

Simulation tools for radiation detectors before and after irradiation

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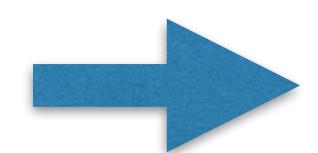
2nd Allpix² User Workshop
17 -19 August 2021

Introduction

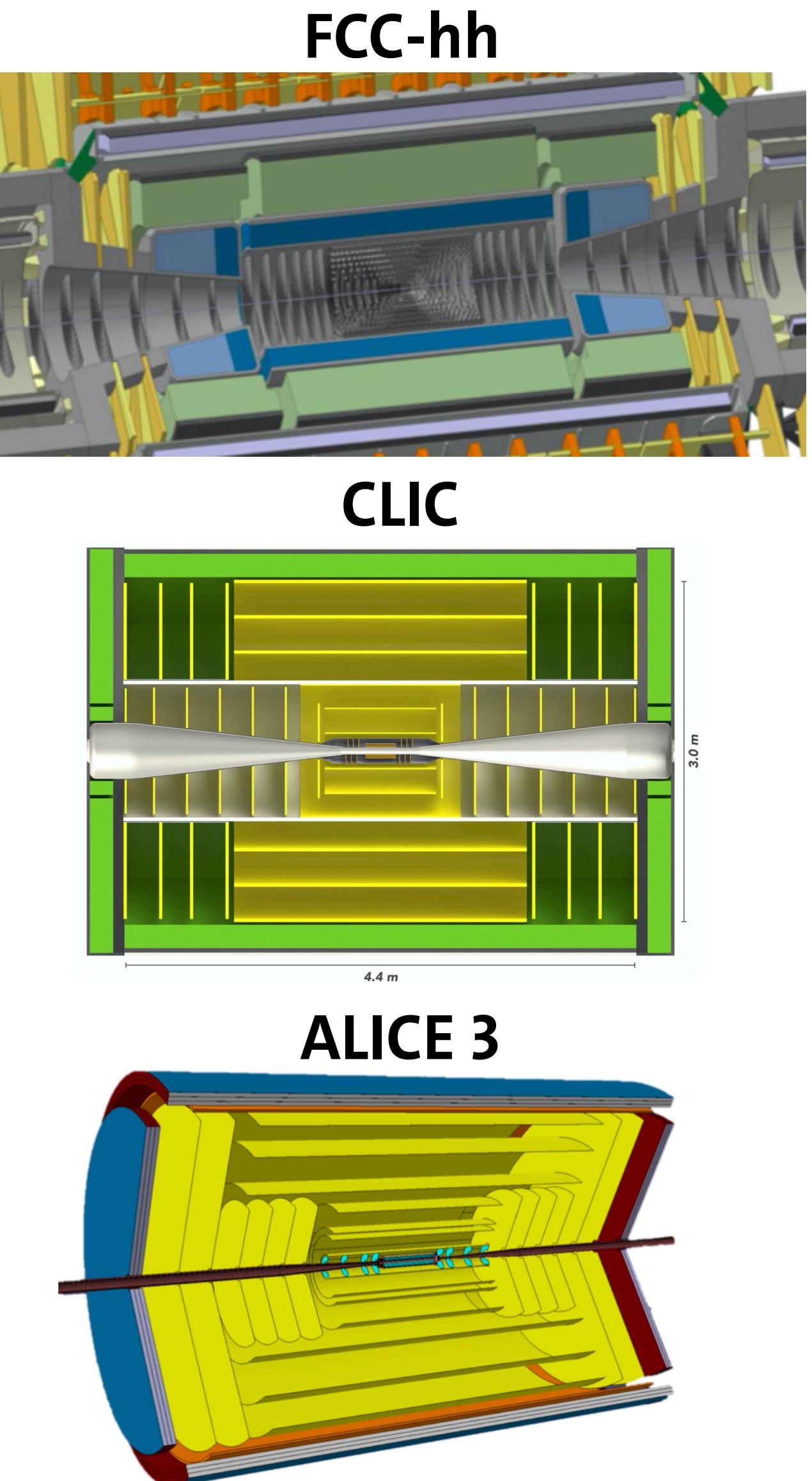
Future requirements for solid state detectors:

- **FCC-hh**
 - Up to $\Phi_{\text{eq}} \approx 1 \times 10^{18} \text{ cm}^{-2}$ 1 MeV neutron equivalent fluence , TID 300 MGy
 - Pixel size: $25 \times 50 \mu\text{m}^2$
 - Timing of tracks at the < 10 ps level
- **Future Linear High energy e⁺e⁻ Machines**
 - Single point resolution: $\approx 3 \mu\text{m}$
 - Lowest possible mass: $\approx 0.2\% X_0$ per layer
 - Pixel size: $\leq 25 \times 25 \mu\text{m}^2$
- **Strong Interaction Experiments**
 - DCA resolution: $\approx 25 \mu\text{m}$ at $p_t = 100 \text{ MeV}/c$
 - Material budget: $0.1\% X_0$ per layer
 - Pixel size: $\leq 10 \times 10 \mu\text{m}^2$

*) DCA = Distance of closest approach



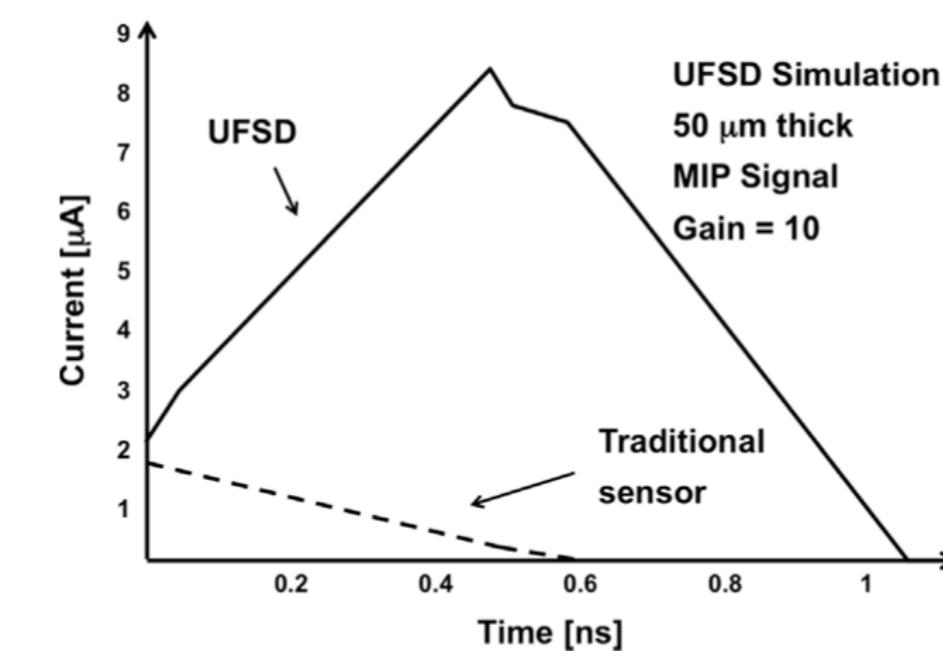
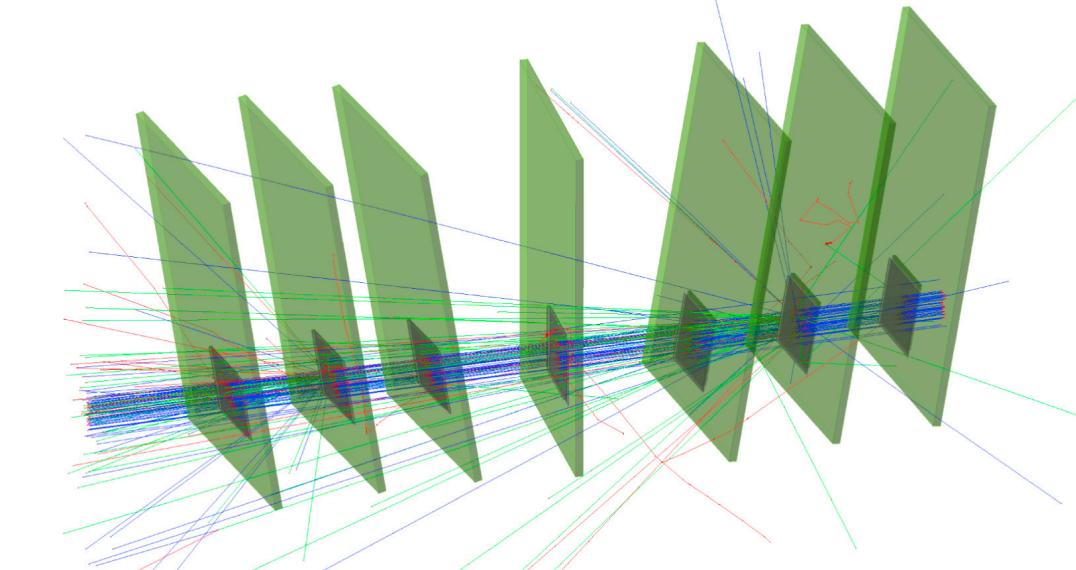
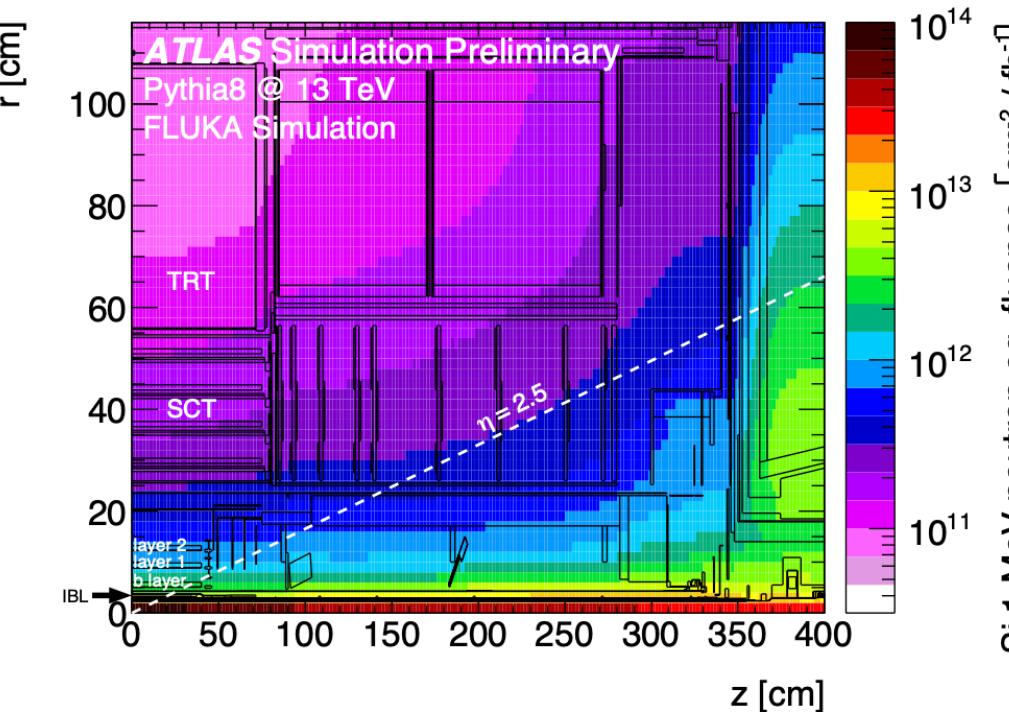
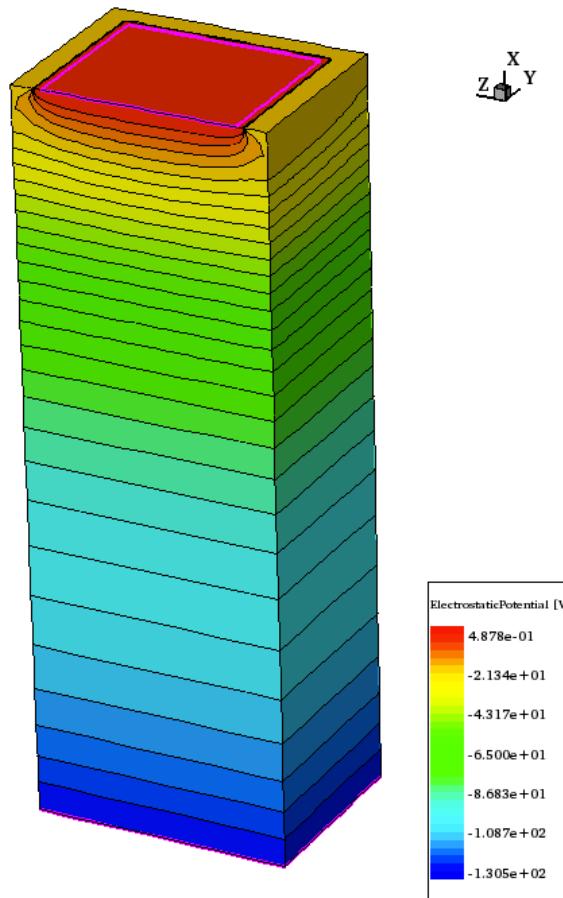
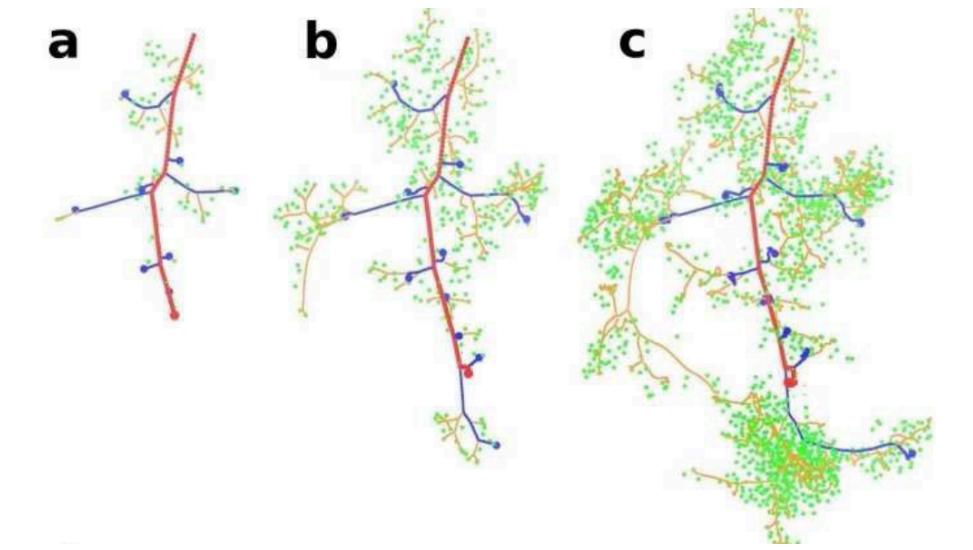
- Extreme radiation tolerance
- Very fast
- Very thin
- High granularity



