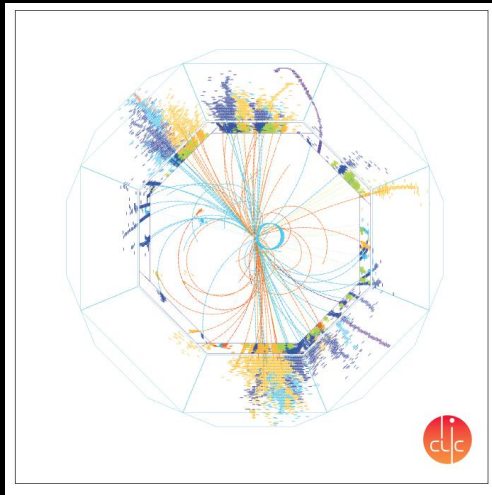


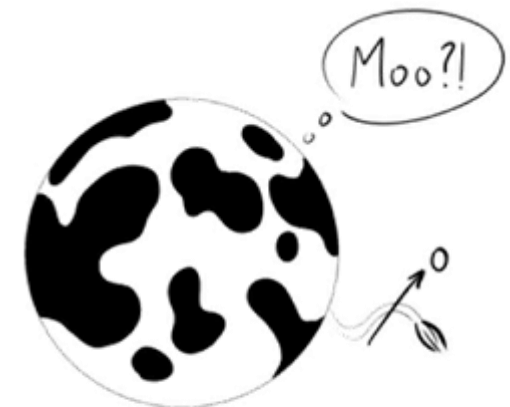
TCAD Simulation of irradiated Silicon radiation detector using commercial simulation products



Mathieu Benoit, CERN, PH-LCD

Outline

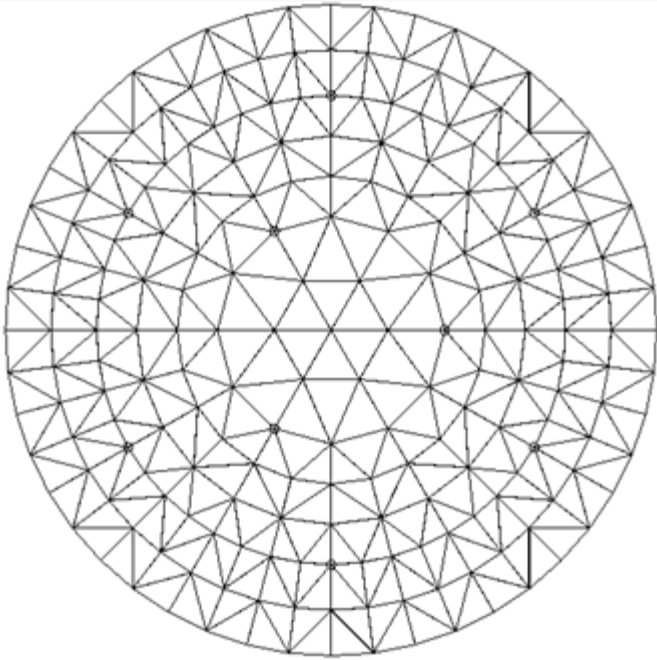
- Short summary of theory of Finite-Element / Difference Method (FEM) in Silicon TCAD simulation
 - Numerical methods
 - Existence of the solution
- Comparison of main commercial TCAD simulation software
 - Physics
 - Functionality (user friendliness)
- Example of TCAD simulation
 - Space-Charge Sign Inversion (SCSI)
 - Double peak in inverted sensors
 - Charge multiplication
- Conclusion



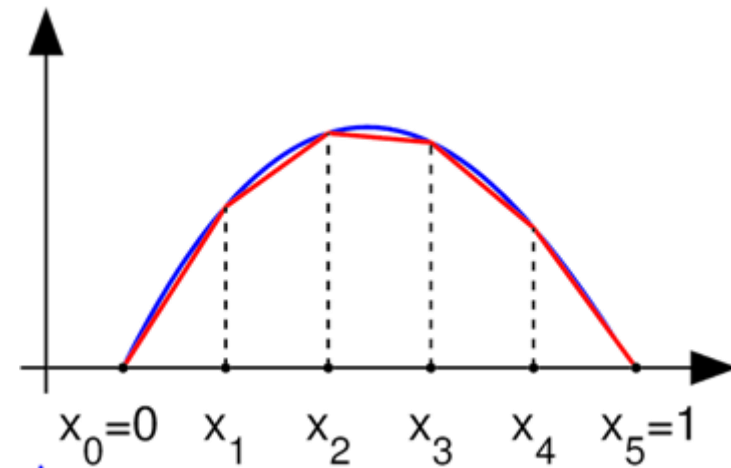
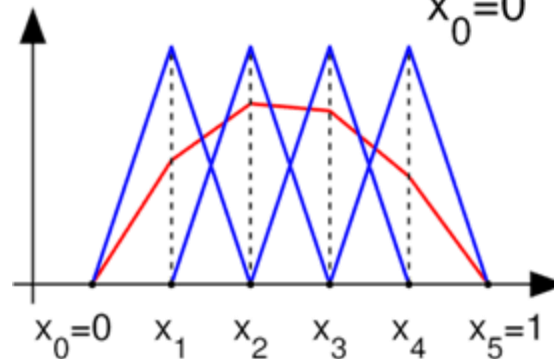
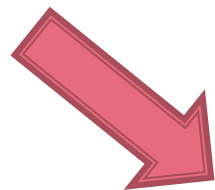
Consider a spherical cow
of radius R ...

Warning this talk
contains spherical cows

TCAD simulation principles



$$q \frac{dn}{dt} = q \left[(G_n - R_n) + \nabla \cdot (n \mu_n \vec{E} + D_n \nabla n) \right]$$
$$-\nabla \cdot (\epsilon \nabla V) = q(c + p - n)$$



TCAD simulation principles : Beyond the standard model !

- I mention here for completeness the possibility in the main TCAD simulation to perform simulation at higher orders of Boltzmann transport equation :
 - The thermodynamic model

$$\vec{J}_n = -nq\mu_n(\nabla\Phi_n + P_n\nabla T)$$

$$\vec{J}_p = -pq\mu_p(\nabla\Phi_p + P_p\nabla T)$$

- The hydrodynamic model

$$\vec{J}_n = q\mu_n \left(n\nabla E_C + kT_n\nabla n - nkT_n\nabla \ln\gamma_n + \lambda_n f_n^{\text{td}} kn\nabla T_n - 1.5nkT_n\nabla \ln m_n \right)$$

$$\vec{J}_p = q\mu_p \left(p\nabla E_V - kT_p\nabla p + pkT_p\nabla \ln\gamma_p - \lambda_p f_p^{\text{td}} kp\nabla T_p - 1.5pkT_p\nabla \ln m_p \right)$$

