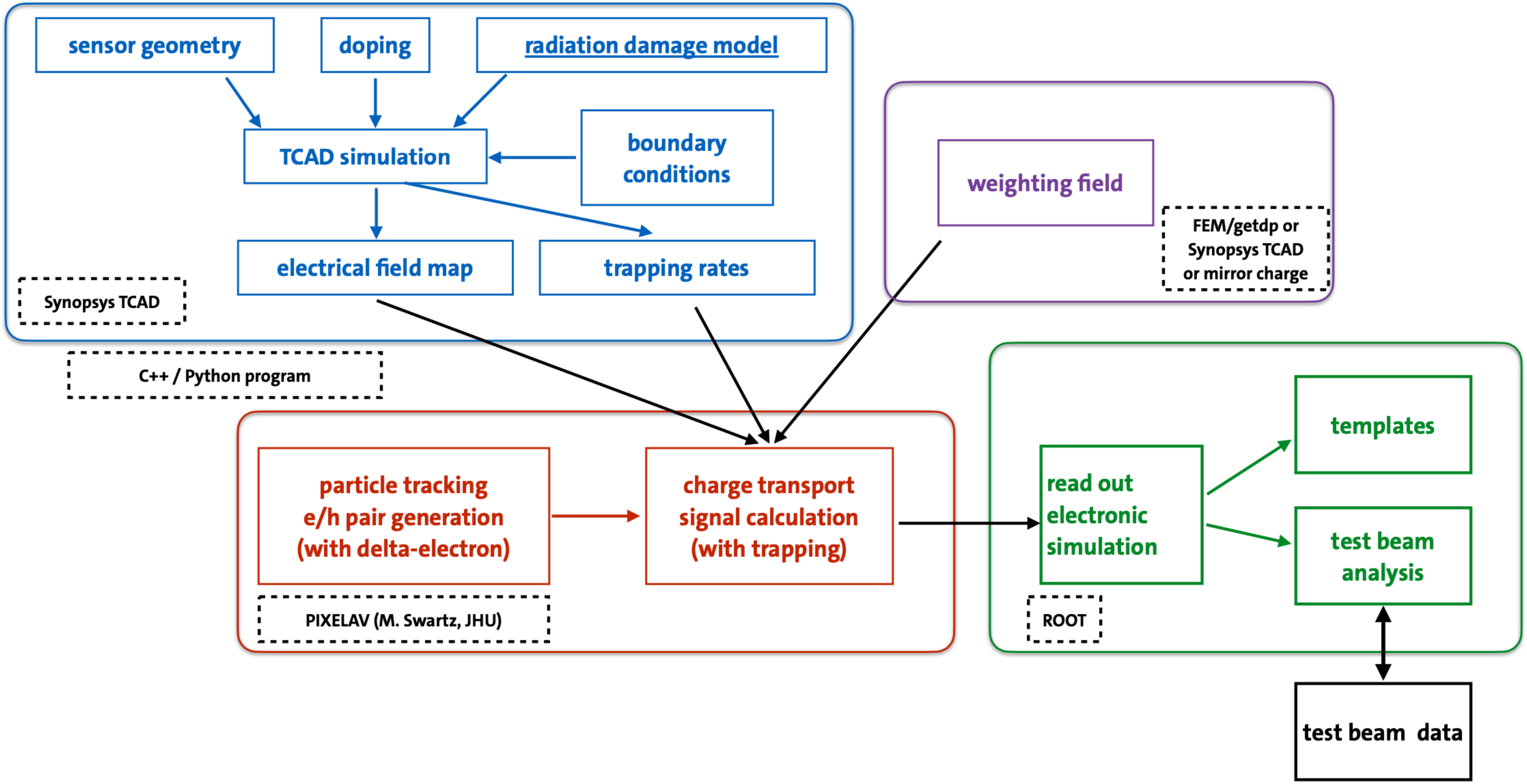
faster signal

radiation hardness

heat dissipation

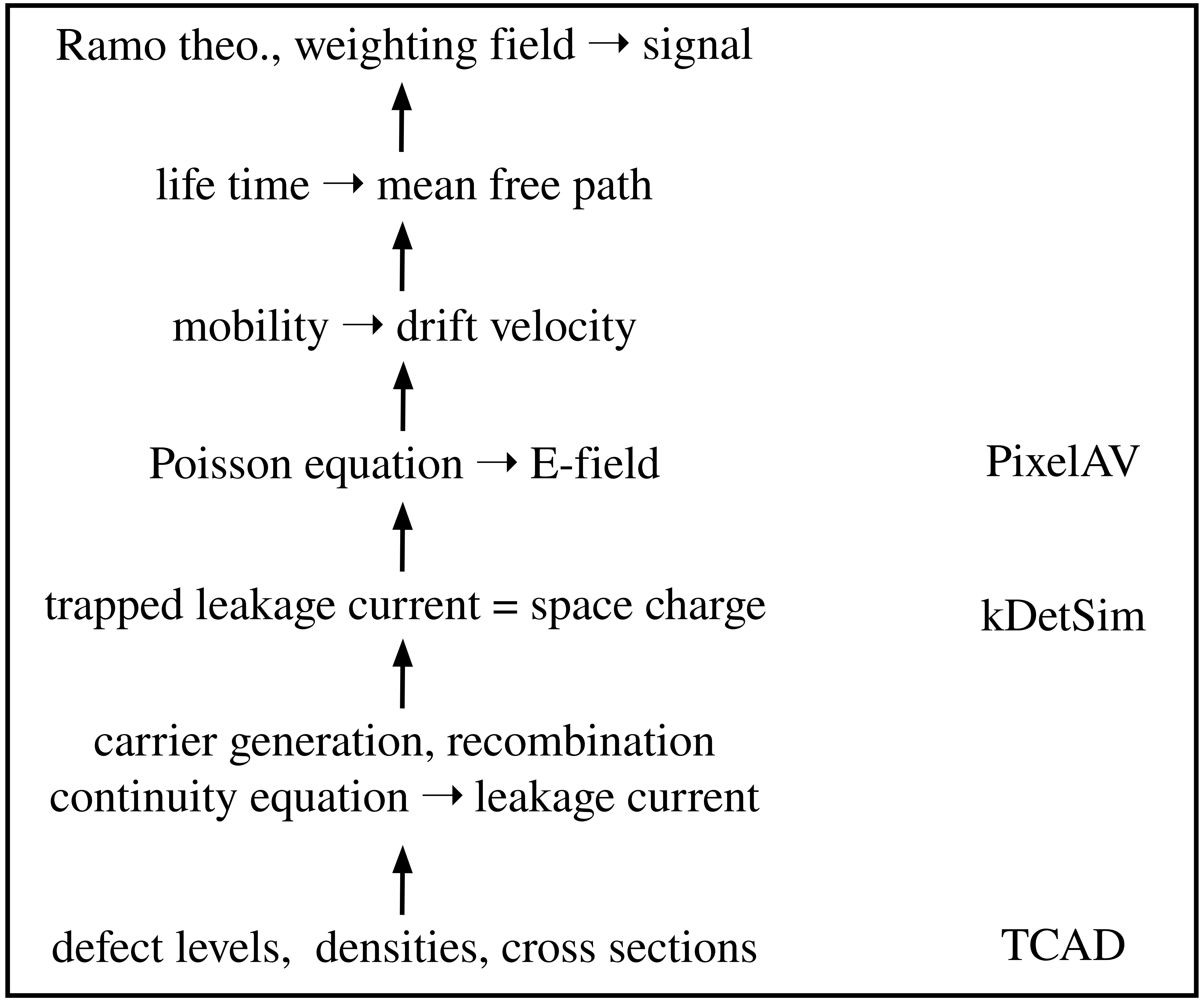
lower signal

SIMULATION FLOW



LEVELS OF MODELLING

Levels of modelling



Ramo theo., weighting field → signal

↑

life time → mean free path

↑

mobility → drift velocity

↑

Poisson equation → E-field — PixelAV

↑

trapped leakage current = space charge — kDetSim

↑

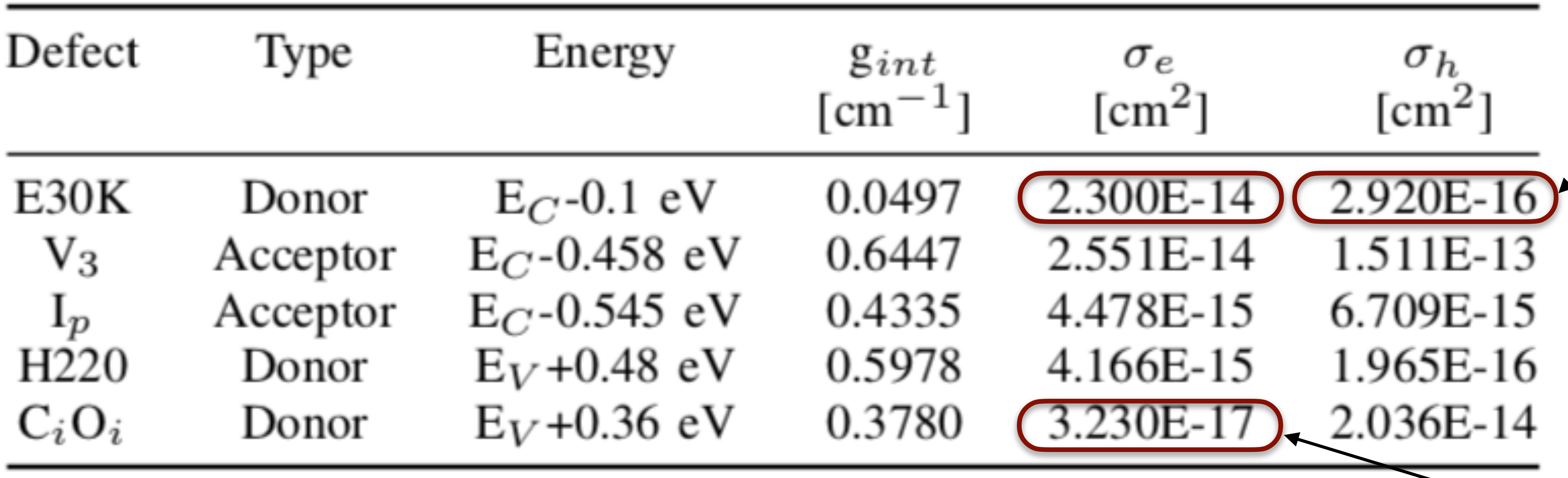