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

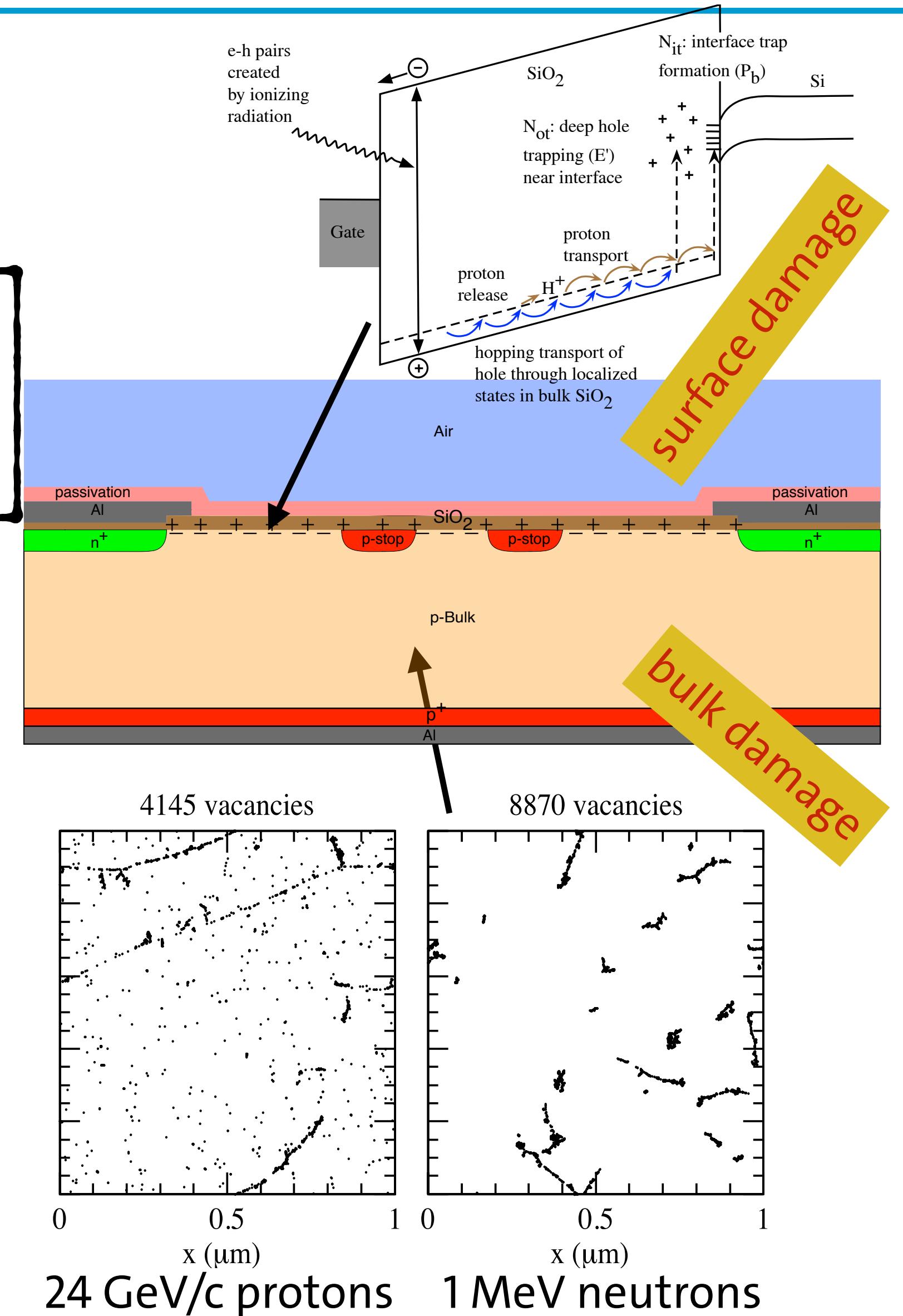


Radiation damage

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-SiO₂ interface
- Trapping near to the Si-SiO₂ 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

TCAD overview

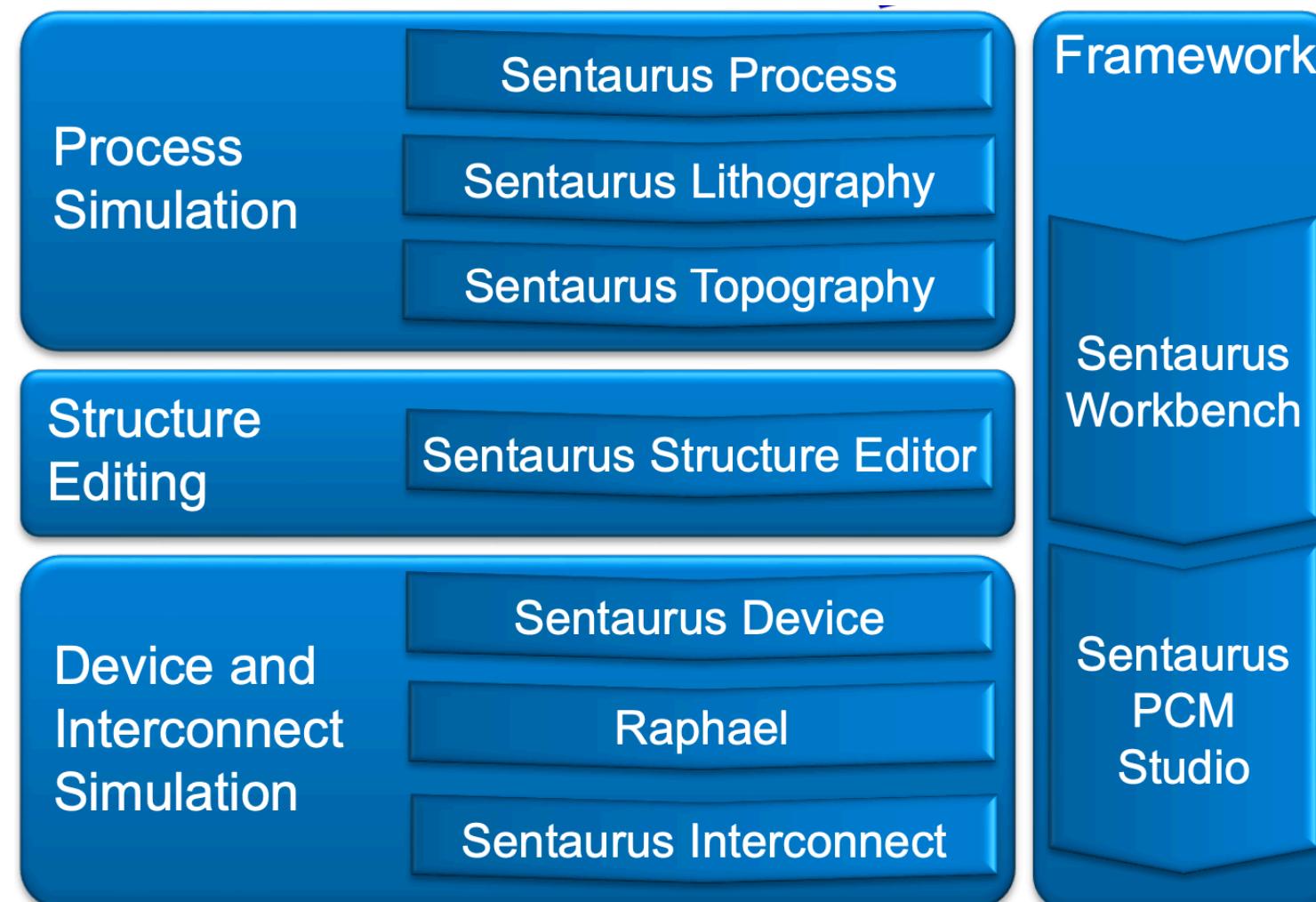
Technology Computer-Aided Design (TCAD):