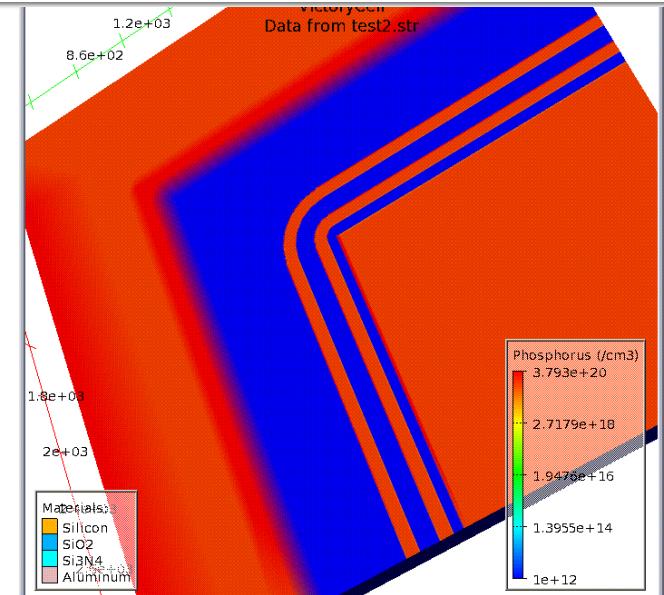
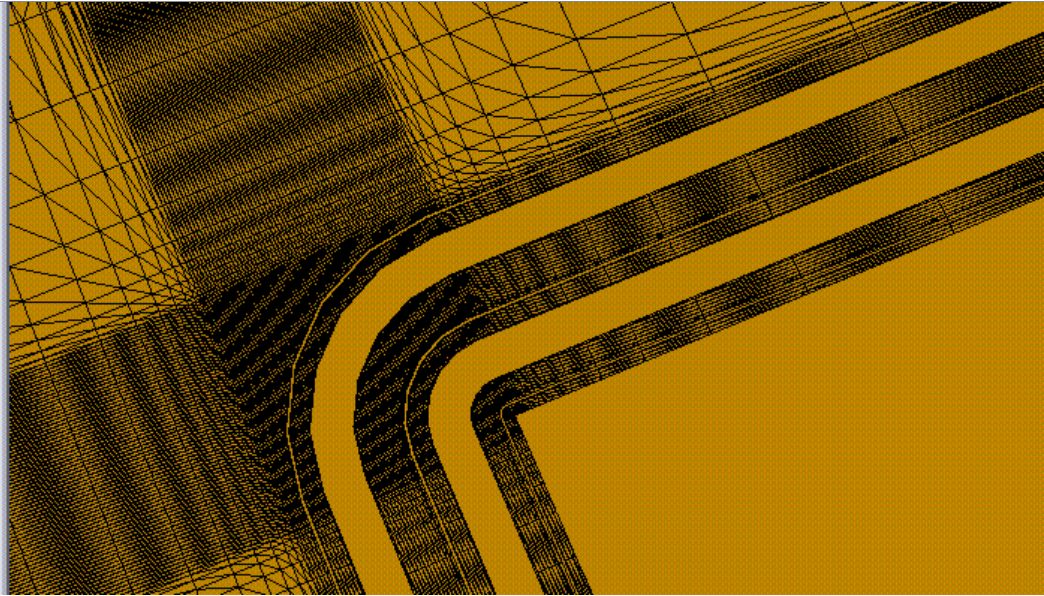
TCAD simulation principles

- The exact solution to the equation needs to be definable as :

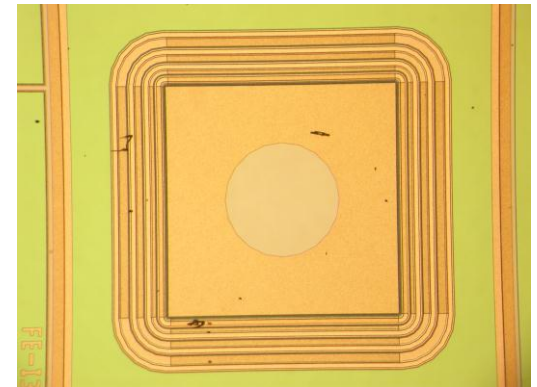
$$u_k = u_g + \sum_{j=1}^n u_j \phi_j$$

- n can be infinite (or not, ex: simple diode etc)
- In FEM, n is fixed by the number of degrees of liberty (nDOF)
 - nDOF is fixed by the mesh defined in your geometry

Importance of meshing properly



- Meshing in the **first main problem you will encounter when doing TCAD simulation**
- Determination of the perfect mesh is not an exact science (a lot of trial and error !)
 - Upper limit of mesh size set by device feature size (implants , electrodes)
 - Lower limit of mesh size set by computational limits (RAM, computing time)
 - Meshing algorithm available in software packages also have internal limitation (!!!)

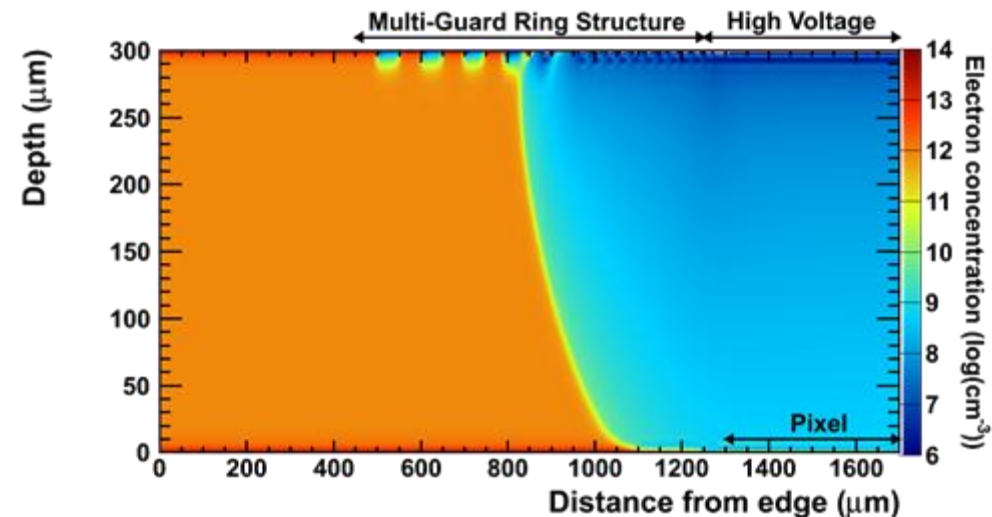
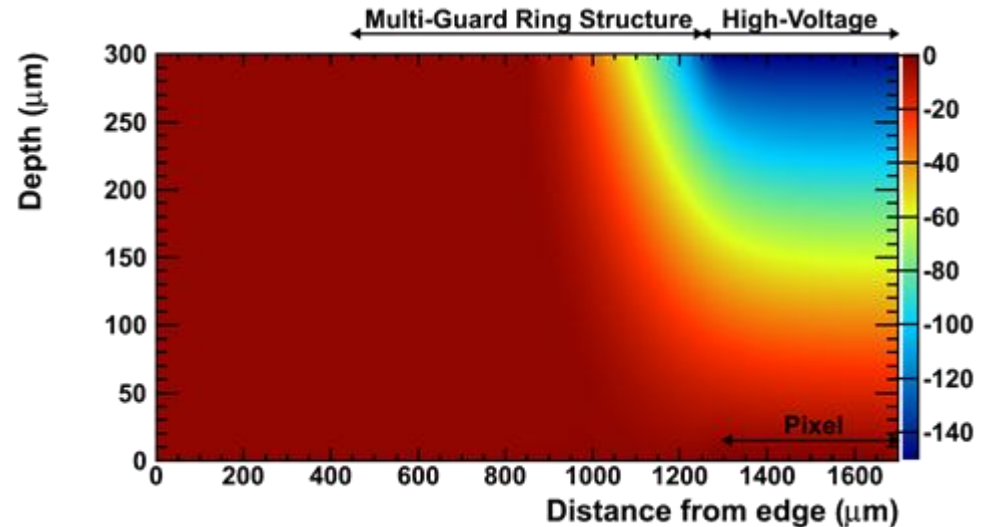


Tricks for meshing properly

- Paradoxically, One need a good idea of the solution to guide the meshing algorithm

- Mesh length not more that $\frac{1}{4}$ of feature length (ex : Junction, electrodes, high E Field area)
- Mesh length must be adjusted to the characteristic length of physical phenomenom important locally in the model (inversion channels, charge multiplication by impact ionization)

- It is much dangerous to reduce mesh size to save time than to add too many nodes
- Convergence study are eventually the best method to see how mesh influence the solution



Physics

Physics	Models
Mobility	Concentration-dependent mobility (fit to experimental data), Parallel field dependent mobility (fit to experimental saturation velocities)
Generation recombination and trapping	Modified concentration dependent Shockley-Read-Hall Generation/recombination (for treatment of defects)
Impact ionization	Selberherr's Impact ionization model
Tunneling	Band-to-band tunnelling, Trap-Assisted tunneling
Oxide physics	Fowler-Nordheim tunnelling, interface charge accumulation

Generation/Recombination

- Modified Shockley-Read-Hall G/R
 - A sum of SRH contribution by each trap
 - Γ is the degeneracy of the trap, n_i the intrinsic concentration of carriers

$$R_{n,p} = \sum R_i$$

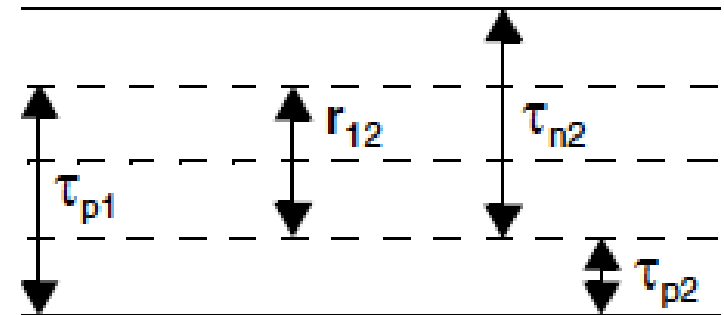
$$R_i = \frac{pn - n_i^2}{\tau_{ni} \left(p + \Gamma n_i e^{(E_f - E_i)/kT} \right) + \tau_{pi} \left(n + \frac{n_i e^{(E_i - E_f)/kT}}{\Gamma} \right)}$$