carrier generation, recombination
continuity equation → leakage current

↑

defect levels, densities, cross sections — TCAD

HPTM PARAMETER

Result of tuning: Hamburg Penta Trap Model (HPTM)



Defect	Type	Energy	g_{int} [cm^{-1}]	σ_e [cm^2]	σ_h [cm^2]
E30K	Donor	E_C-0.1 eV	0.0497	2.300E-14	2.920E-16
V_3	Acceptor	E_C-0.458 eV	0.6447	2.551E-14	1.511E-13
I_p	Acceptor	E_C-0.545 eV	0.4335	4.478E-15	6.709E-15
H220	Donor	E_V+0.48 eV	0.5978	4.166E-15	1.965E-16
C_iO_i	Donor	E_V+0.36 eV	0.3780	3.230E-17	2.036E-14

fixed

fixed

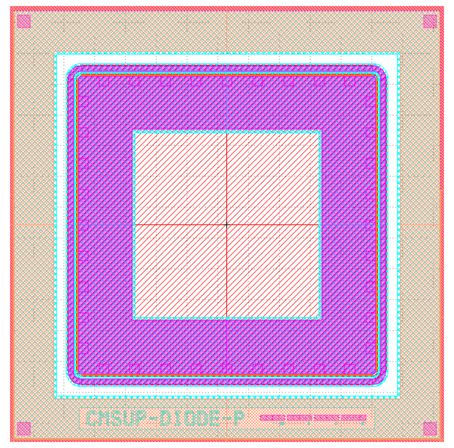
- **Type** and **energy** of defects were **fixed**. Values taken from R. Radu et al. JAP 117, 164503 (2015)
- Trap **concentration** of defects: **$N = g_{int} \cdot \Phi_{eq}$**
- **E30K** electron and hole cross section were fixed
- **C_iO_i** electron cross section was fixed
  ➡12 free parameter
- Optimisation done with the nonlinear simplex method