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

SYNOPSYS®

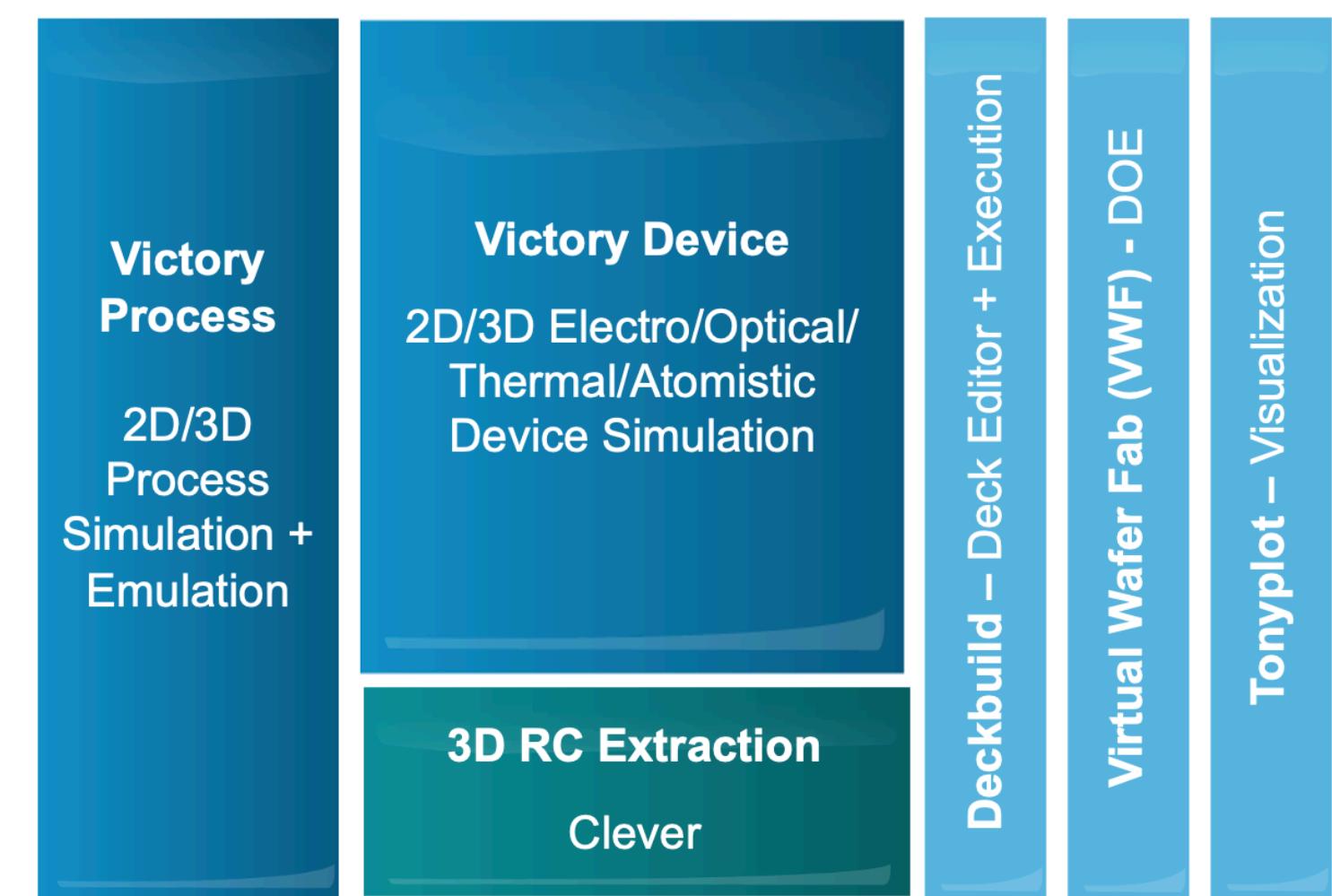
Silicon to Software™

<https://www.synopsys.com>



SILVACO

<https://silvaco.com>



- Licences for Synopsys via



→ Majority of users in HEP

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

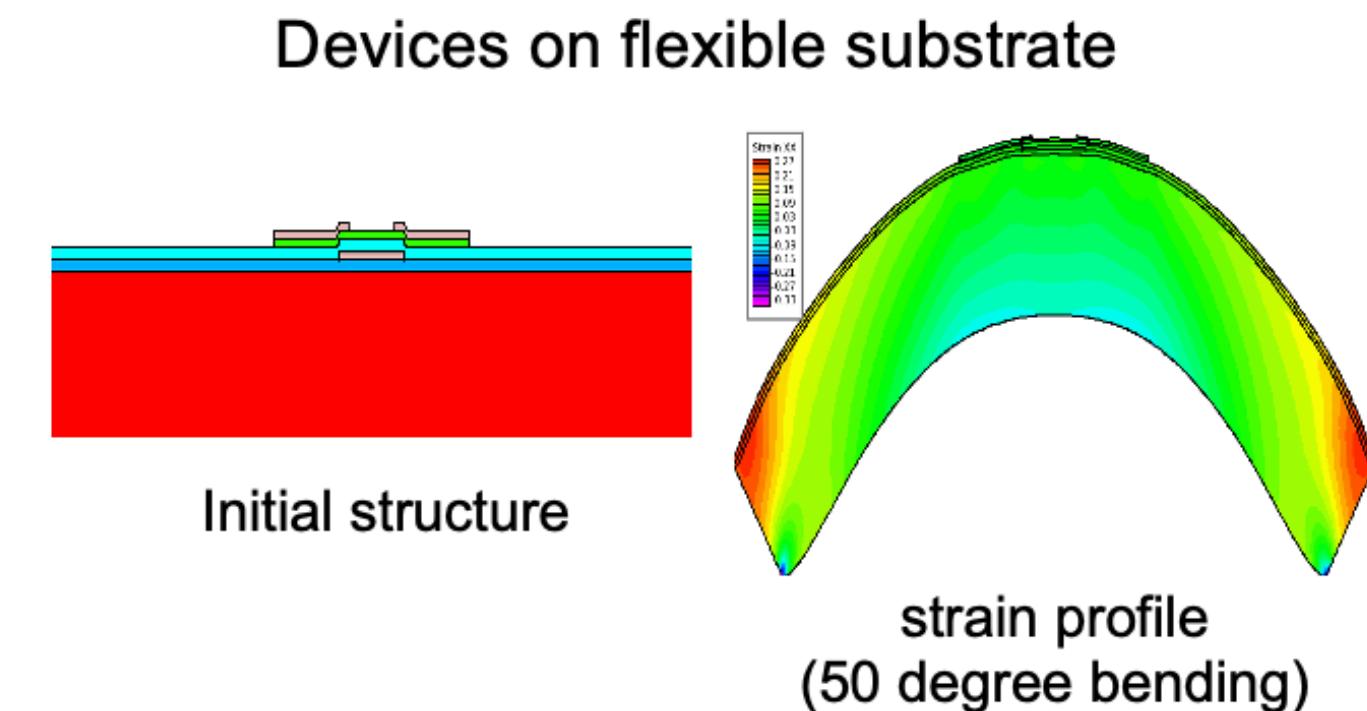
PROCESS simulation I

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.



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 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

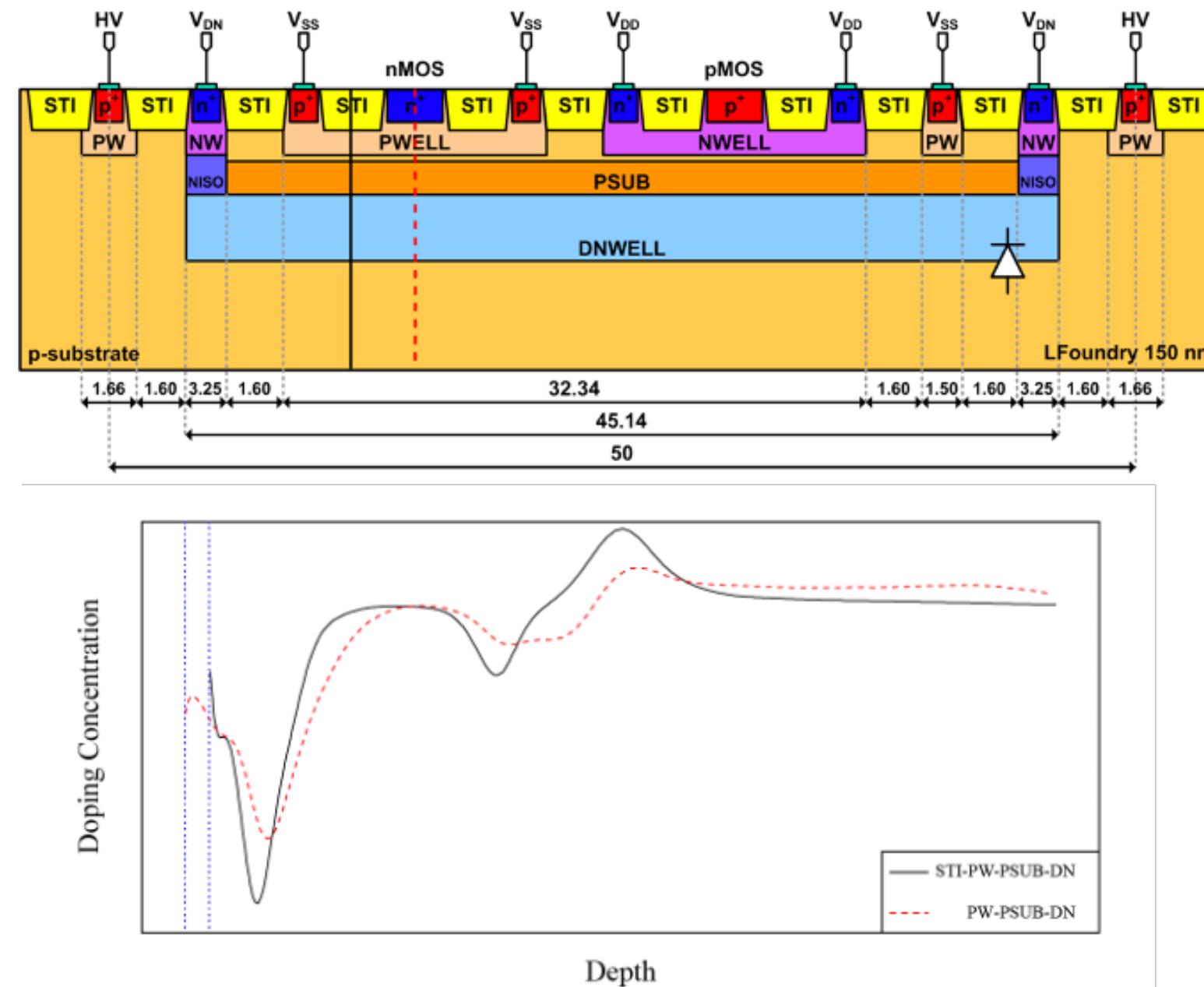
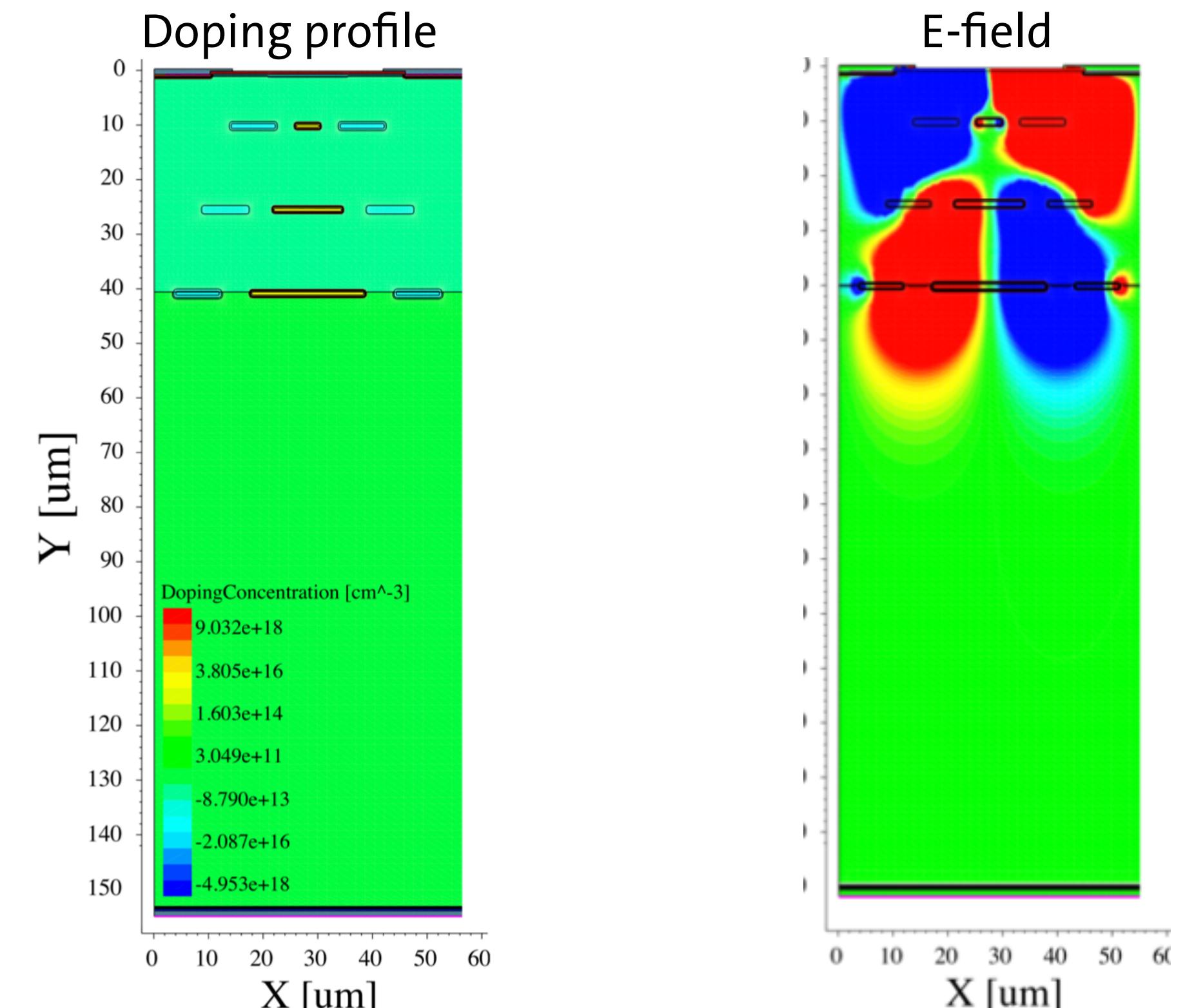


Figure 5.36: Comparison of doping profiles extracted from process simulation. Black solid line represents the doping profile of a region under an STI and red dashed line is the profile in regions without STI for the same implants PW-PSUB-DN, corresponding to the cut lines in Fig. 5.35 without the n⁺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

2. Enhanced Lateral Drift Sensor(ELAD)



A. Velyka, DESY-THESIS-2020-014

-
- 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

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

Electron continuity $\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_n + R_{net}$ where $\mathbf{J}_n = qn\mu_n \mathbf{E} + qD_n \nabla n$

Hole continuity $\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{J}_p + R_{net}$ where $\mathbf{J}_p = qp\mu_p \mathbf{E} - qD_p \nabla p$