Generation/Recombination

Other models, or further parametrizations, are available in both the main TCAD simulation packages :

- Temperature dependence of SRH
- Doping dependence of SRH
- Field Dependence of G/R (Trap to band tunneling, band-to-band tunnelling)
- Coupled-Defect-Level models (CDL)
- Impact ionization

Selection of physics to model the terms of the Drift-Diffusion equation should be selected carefully. Including all physics in all simulation can lead to wrong results or difficulties in converging to a solution (Large relative errors on mostly zero values quantities)



Generation/Recombination

■ Transient behaviour of traps

$$\begin{aligned}
 \frac{dN_{tD}^+}{dt} &= \rho_t \left\{ \overbrace{v_p \sigma_p (p(1 - F_{tD}) - F_{tD} n_i \Gamma e^{E_i - E_t / kT})}^{\text{hole capture}} - \overbrace{v_n \sigma_n (n F_{tD} - \frac{(1 - F_{tD}) n_i}{\Gamma} e^{E_t - E_i / kT})}^{\text{electron emission}} \right\} \\
 \frac{dN_{tA}^-}{dt} &= \rho_t \left\{ \overbrace{v_n \sigma_n (n(1 - F_{tA}) - F_{tA} n_i \Gamma e^{E_t - E_i / kT})}^{\text{Electron capture}} - \overbrace{v_p \sigma_p (p F_{tA} - \frac{(1 - F_{tA}) n_i}{\Gamma} e^{E_i - E_t / kT})}^{\text{Hole emission}} \right\}
 \end{aligned}$$

$\sigma_{n,p}$ is trap capture cross-section
 $v_{n,p}$ is thermal velocity
 n_i is intrinsic concentration
 $F_{tA,TD}$ the probability of ionization
 $N_{tA,TD}$ space charge density

$$\sigma_n = \frac{1}{\rho_{trap} \tau_n v_n} \sigma_p = \frac{1}{\rho_{trap} \tau_p v_p}$$

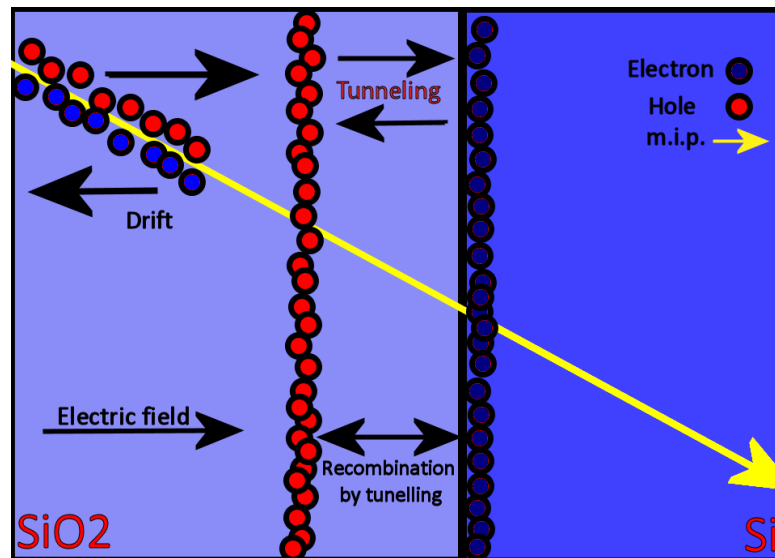
Radiation damage

P-TYPE RADIATION DAMAGE MODEL

Non-ionizing
Energy loss

Defect's energy (eV)	Introduction rate (cm^{-1})	Electron capture cross-section (cm^{-2})	Hole capture cross-section (cm^{-2})
$E_c - 0.42$	1.613	$2.e-15$	$2e-14$
$E_c - 0.46$	0.9	$5e-15$	$5e-14$
$E_c - 0.10$	100	$2e-15$	$2.5e-15$
$E_v + 0.36$	0.9	$2.5e-14$	$2.5e-15$

Ionizing
Energy loss



D. Menichelli, M. Bruzzi, Z. Li, and V. Eremin, "Modelling of observed double-junction effect," *Nucl. Instrum. Meth. A*, vol. 426, pp. 135-139, Apr. 1999.

F. Moscatelli et al., "An enhanced approach to numerical modeling of heavily irradiated silicon devices," *Nucl. Instrum. Meth. B*, vol. 186, no. 1-4, pp. 171-175, Jan. 2002.

F. Moscatelli et al., "Comprehensive device simulation modeling of heavily irradiated silicon detectors at cryogenic temperatures," *IEEE Trans. Nucl. Sci.*, vol. 51, no. 4, pp. 1759-1765, Aug. 2004.

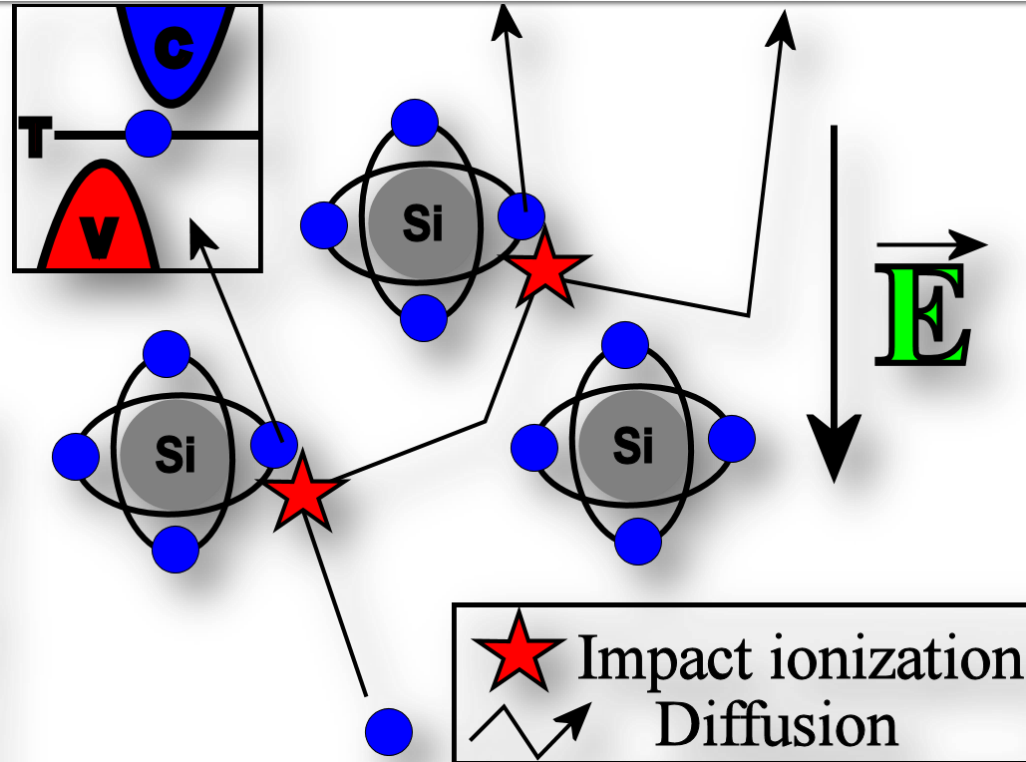
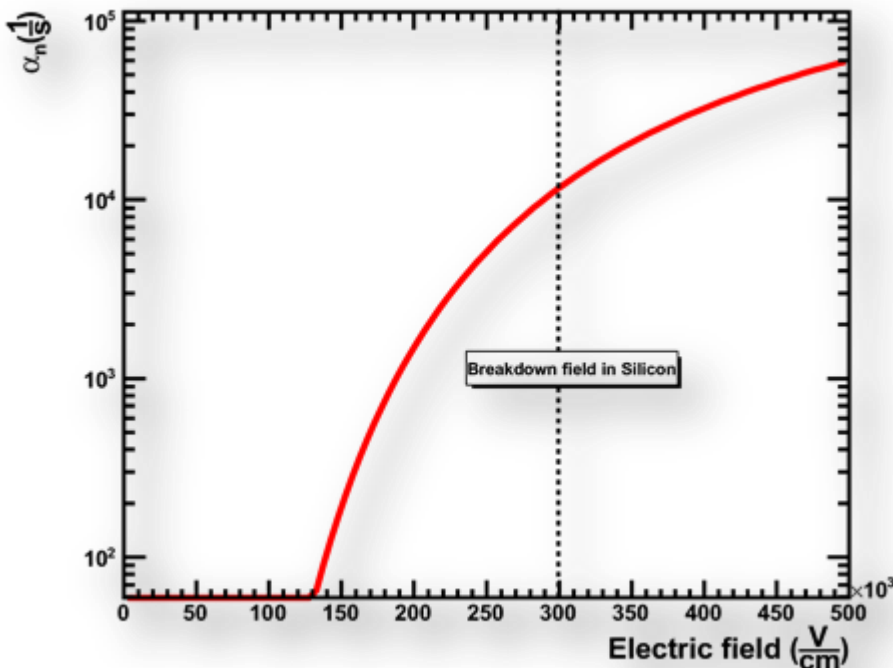
M. Petasecca, F. Moscatelli, D. Passeri, G. Pignatelli, and C. Scarpello, "Numerical simulation of radiation damage effects in p-type silicon detectors," *Nucl. Instrum. Meth. A*, vol. 563, no. 1, pp. 192-195, 2006.