HPTM COMPARISON TO DATA

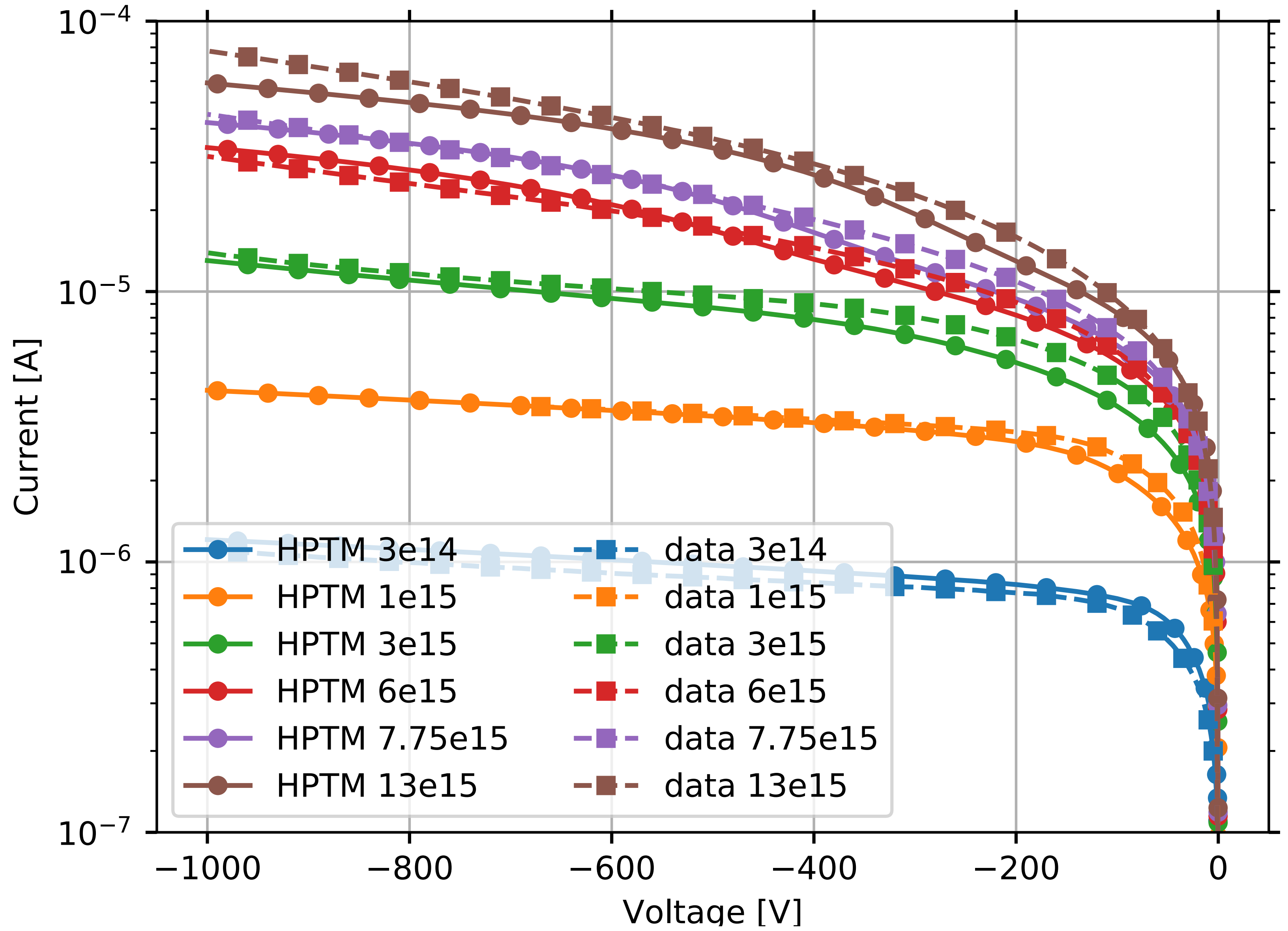
I-V, C-V and CCE(IR) for fluences from 0.3 - 13x10^{15} n$_{eq}$/cm^2 at T= -20 °C (for T= -30 °C see backup)

- HPK **p-type** 200 µm thick diodes
- Irradiated with **24 GeV/c protons** at CERN IRRAD
  - Fluences: 0.3, 1, 1.5, 2.4, **3**, **6**, 7.75, **13x10^{15} n$_{eq}$/cm^2**