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

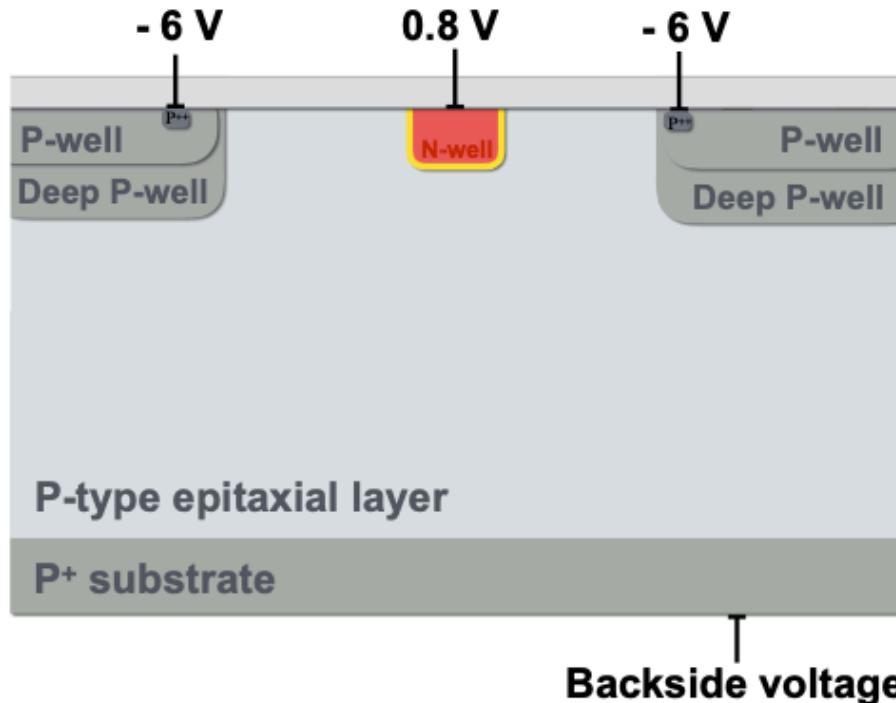
Device simulation II

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

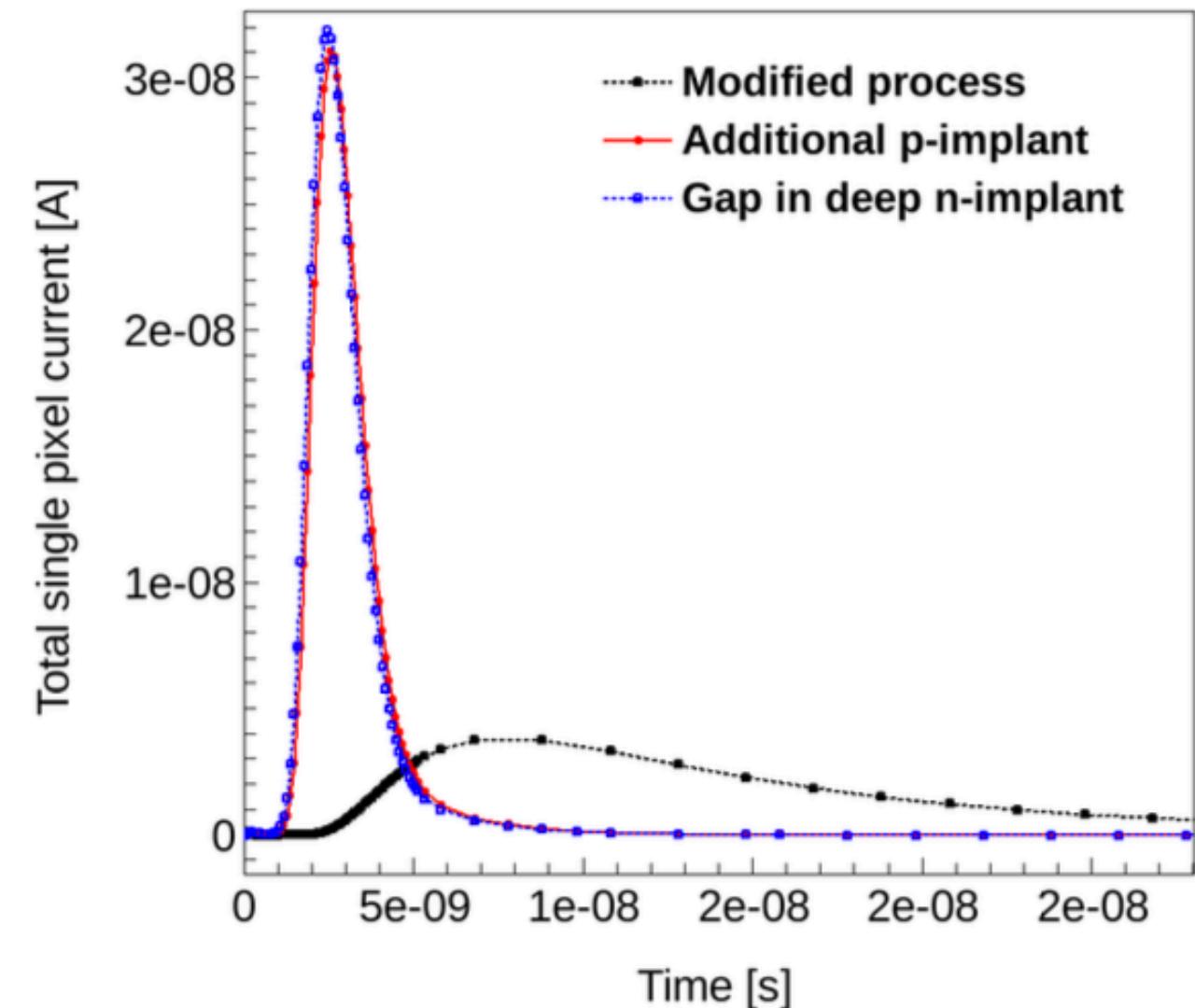
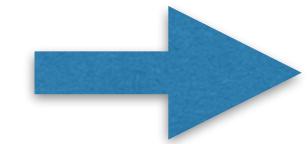
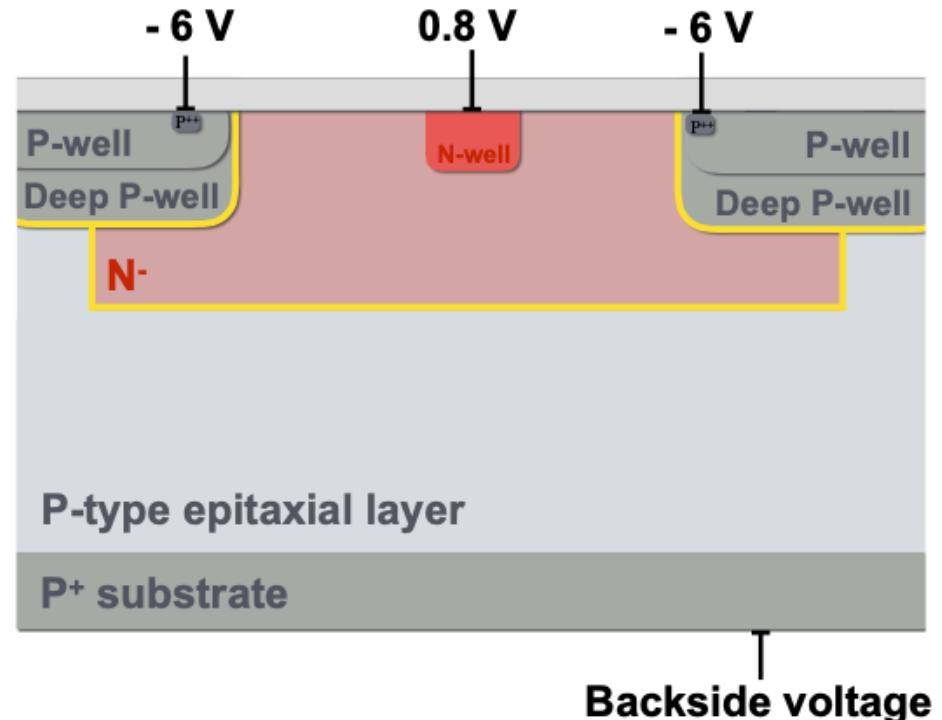
Examples of device simulations:

- Improving CMOS pixel sensor for faster charge collection

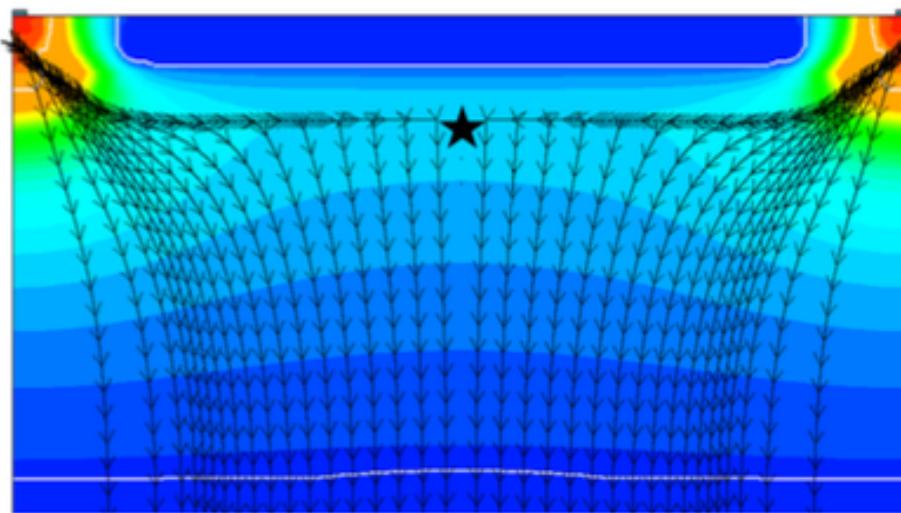
Standard process:



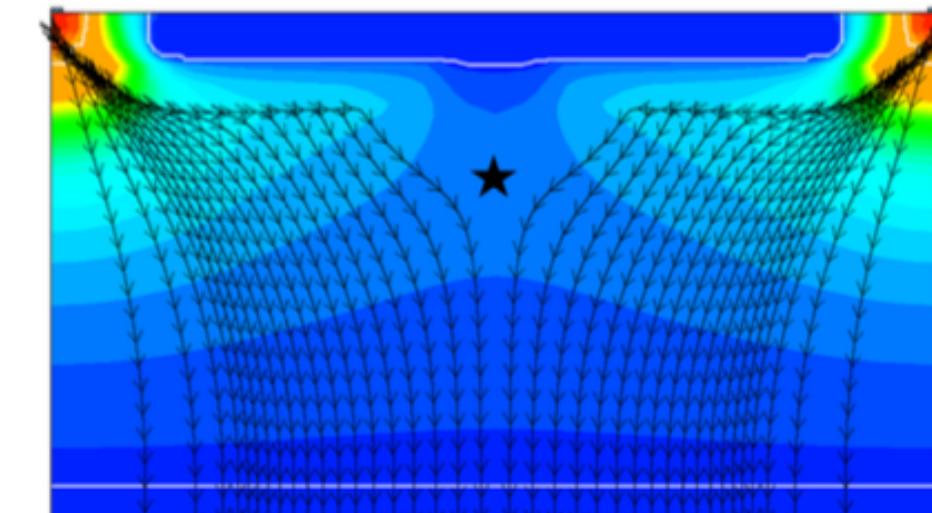
Gap in deep n-implant:



Electrostatic potential:



Electrostatic potential:



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

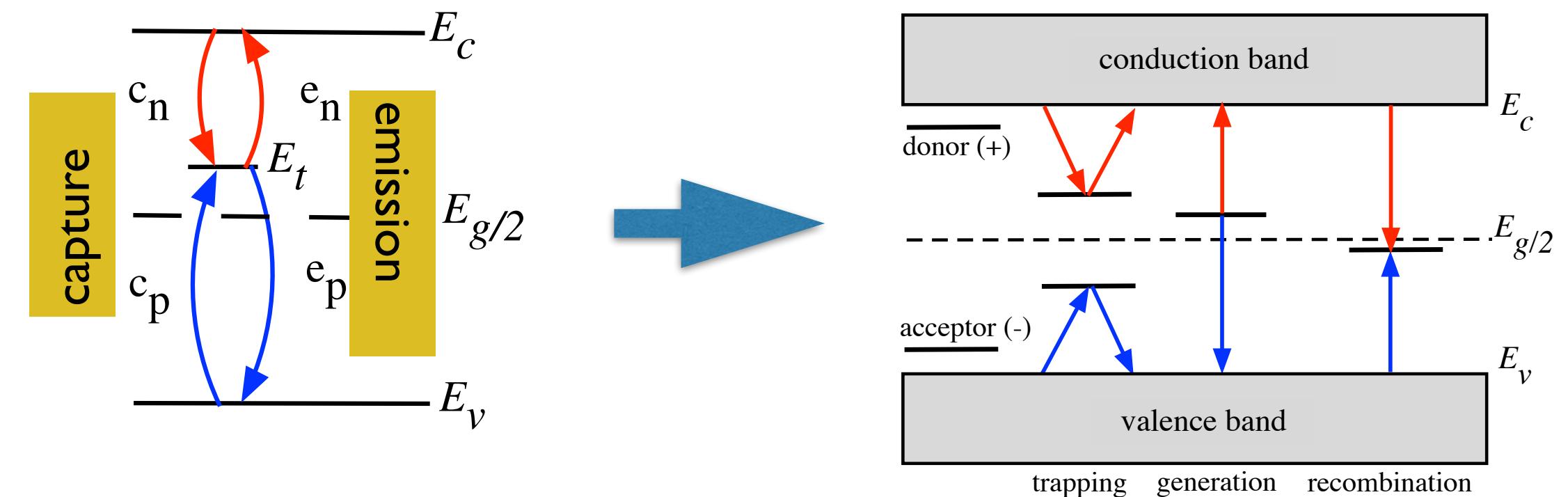
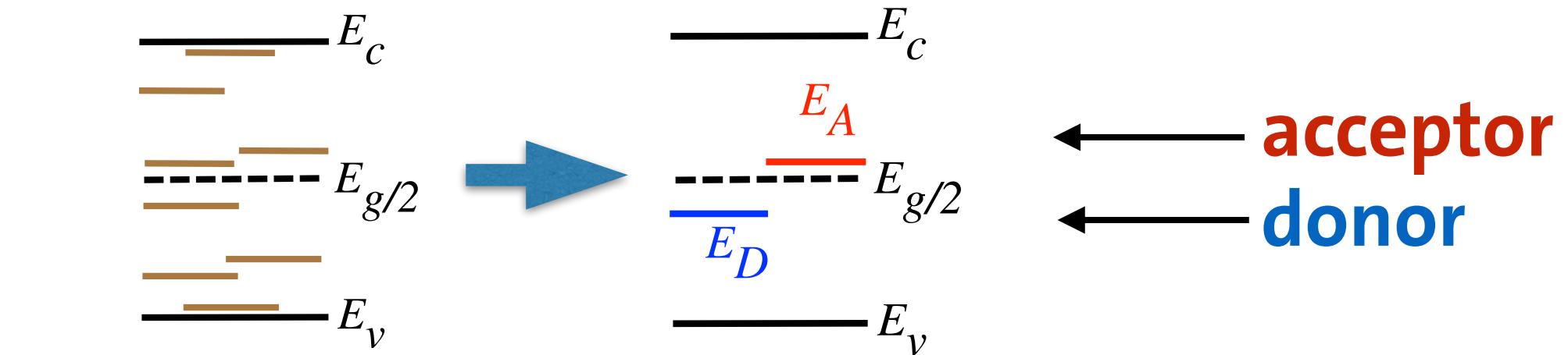
Radiation damage modelling I