Impact ionization

$$G = \alpha_n(E)J_n + \alpha_p(E)J_p$$

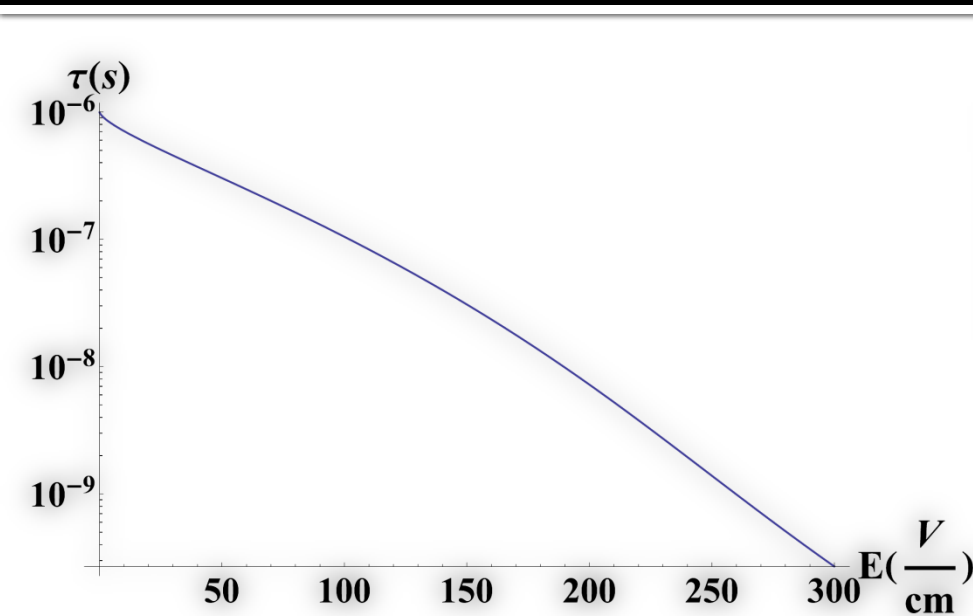
$$\alpha_n = A_n e^{-(B_n/E)^{\beta_n}}$$

$$\alpha_p = A_p e^{-(B_p/E)^{\beta_p}}$$



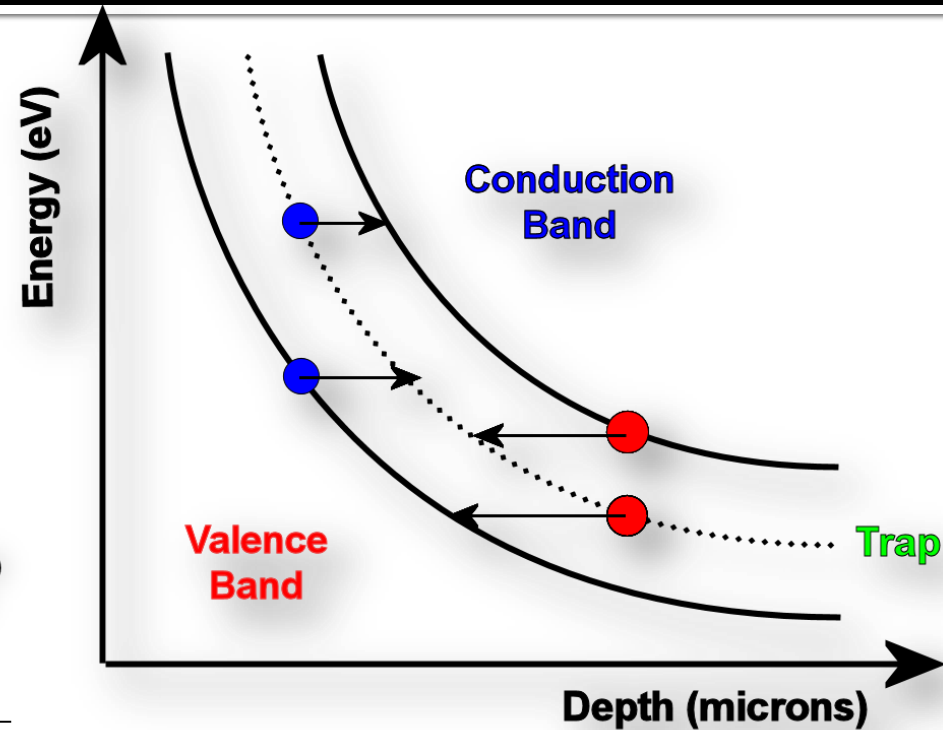
Selberherr, S., "Analysis and Simulation of Semiconductor Devices", Springer-Verlag Wien New York, ISBN 3-211-81800-6, 1984.

Phonon-assisted trap-to-band tunnelling



$$R_i = \frac{pn - n_i^2}{\frac{\tau_{n0}}{1 + \Gamma_n^{DIRAC}} (p + \Gamma n_i e^{\frac{(E_f - E_i)}{kT}}) + \frac{\tau_{p0}}{1 + \Gamma_p^{DIRAC}} (n + \frac{n_i e^{\frac{(E_i - E_f)}{kT}}}{\Gamma})}$$

Hurkx, G.A.M., D.B.M. Klaasen, M.P.G. Knuvers, and F.G. O'Hara, "A New Recombination Model Describing Heavy-Doping Effects and Low Temperature Behaviour", *JEDM Technical Digest*(1989): 307-310.



$$\Gamma_n^{DIRAC} = \frac{\Delta E_n}{kT_L} \int_0^1 e^{\left(\frac{\Delta E_n}{kT_L} u - K_n u^{\frac{3}{2}}\right)} du$$

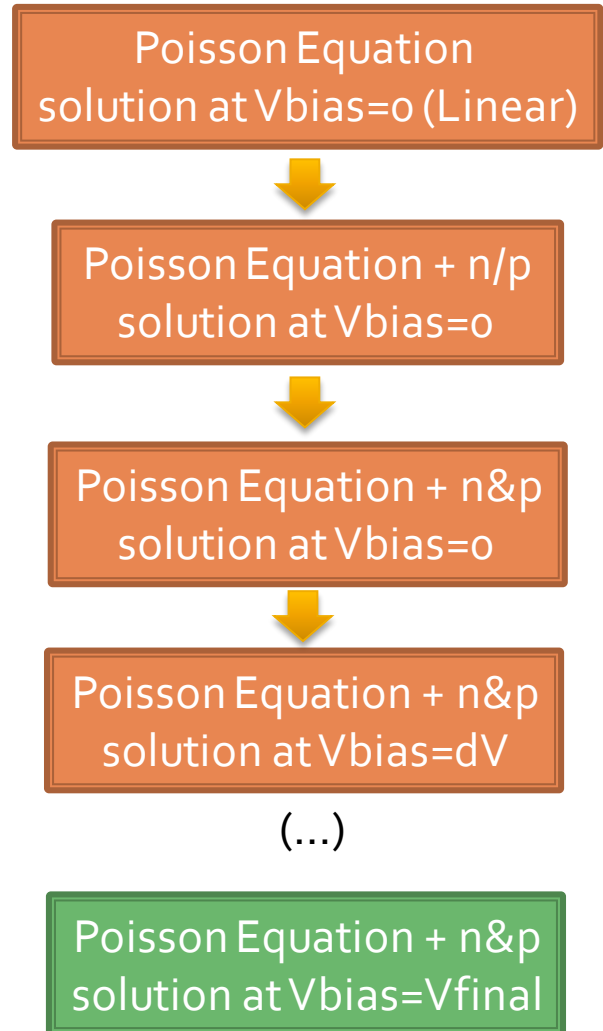
$$K_n = \frac{4}{3} \frac{\sqrt{2m_0 m_{tunnel}} \Delta E_n^3}{3q\hbar|E|}$$