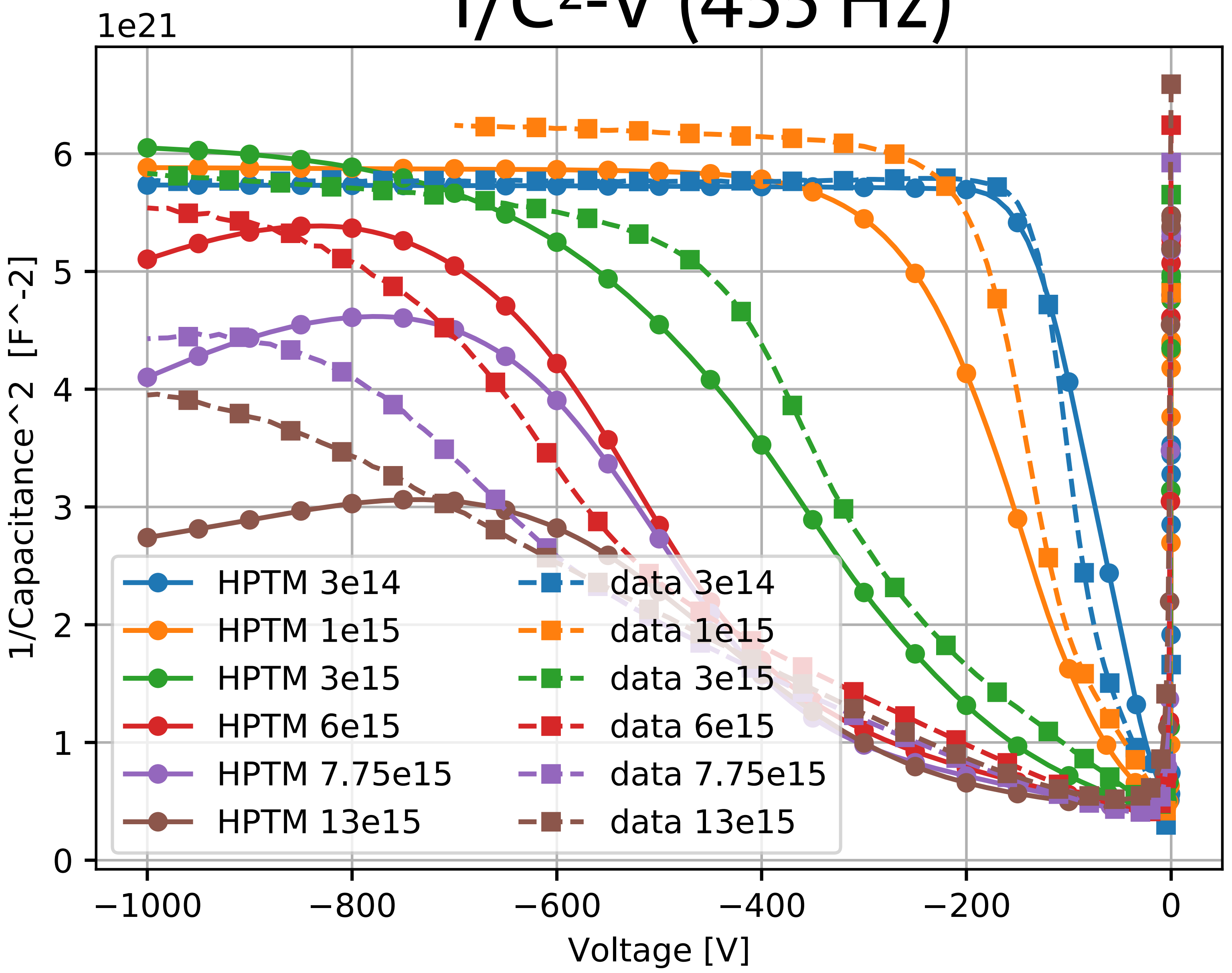
5 mm x 5 mm



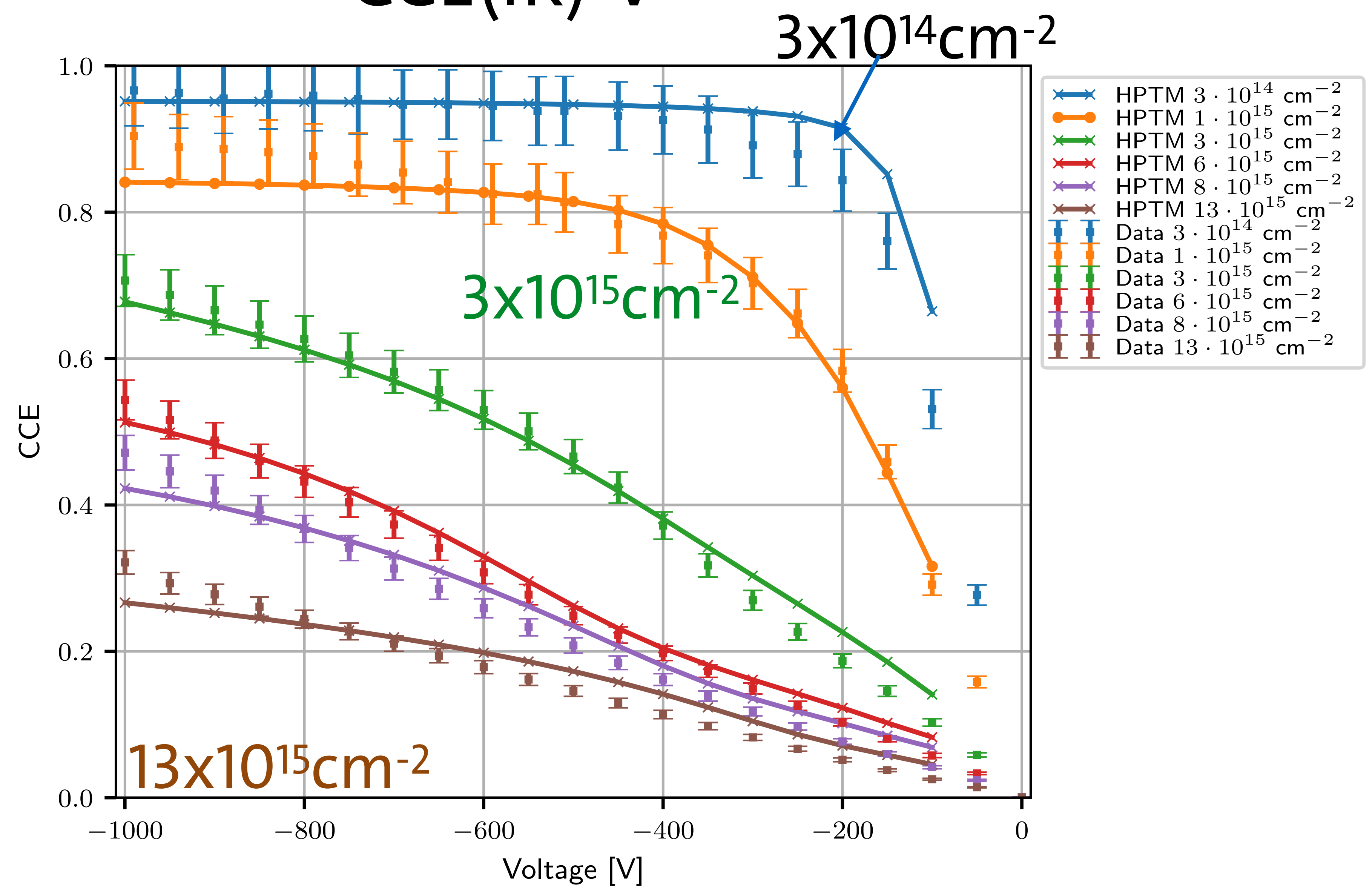
I-V



1/C^2-V (455 Hz)



CCE(IR)-V



- The simulation for 0.3 and 1x10^{15} n$_{eq}$/cm^2 are **extrapolations** and the 7.75x10^{15} n$_{eq}$/cm^2 is a **interpolation**
- The simulation **agrees** with the measurements within **20%** for **all fluences** and **voltages**
- **Double peak structure** in the electrical field for fluences ≥ 3•10^{15} n$_{eq}$/cm^2 (see backup)