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

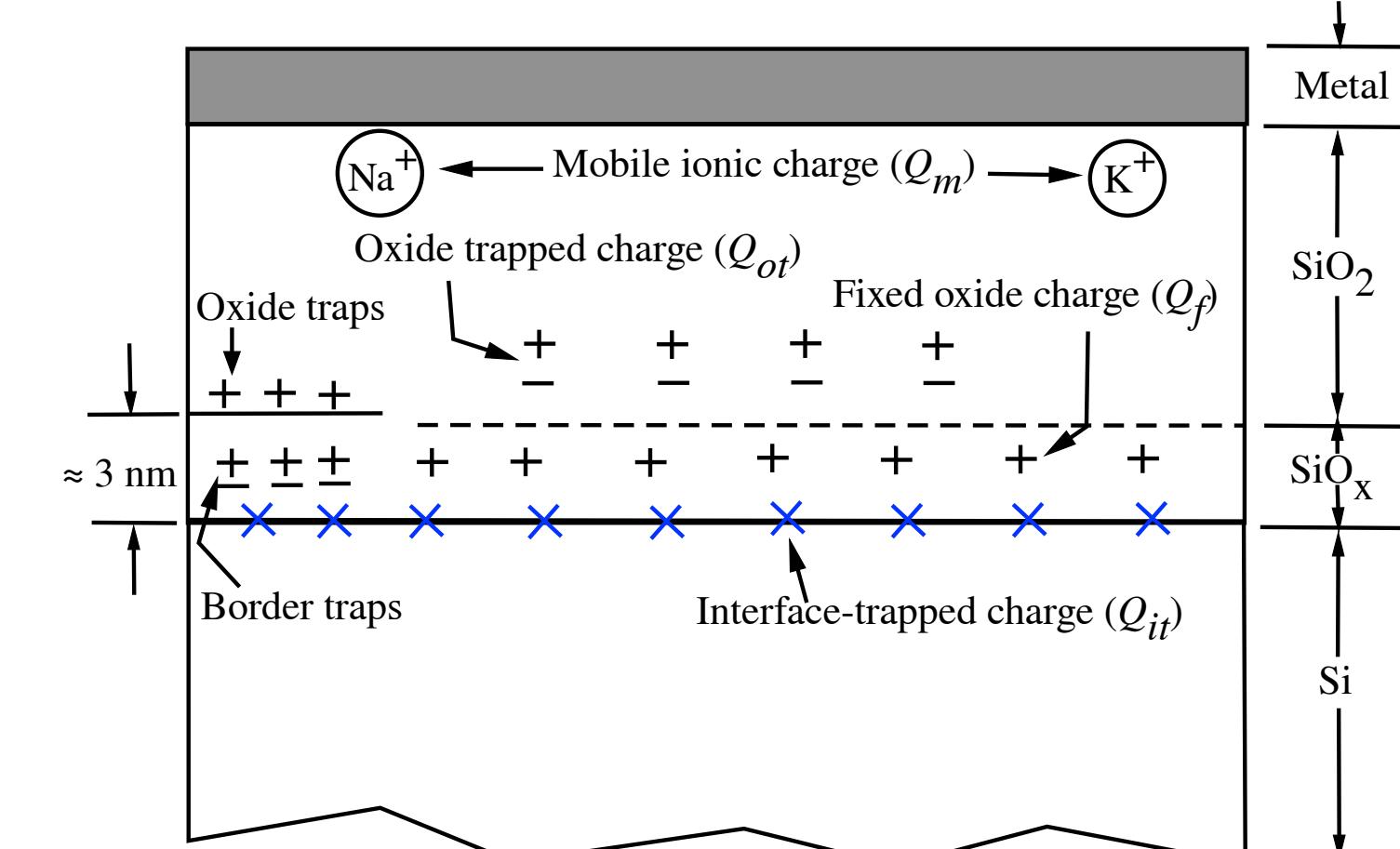
- Energy levels + type:** E_A , E_D fixed
 - Concentrations:** N_A , N_D
 - Cross sections:** σ^A_e , σ^A_h , σ^D_e , σ^D_h
- $\rho_{trap} = q[N_D f_D - N_A f_A], f_D, f_A, R_{net}$



Surface damage modelling:

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

*) SRH = Shockley-Reed-Hall



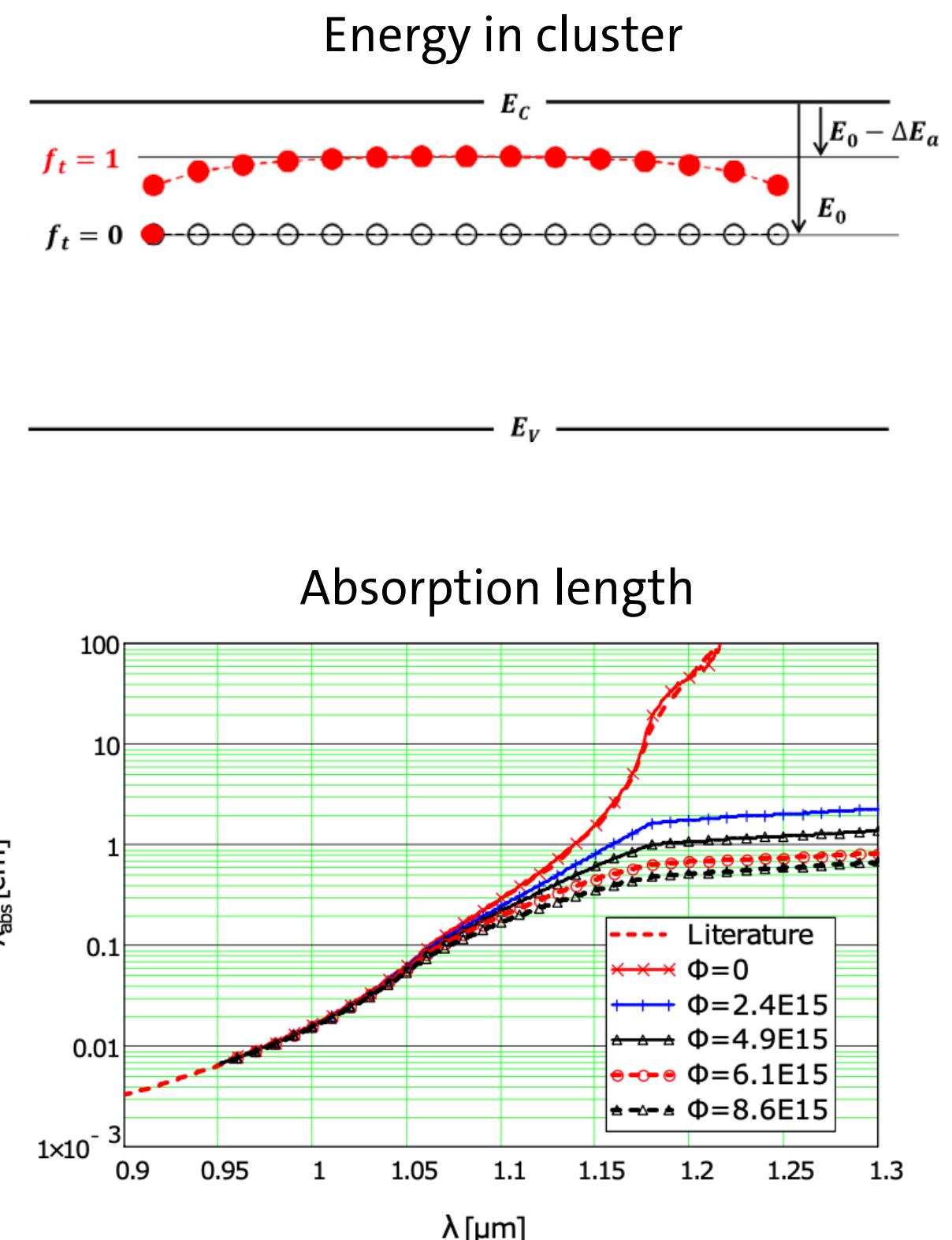
Radiation damage modelling II

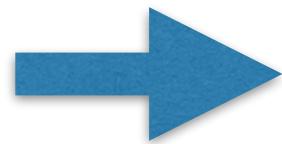
Radiation damage models up to $2 \times 10^{16} \text{ n}_{\text{eq}}/\text{cm}^2$:

- 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 $1 \times 10^{18} \text{ n}_{\text{eq}}/\text{cm}^2$:

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




 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
- Within 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

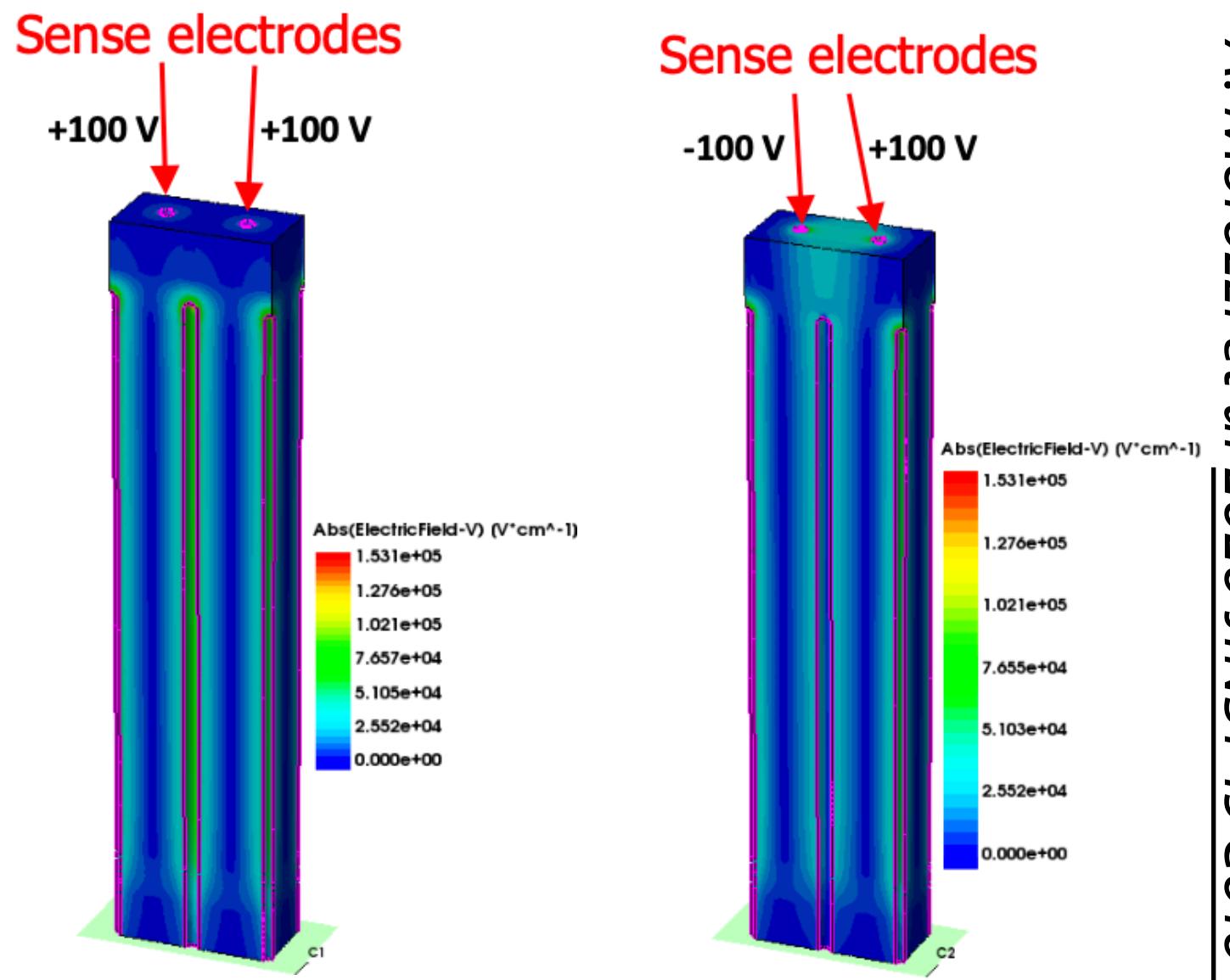
Gallium Nitride (GaN):

- 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

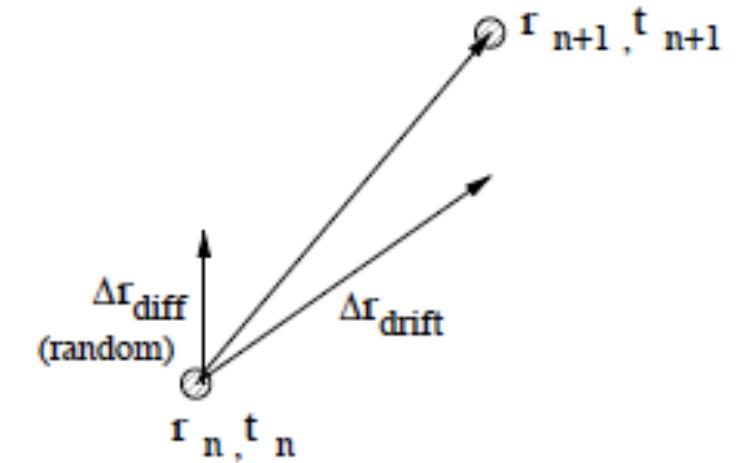


Radiation damage models for alternative materials need to be developed and incorporated in TCAD

Signal simulation tools I

Main features:

- They solve Poisson Equation for an input N_{eff} rather than 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