$$\Gamma_p^{DIRAC} = \frac{\Delta E_p}{kT_L} \int_0^1 e^{\left(\frac{\Delta E_p}{kT_L} u - K_p u^{\frac{3}{2}}\right)} du$$

$$K_p = \frac{4}{3} \frac{\sqrt{2m_0 m_{tunnel}} \Delta E_p^3}{3q\hbar|E|}$$

Numerical methods and convergence

- The second major issue you will encounter when doing TCAD simulation is convergence
 - In practice most problems will have large non-linearities due to the model used for G/R -> Newton method
 - More complex solver must be used to obtain solution in practice
 - A good initial solution is needed for all practical purposes



Comparison of main commercial TCAD software packages

SILVACO TCAD Suite

<http://www.silvaco.com/>

Silvaco Data Systems was founded in 1984 by Dr. Ivan Pesic. The initial product, UTMOST, quickly became the industry standard for parameter extraction, device characterization and modeling.

In 1985 Silvaco entered the SPICE circuit simulation market with SmartSpice.

In 1987 Silvaco entered into the technology computer aided design (TCAD) market. By 1992 Silvaco became the dominant TCAD supplier with the ATHENA process simulator and ATLAS device simulator.

Educational prices available on request from Silvaco

Sentaurus TCAD Suite

<http://www.synopsys.com/Tools/TCAD/Pages/default.aspx>

Formerly ISE TCAD, bought by Synopsys

Synopsys is a world leader in electronic design automation (EDA), supplying the global electronics market with the software, IP and services used in semiconductor design and manufacturing. Synopsys' comprehensive, integrated portfolio of implementation, verification, IP, manufacturing and FPGA solutions helps address the key challenges designers and manufacturers face today, such as power and yield management, system-to-silicon verification and time-to-results. These technology-leading solutions help give Synopsys customers a competitive edge in bringing the best products to market quickly while reducing costs and schedule risk. Synopsys is headquartered in Mountain View, California, and has more than 60 offices located throughout North America, Europe, Japan, Asia and India.

Available from EUROPractice

Disclaimer: I do not have any link with any of the company producing TCAD software. Recommendation here are strictly personal based on my experience with both software during my work in HEP

Comparison of main commercial TCAD software packages

SILVACO	Sentaurus
Athena : 2D SSUPREM4 based process simulator	Sprocess : 2D/3D SSUPREM4 based process simulation
ATLAS : 2D (and basic 3D) device simulation	Sdevice : 2D and 3D device simulation
VICTORYCELL : GDS based 3D process simulation	SnMesh : Adaptativ meshing tool for process and device simulation
VICTORYPROCESS : 3D Process simulation	Swb : Sentaurus WorkBench, GUI controlling simulation process flow, parametrization etc..
VICTORY DEVICE : 3D device simulation	
Virtual Wafer Fab : wrapper of the different tool in a GUI	

• Advantages

- 3D Simulation built-in
 - Seamless transition from 2D to 3D
- Excellent user interface
- Support for LSF (lxbatch !!!)
- Parallel 3D solver (takes advantage of modern multi-core CPU)
- Adaptive meshing and clever 3D meshing algorithm

Inconvenients

- User support very slow
 - ~1-2 months for an answer
- Syntax of the simulation protocol is a bit more tedious than for equivalence in the competitor (learning curve steeper)
- Set of example smaller and less relevant for HEP than the competitor

Advantages

- Simple scripting language make it easy to start real work within a short time
- Extensive litterature supporting the validity of the software
- Very responsive user support:
 - Email exchange directly with the engineers
 - Custom patches produced following our needs

Inconvenients

- More complex parametric simulation planification (Design-Of-Experiment)
- GUI rather old and in need of a rejuvenation
- No parallel solver for 3D device simulation
- No 3D process simulation without the purchase of an expensive supplementary licence
- Meshing methods not adapted to 3D simulation

Common aspects

- The physics included in both simulation software are very similar :
 - Both software based on the same open-source base programs.
 - Syntax, outputs in most case identical
 - Models are based on same publications
 - Solving methods essentially the same
 - Matrix handling however differ between software
 - Both, unsurprisingly, claim to be the best on the market !

Common aspects

- Both software allow for redefinition of any constants, input parameters of the models used, ex :
 - Lifetime, cross-section, bandgap, impact ionization coefficient etc...
- Many (not all) models can be redefined using the internal C interpreter, ex :
 - Redefined impact ionization coefficient variation with electric field
 - Redefined mobility dependence on $T, E, N_{A/D}$

TCAD simulation as a black box (1)

- Both software are sold as compiled software with no access to source code, however :
 - Both software are extensively used in the industry with a lot of success translating in a major contribution to the improvement of the microelectronics
 - Both software are extensively documented with references provided :
 - SILVACO ATLAS Manual -> 898 pages
 - SENTAUROS DEVICE Manual -> 1284 pages

TCAD simulation as a black box (2)

- The benefit of using a commercial software w.r.t Home-Made solution are :
 - to benefit from a large user base (debugging, feedback and new features) 😊
 - Less focus on mathematics and coding more focus on physics 😊 (physicist can't do everything, we should stick to what we know best !)
 - Ex: Writing a Navier-Stokes solver for a 2D very specific geometry (given a recipe and all equation and numerical methods) ~ 1-2 months for a master student

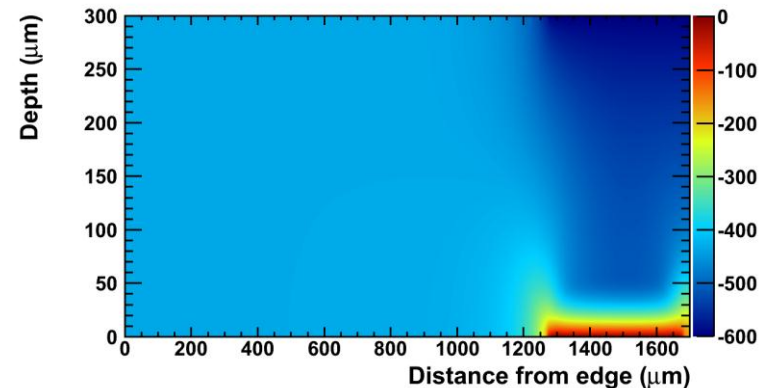
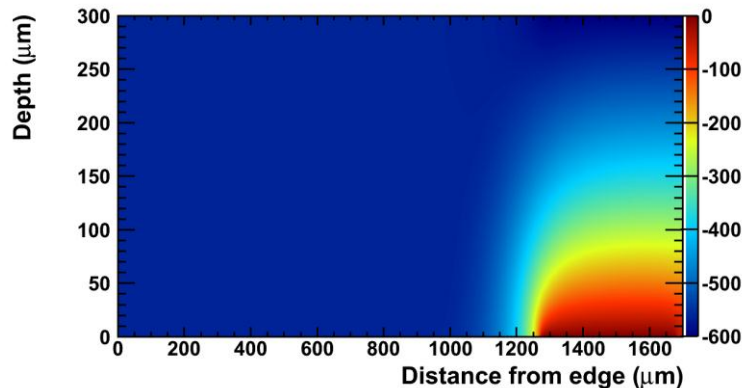
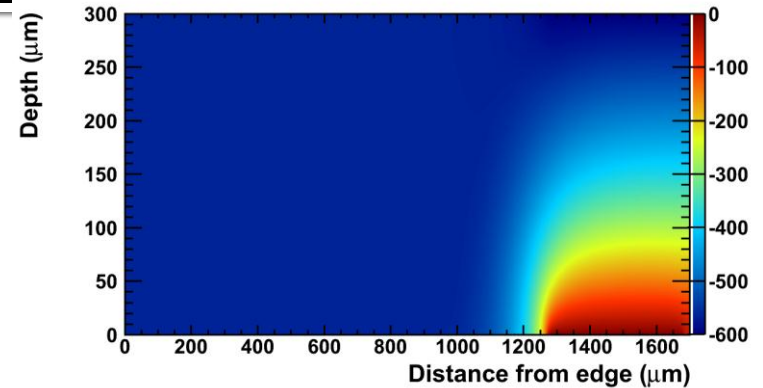
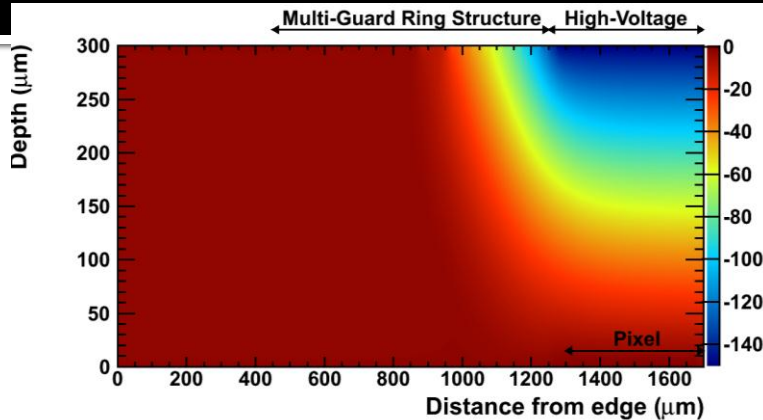
TCAD simulation as a black box (3)