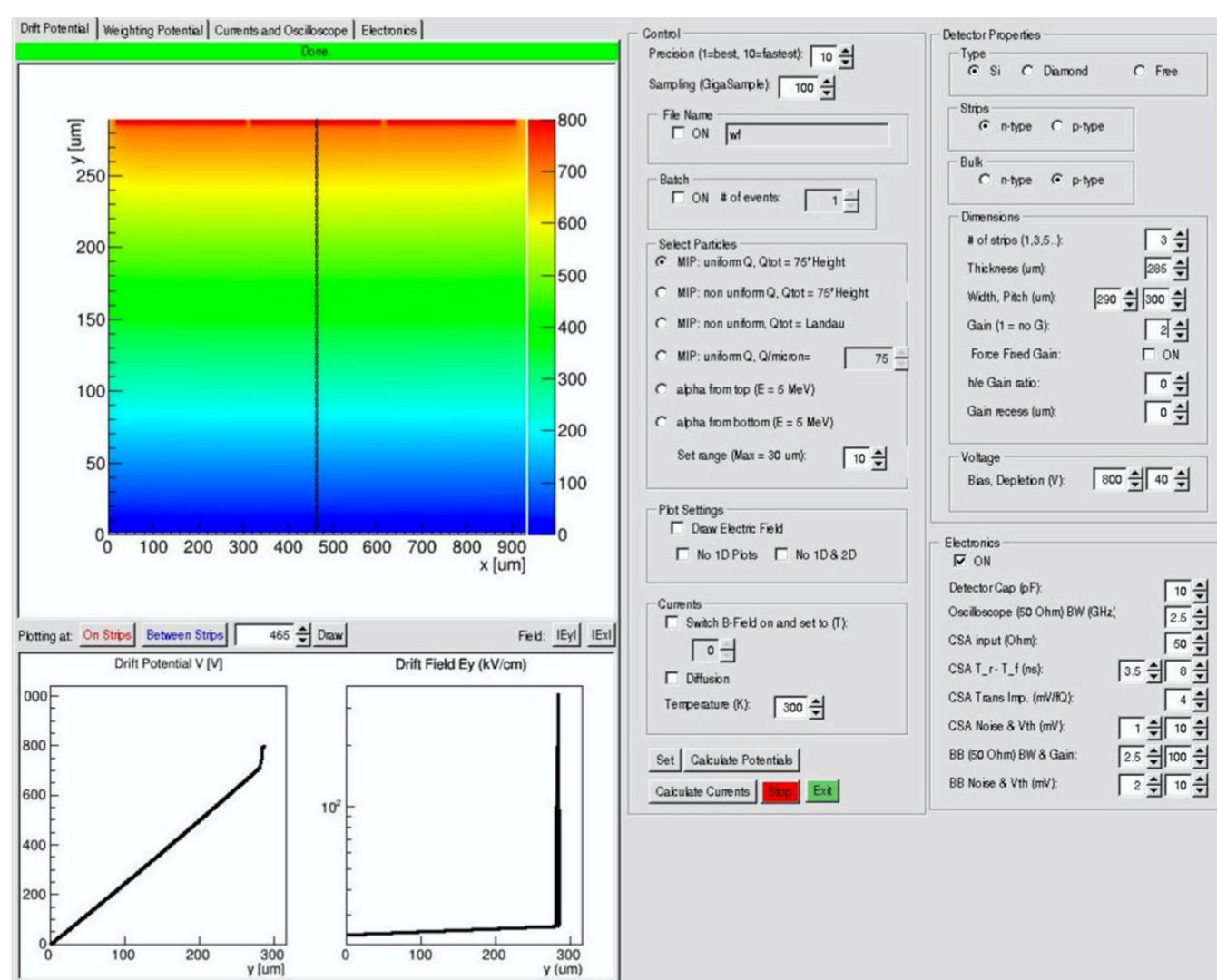
Signal simulation tools II

Many available:

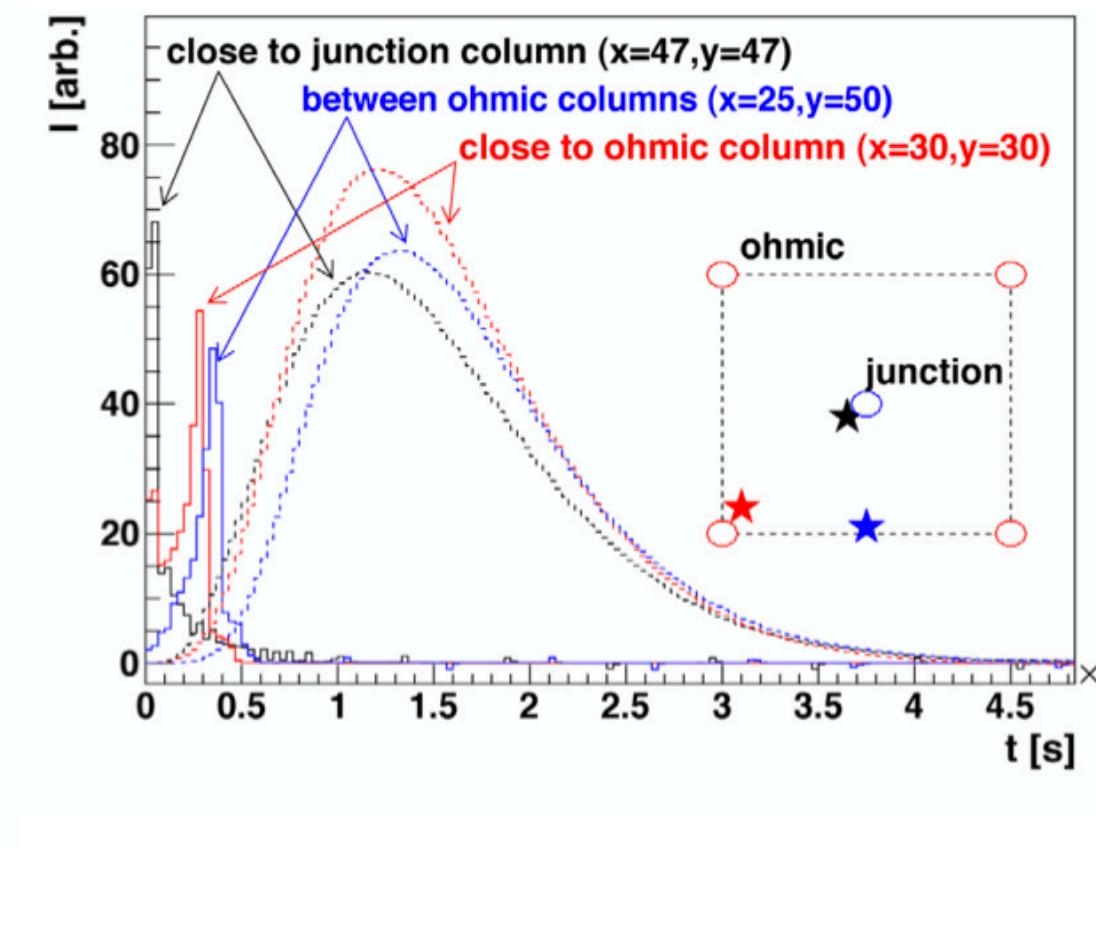
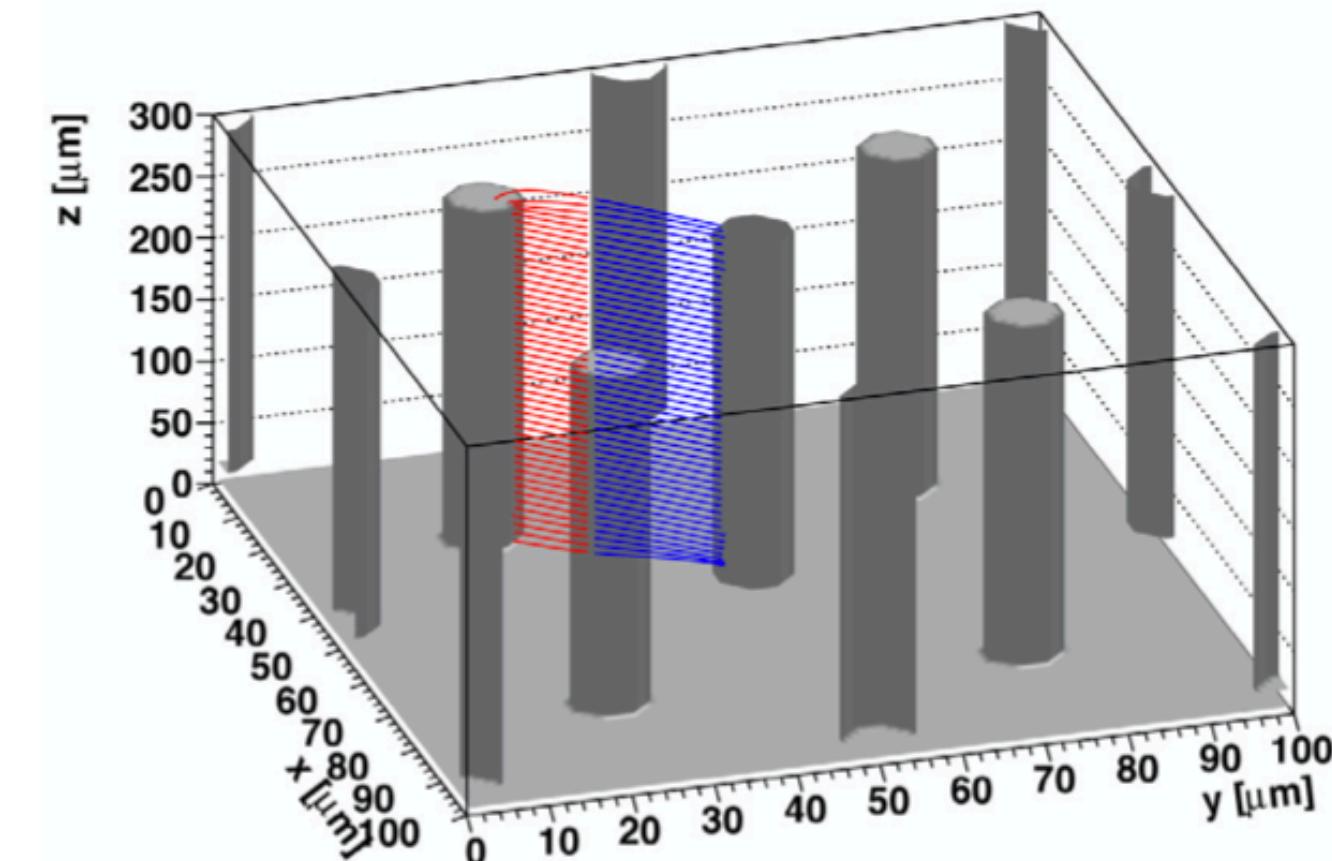
- Weightfield2, KDetSim, PixelAV, TRACS, TCODE, GARFIELD++, Allpix², etc.

Examples:

Weightfield2



KSetSim



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)

$$\frac{1}{\tau_e} = \sum_{defects} v_e^{th} \sigma_{t,n} (1 - f_t) N_t$$

$$\frac{1}{\tau_h} = \sum_{defects} v_h^{th} \sigma_{t,p} f_t N_t$$

Experimental setup simulation

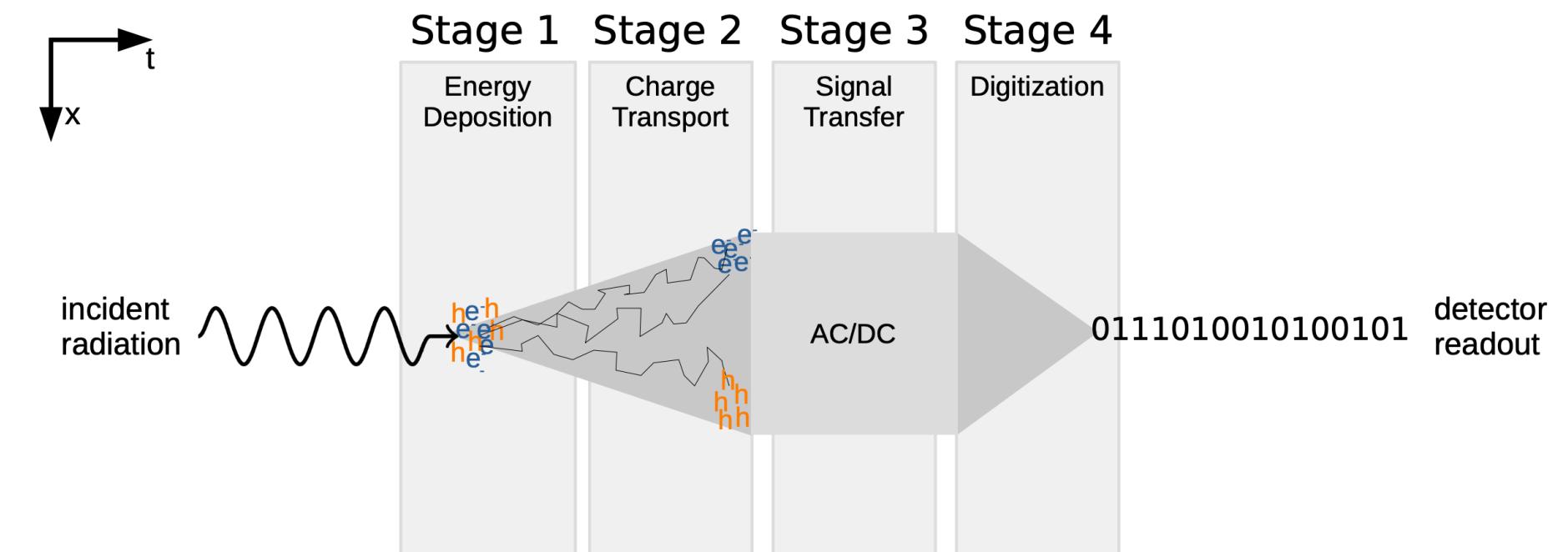
S. Spannagel et al., doi:[10.1016/j.nima.2018.06.020](https://doi.org/10.1016/j.nima.2018.06.020)

Allpix² Framework:

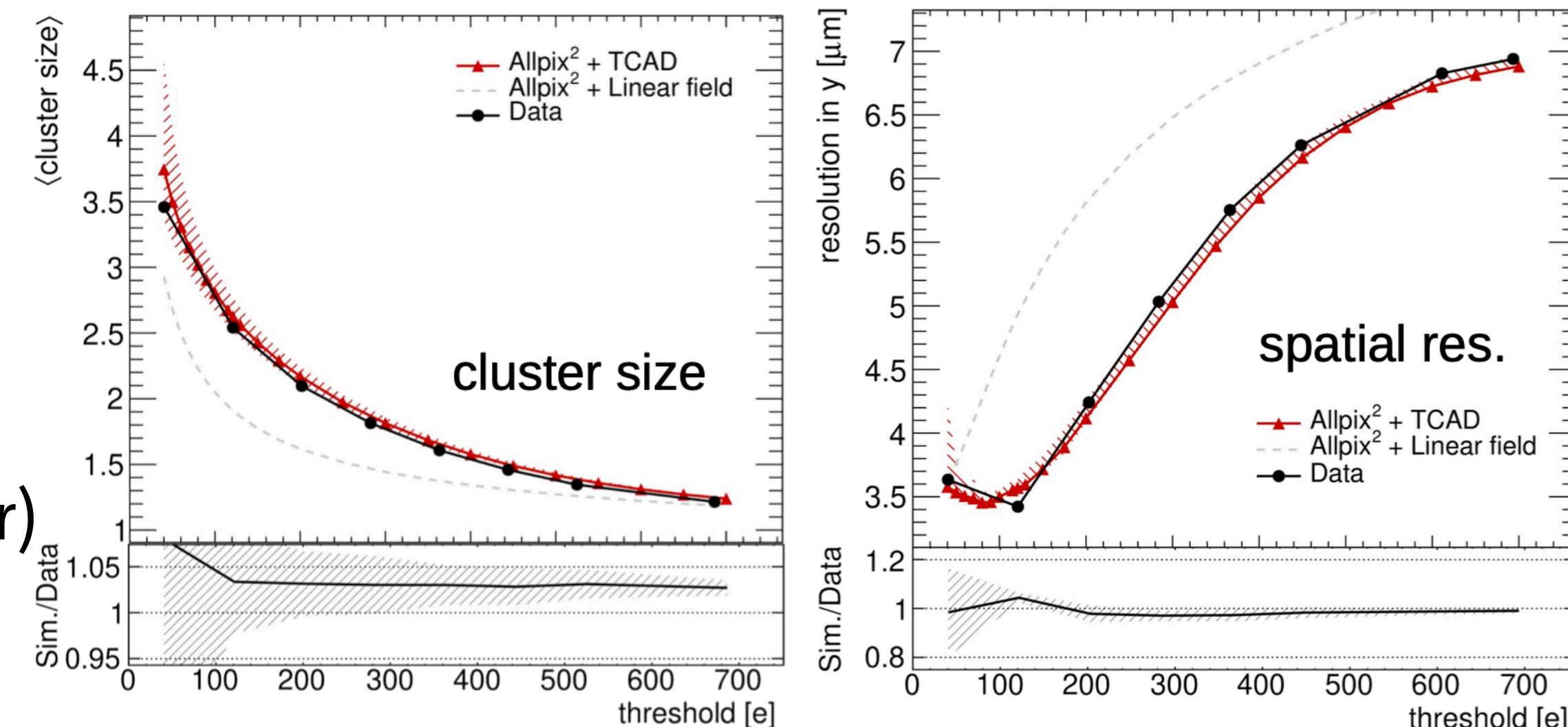
- Simulate full chain: energy deposition, signal formation, transfer and digitisation
- Include stochastic effects, fluctuations, secondaries
- Requires simplifications:
 - No self-interaction, static electric field, empirical models for different stages, ...
- Allows to derive performance parameters:
 - 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](https://doi.org/10.1016/j.nima.2020.163784)

Full detector system simulation

Aim:

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

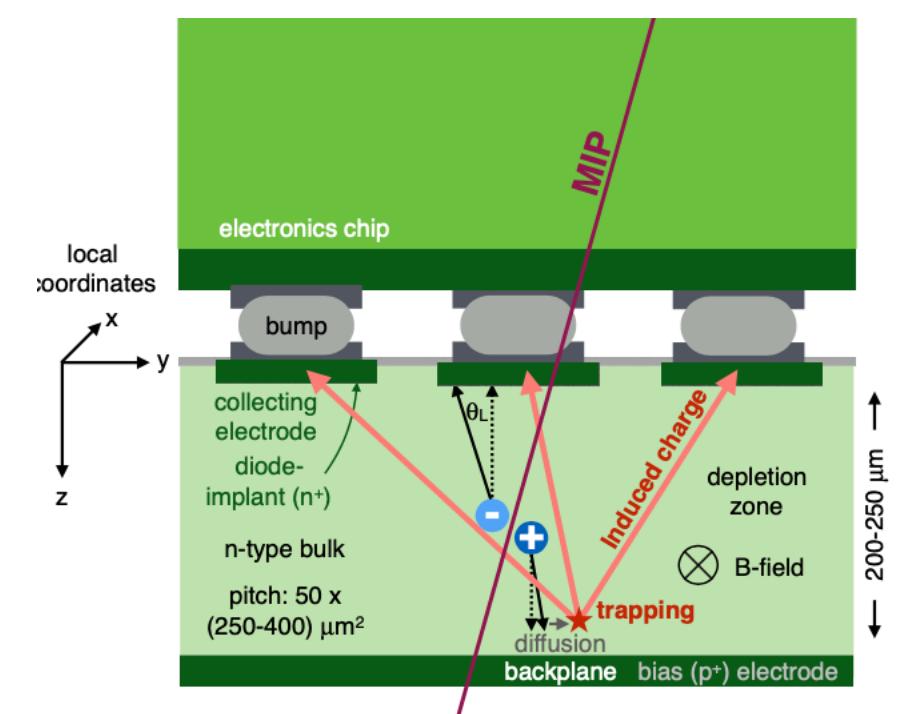
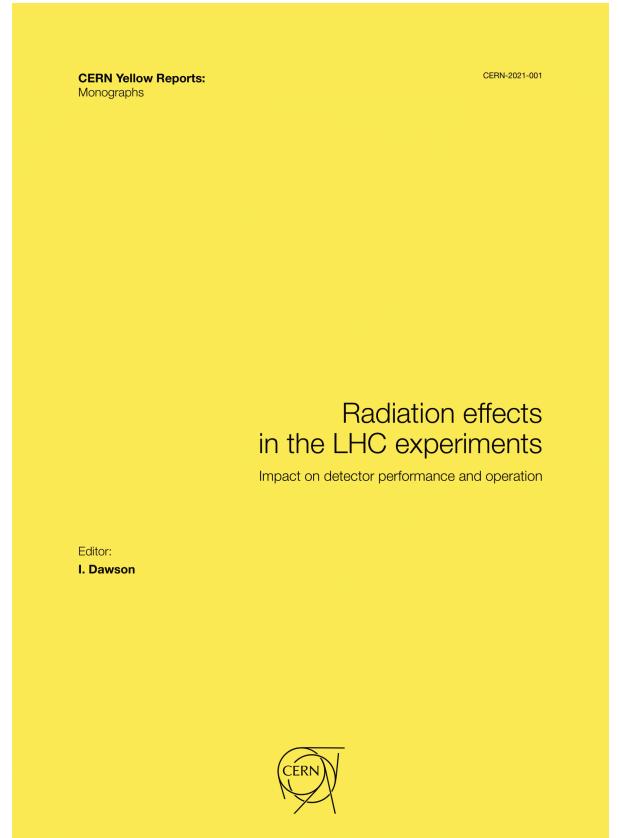
Requires:

- Simulation of radiation environments
 - Event generation (e.g. PYTHIA8),
 - 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

I. Dawson (Ed.), [CERN-2021-001](#)



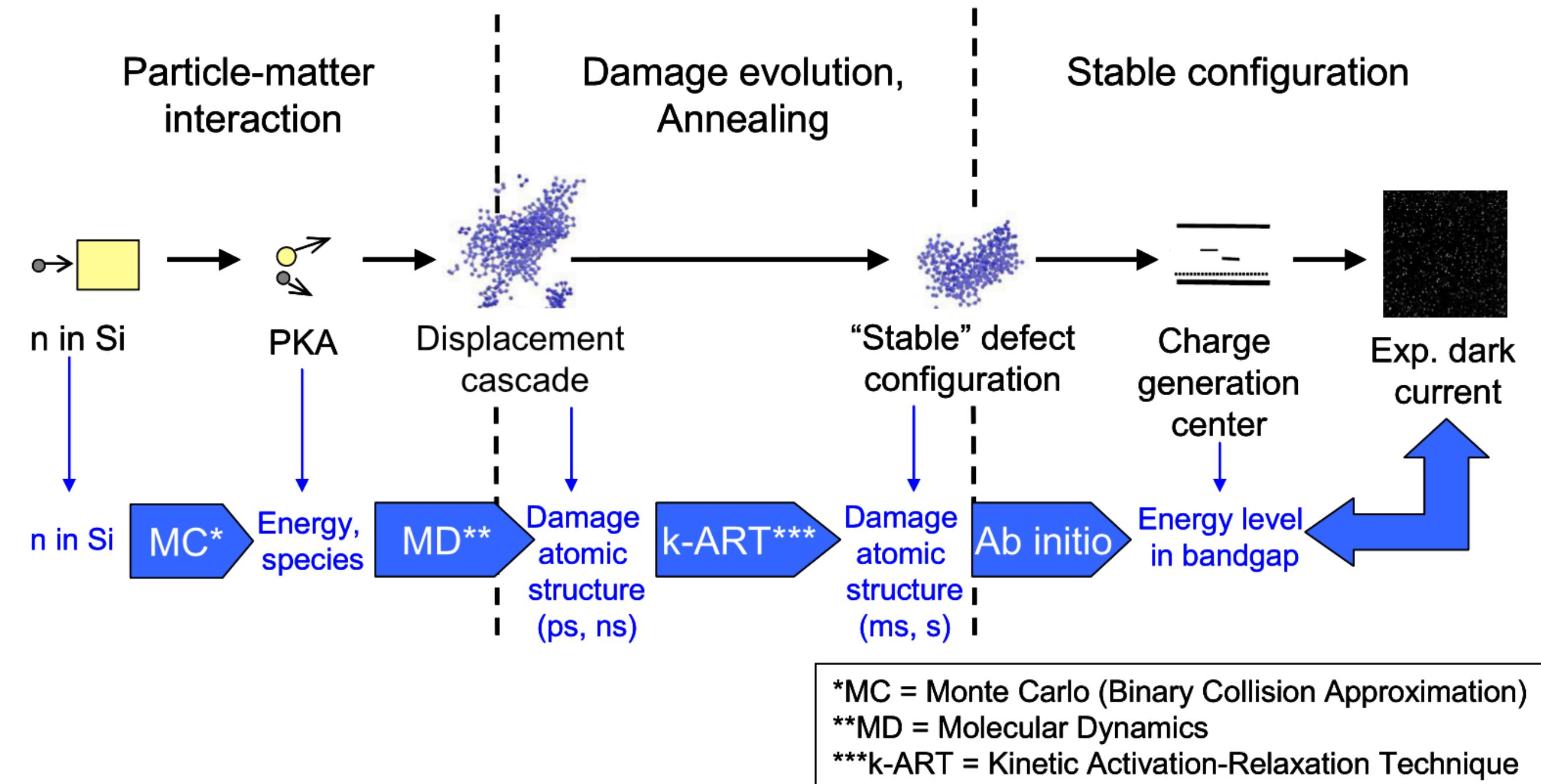
Displacement damage simulation

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



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

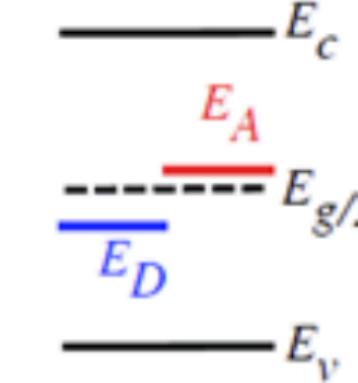
Synopsys TCAD	https://www.synopsys.com/silicon/tcad.html
Silvaco TCAD	https://silvaco.com/tcad/
COGENDA TCAD	https://cogenda.com
Weightfield2	http://personalpages.to.infn.it/~cartigli/Weightfield2
KDetSim	http://kdetsim.org
PixelAV	https://physics-astronomy.jhu.edu/directory/morris-swartz/
TRACS	https://github.com/IFCA-HEP/TRACS
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

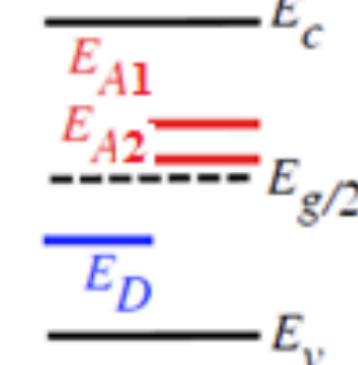
EVL model

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 CiO_i, 1st acceptor to V₂ and 2nd acceptor to V₃

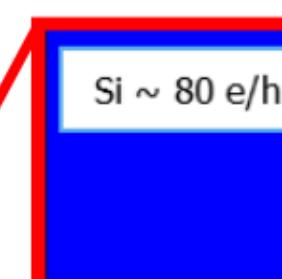


Model	E [eV]	g _{int} [cm ⁻¹]	σ _e [cm ²]	σ _h [cm ²]
EVL	Ev+0.48	6	1e-15	1e-15
Neutrons	Ec-0.525	3.7	1e-15	1e-15
Delphi	Ev+0.48	4	2e-15	2.6e-15
23 MeVp	Ec-0.51	3	2e-15	2e-15
KIT (Eber)	Ev+0.48	5.598 (-3.949e14)	2e-15	2.6e-15
23 MeVp	Ec-0.525	1.198 (+6.5434e13)	2e-15	2e-15
HIP	Ev+0.48	5.598 (-3.949e14)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