- FEM is commonly use to provide reliable simulation for design of the plane that flew you here , or the cooling system of your laptop
- Simulation of non-irradiated semiconductor device has reached a similar level or reliability
- A lot of work from the RD50 collaboration could very much bring the simulation of irradiated sensors to the same stat !

TCAD Simulation capabilities

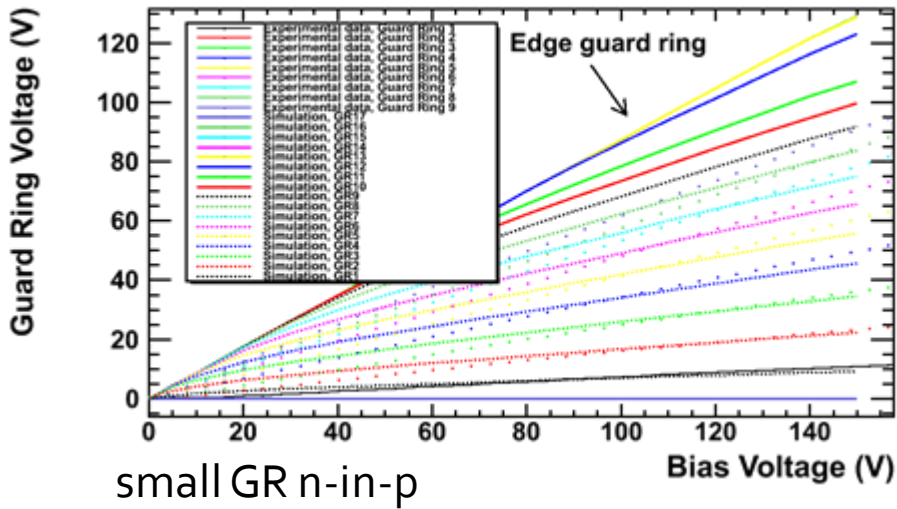
- TCAD is suitable for simulation of complex structure
 - Guard rings , punch-trough
 - E-Field distribution in presence of complex doping profiles
- Transient simulation
 - Apply a stress to a DC-Stable system and relax it back to equilibrium (ie. Virtual TCT)
- AC Analysis (CV Curves, inter-pixel/strip capacitance)

Guard ring simulation and SCS

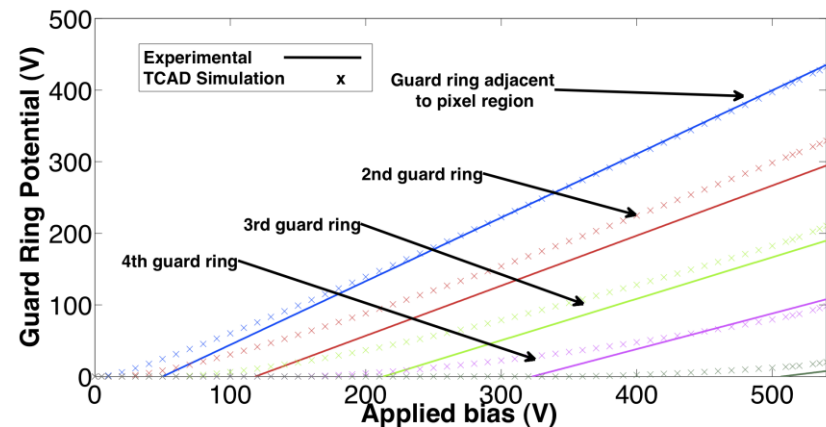
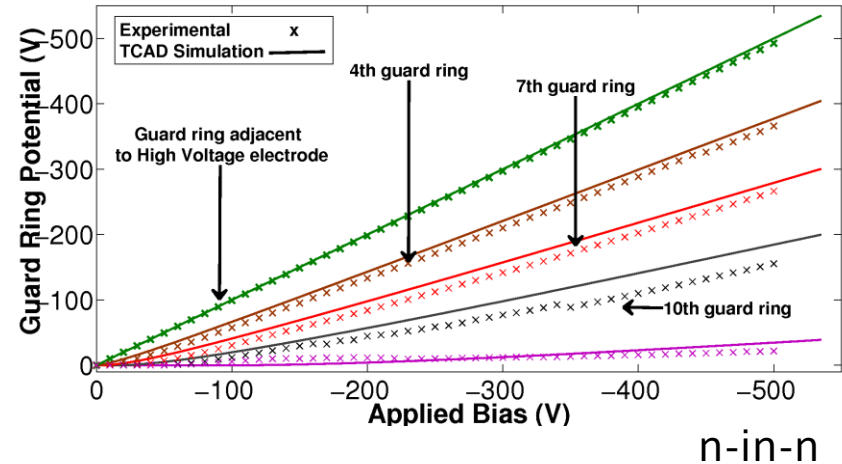


Simulation of Radiation Damage Effects on Planar Pixel Guard Ring Structure for ATLAS Inner Detector Upgrade
by: M. Benoit, A. Lounis, N. Dinu
Nuclear Science, IEEE Transactions on, Vol. 56, No. 6. (08 December 2009), pp. 3236-3243,
doi:10.1109/TNS.2009.2034002

Experimental data

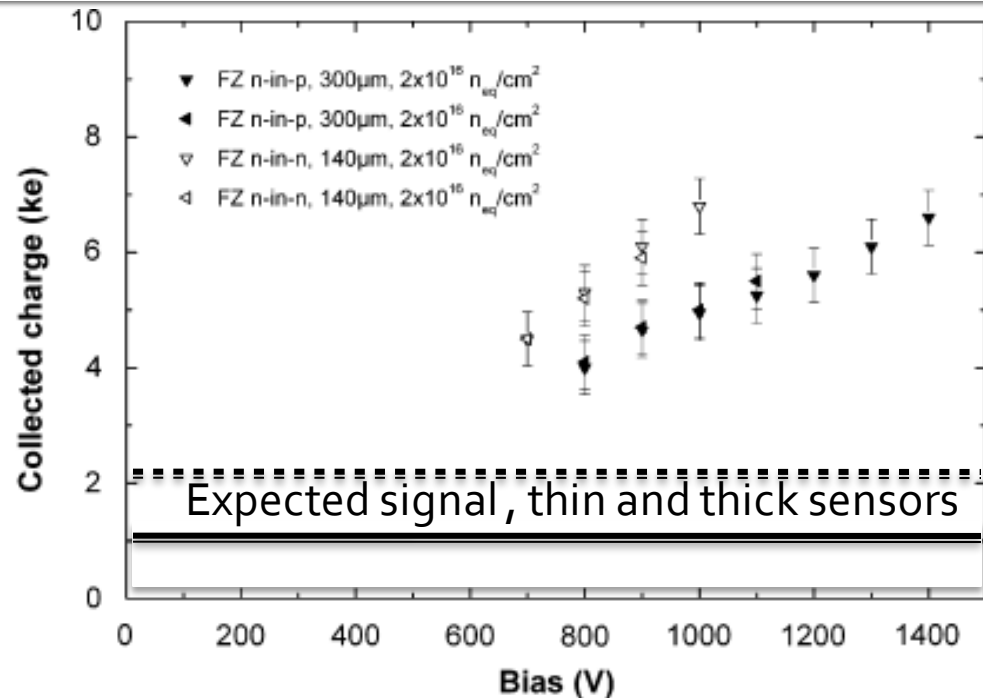


Very good agreement between simulation and data when using adequate technological parameters!



Charge multiplication in silicon planar sensors

- Recent measurements performed on diodes irradiated to sLHC fluence show anomalous charge collection
- My idea has been to use the radiation damage model in TCAD and include the impact ionization and trap-to-band tunnelling into the simulation to see if these physical effects can reproduce the observed behavior



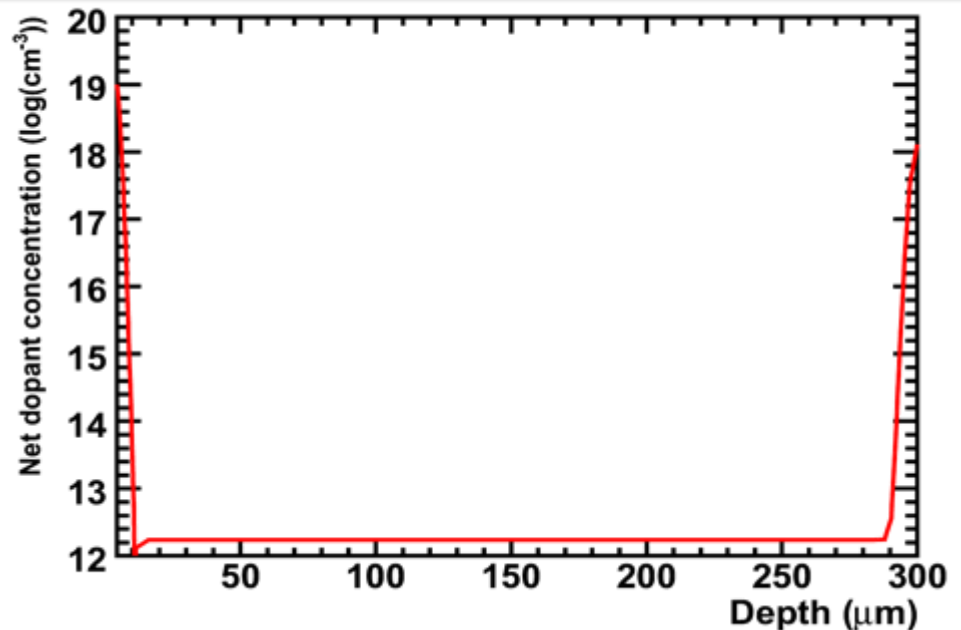
G. Casse and al., "Evidence of enhanced signal response at high bias voltages in planar silicon detectors irradiated up to $2.2 \times 10^{16} \text{ n}_{\text{eq}}/\text{cm}^2$," Nucl. Instrum. Meth. A, j.nima.2010.04.085,, vol. In Press, Corrected Proof, pp. -, 2010.

M. Mikuz, V. Cindro, G. Kramberger, I. Mandic, and M. Zavrtanik, "Study of anomalous charge collection efficiency in heavily irradiated silicon strip detectors, -, j.nima, 2010.

An example : 1D heavily irradiated n-in-p diode

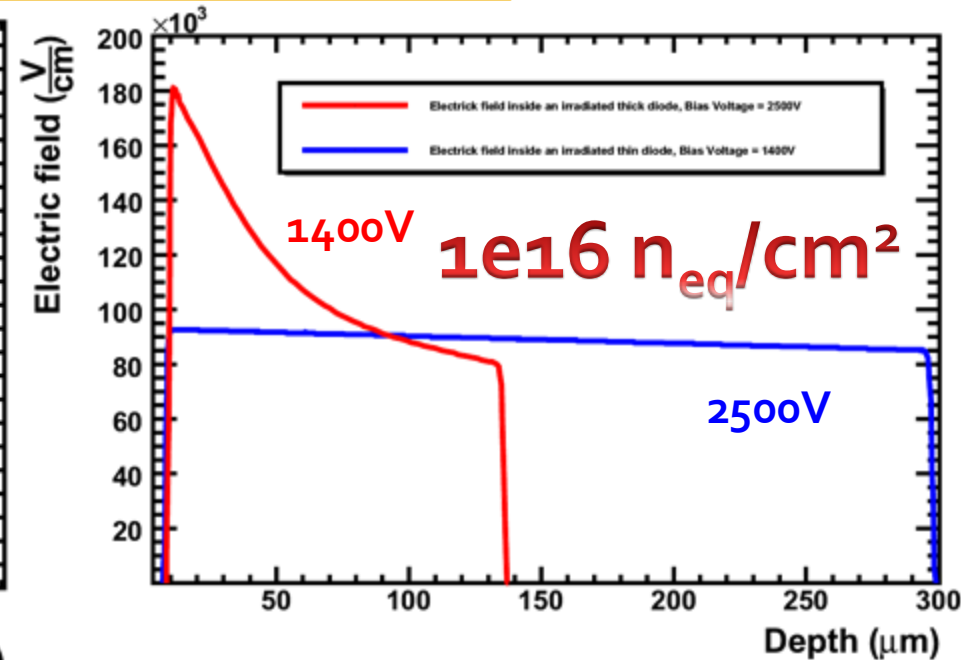
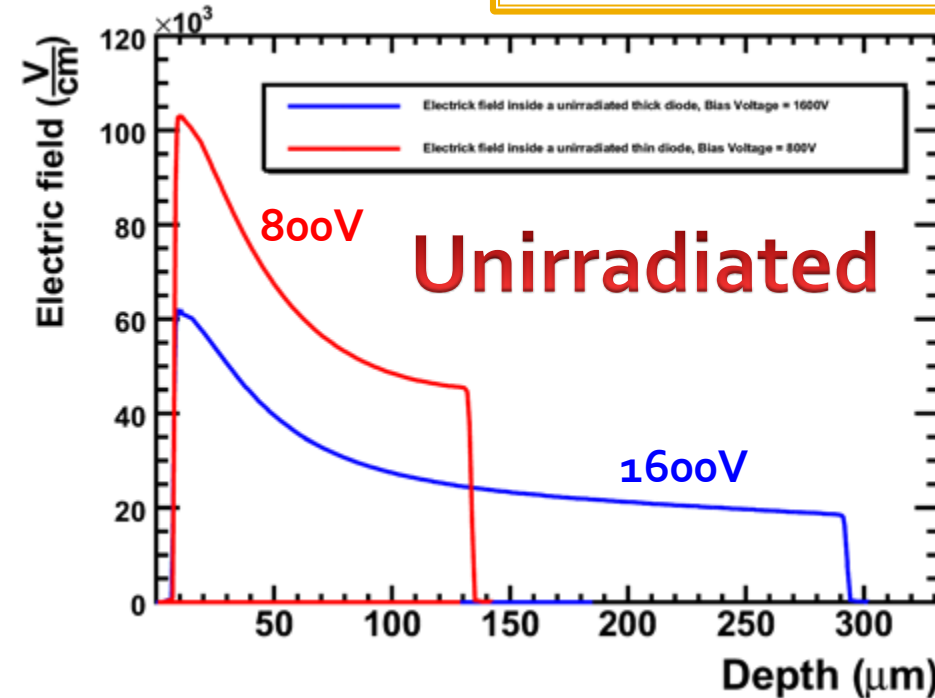
- A simple 1D p-type diode, n readout
- $N_{\text{eff}} = 1.74 \times 10^{12} / \text{cm}^3$
- 140 and 300 microns thickness
- $2 \text{K} \Omega \text{cm}$ resistivity, high implant peak concentration ($1 \times 10^{17} - 10^{18} / \text{cm}^3$)

- To simulate the CCE curve of the irradiated detector, we:
 - 1. Generate a mip-like charge distribution with a 1060nm laser, $0.05 \text{W}/\text{cm}^2$
 - 2. Perform transient simulation over 25ns for each bias
 - 3. Numerical integration of resulting current minus pedestal
 - 4. Numerical integration of available photocurrent
 - 5. $\text{CCE} = Q_{\text{pulse}} / Q_{\text{photocurrent}}$