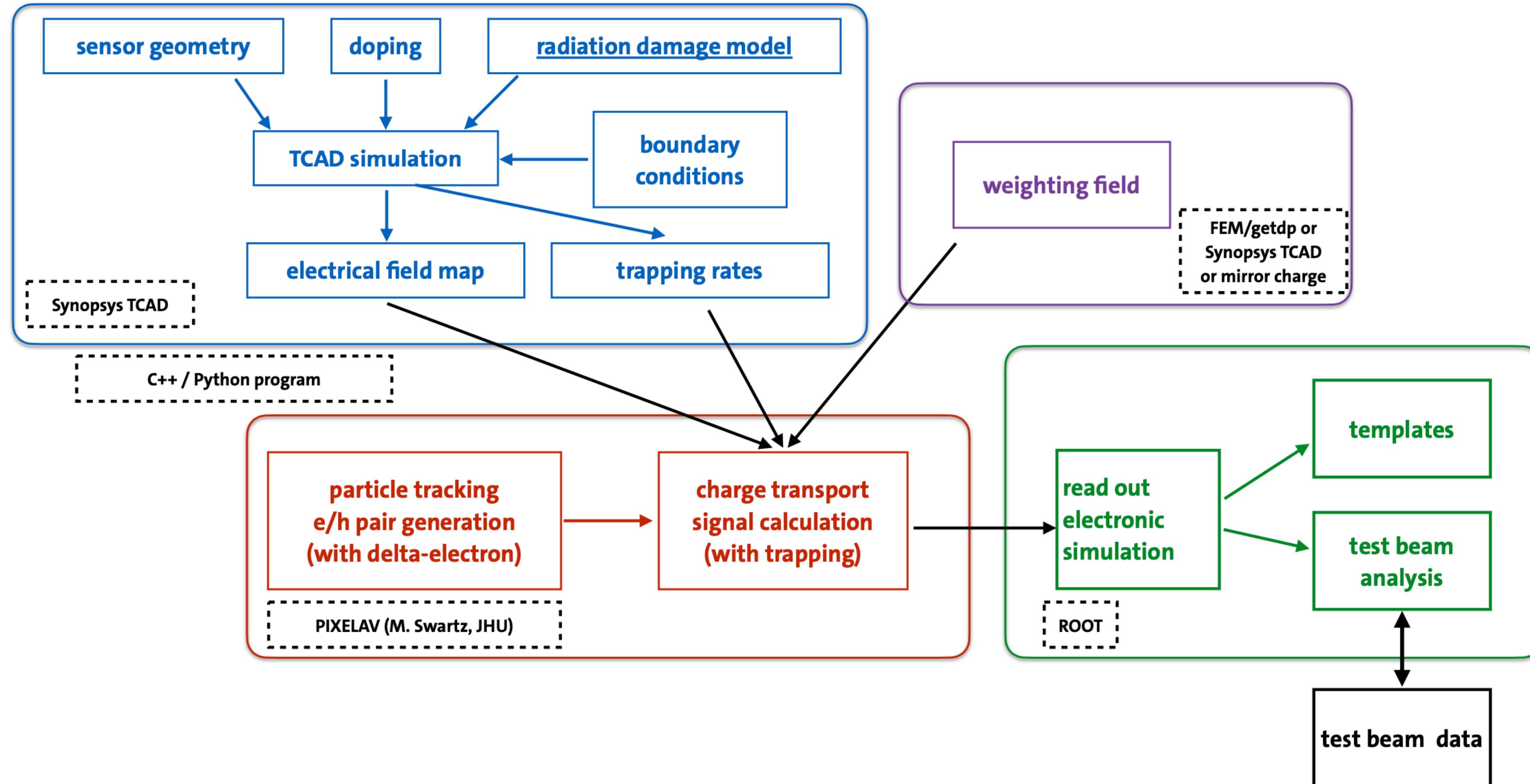
Model	E [eV]	g _{int} [cm ⁻¹]	σ _e [cm ²]	σ _h [cm ²]
Perugia	Ev+0.36	0.9	2.5e-13	2.5e-15
p-type	Ec-0.42	1.6	2e-15	2e-14
	Ec-0.46	0.9	5e-15	5e-14
Perugia	Ev+0.36	1.1	2e-18	1.2e-14
n-type	Ec-0.42	13	2.5e-15	1.2e-14
	Ec-0.50	0.08	5e-15	3.5e-14
Peniccard	Ev+0.36	0.9	3.23e-13	3.23e-14
	Ec-0.42	1.613	9.5e-15	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

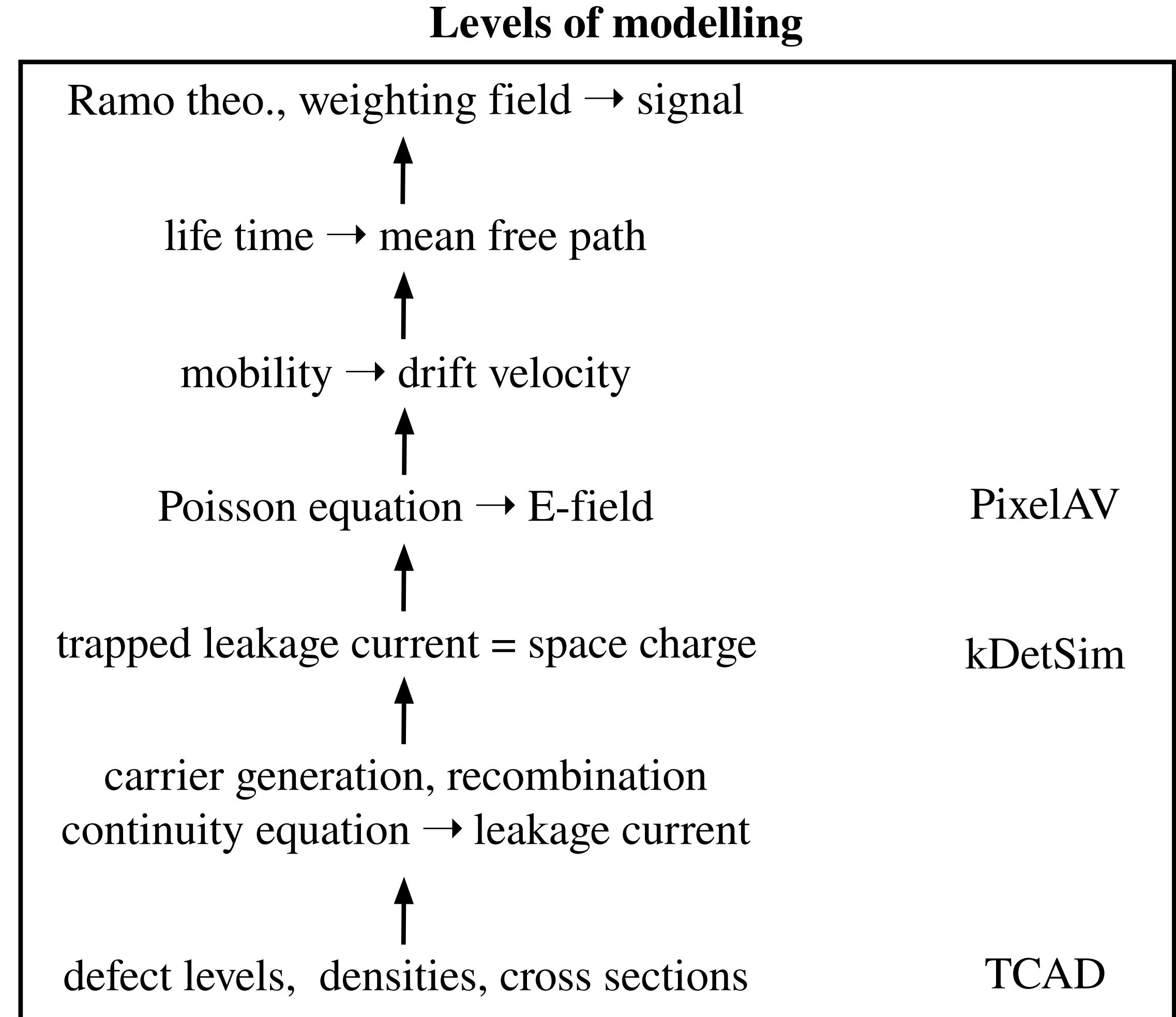
	Silicon	Diamond	
Bandgap [eV]	1,12	5,47	Higher-Field operation
Breakdown Field [MV/cm]	0,4	20	
Intrinsic Resistivity@R.T. [Ω cm]	$2,3 \times 10^5$	$> 10^{11}$	
Intrinsic Carrier Density [cm^{-3}]	$1,5 \times 10^{10}$	10^{-27}	{ lower leakage current }
Dielectric Constant	11,9	5,7	
Electron Mobility	1350	1900-3800	
Hole Mobility	480	2300-4500	{ faster signal }
Saturation Velocity	1×10^7	$2,7 \times 10^7$	
Displacement Energy [eV/atom]	13-20	43	radiation hardness
Thermal Conductivity [$\text{W cm}^{-1} \text{K}^{-1}$]	1,5	20	heat dissipation
Energy to create e-h pair [eV]	3,62	11,6 - 16	$\sim 12000 \text{ e}$
Radiation Length [cm]	9,36	12,2	
Energy Loss for MIPs [MeV/cm]	3,21	4,69	
Aver. Signal Created / 100 μm	8892	3602	lower signal



Simulation flow



Levels of modelling



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	fixed
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

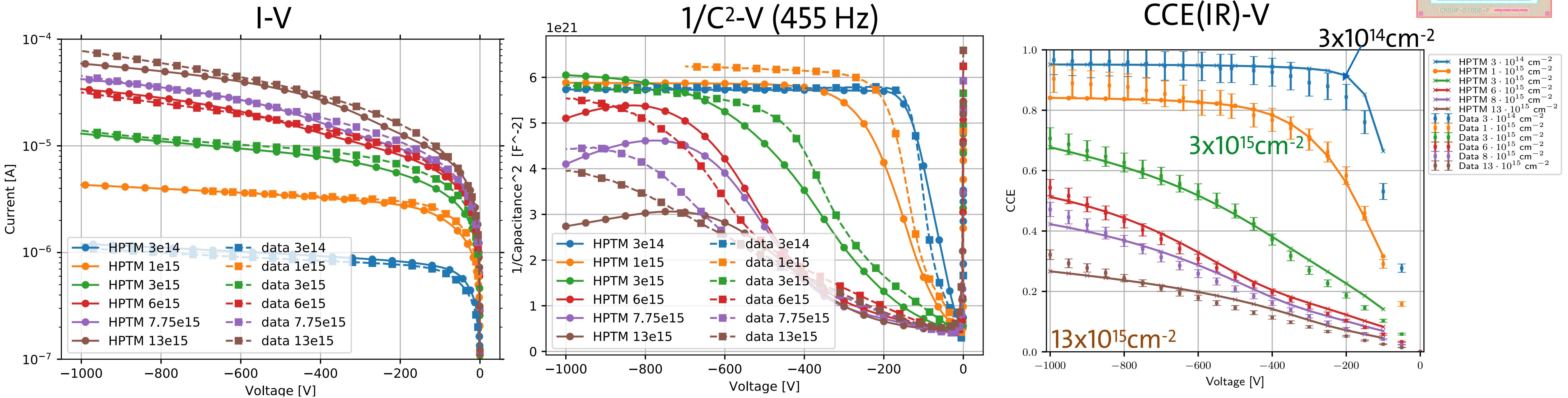
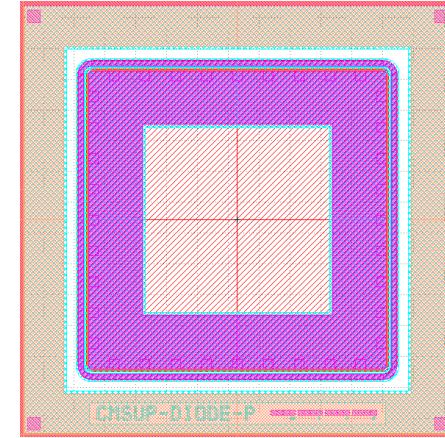
- Type and energy of defects were fixed. Values taken from R. Radu et al. JAP 117, 164503 (2015)
- Trap concentration of defects: $N = g_{int} \cdot \Phi_{eq}$
- E30K electron and hole cross section were fixed
- C_iO_i electron cross section was fixed
→12 free parameter
- Optimisation done with the nonlinear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

HPTM comparison to data

I-V, C-V and CCE(IR) for fluences from $0.3 - 13 \times 10^{15} n_{eq}/cm^2$ at $T = -20^\circ C$ (for $T = -30^\circ C$ see backup)

- HPK p-type 200 μm thick diodes
- Irradiated with **24 GeV/c protons** at CERN IRRAD
- Fluences: $0.3, 1, 1.5, 2.4, 3, 6, 7.75, 13 \times 10^{15} n_{eq}/cm^2$

5 mm x 5 mm



- The simulation for 0.3 and $1 \times 10^{15} n_{eq}/cm^2$ are **extrapolations** and the $7.75 \times 10^{15} n_{eq}/cm^2$ 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 $\geq 3 \cdot 10^{15} n_{eq}/cm^2$ (see backup)