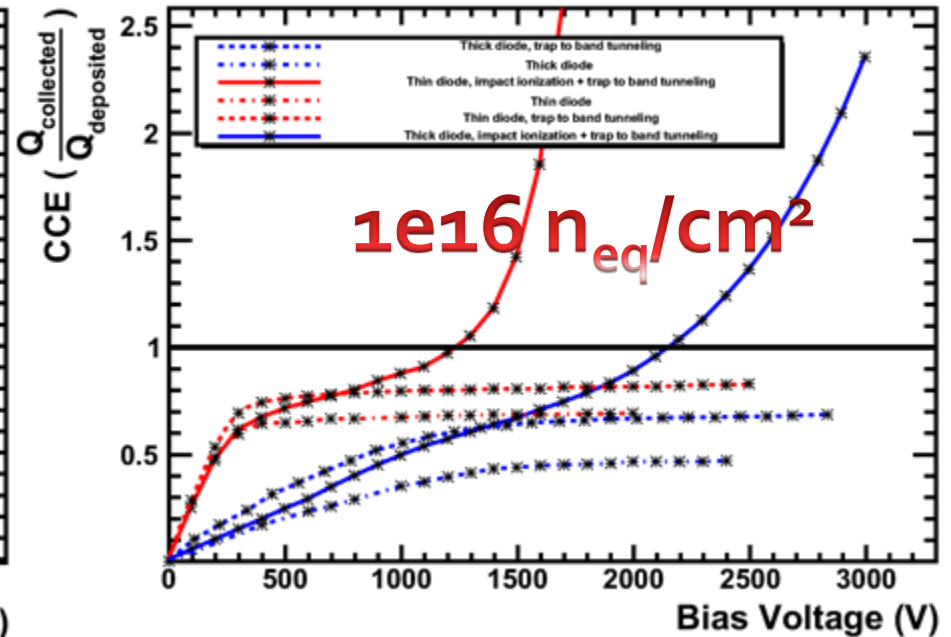
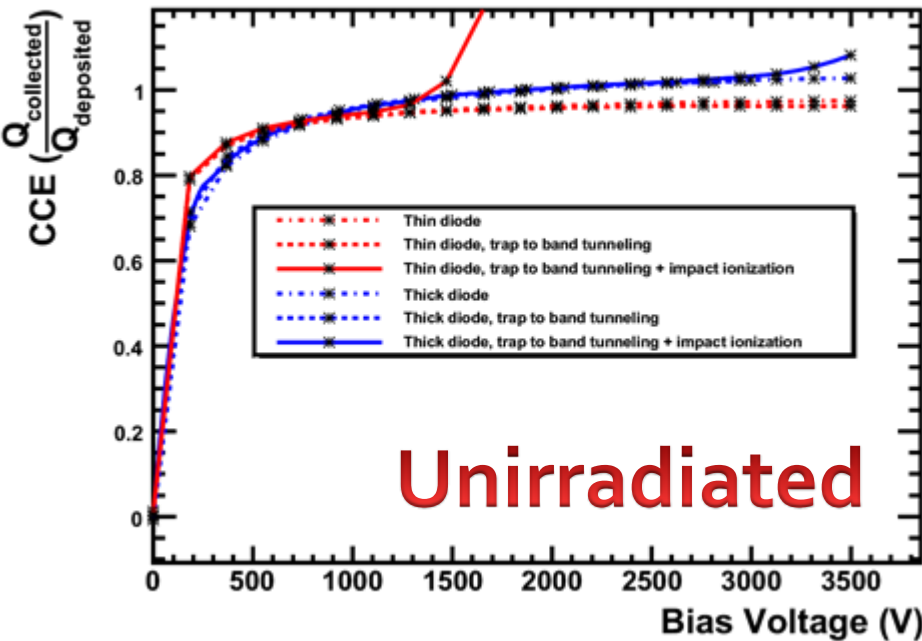
Electric field profiles

Electric field before hard junction breakdown.



Sensor can be biased to HV after irradiation without reaching hard breakdown allowing multiplication in the high electric field produced by this bias

Charge collection efficiency



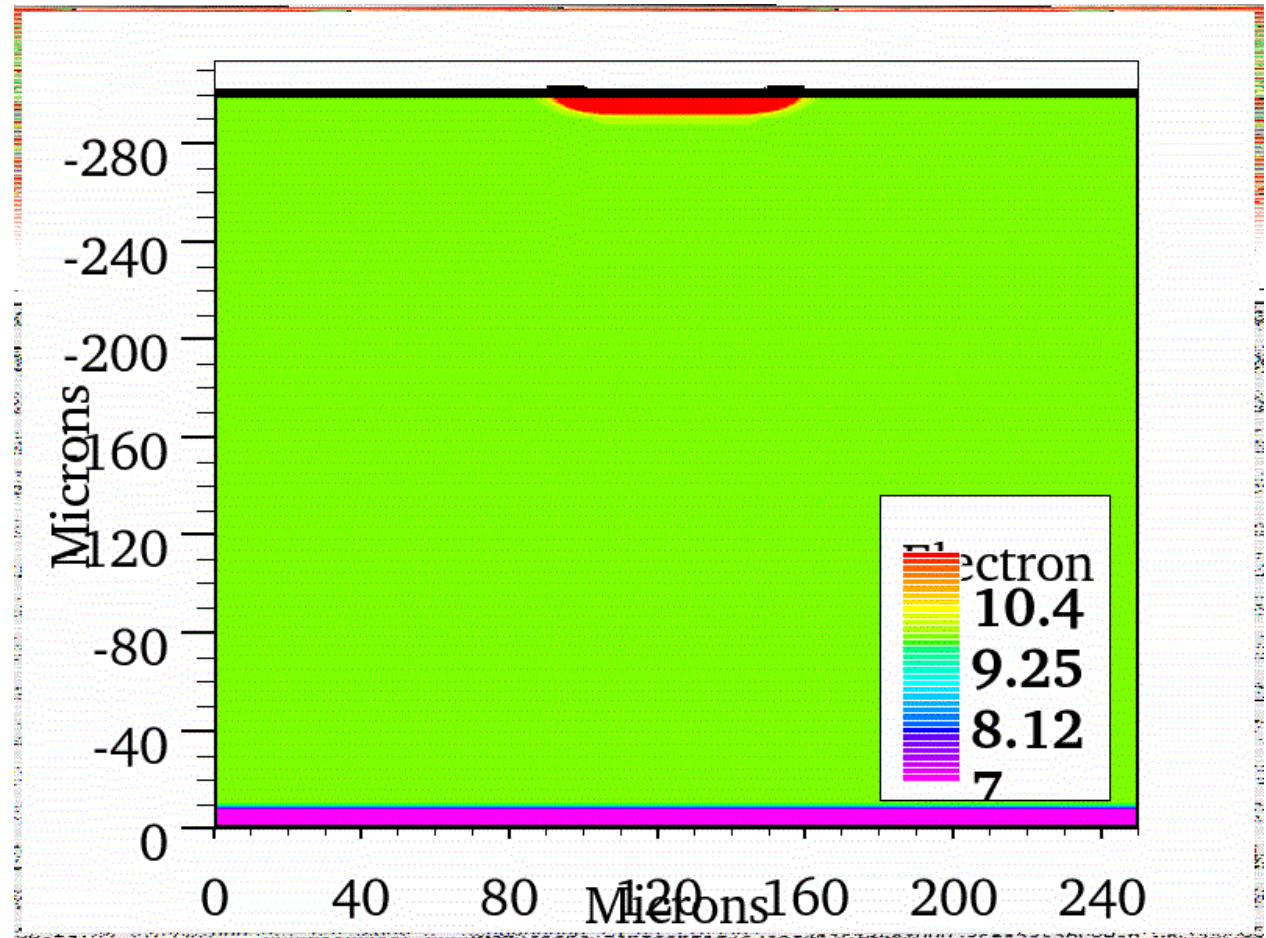
Unirradiated diode unaffected by TTBT and II are off. However, they both contribute to CCE after irradiation because of the presence of the $> 200 \text{ kV/cm}$ field

Simulation of charge multiplication and trap-assisted tunneling in irradiated planar pixel sensors

by: M. Benoît, A. Lounis, N. Dinu

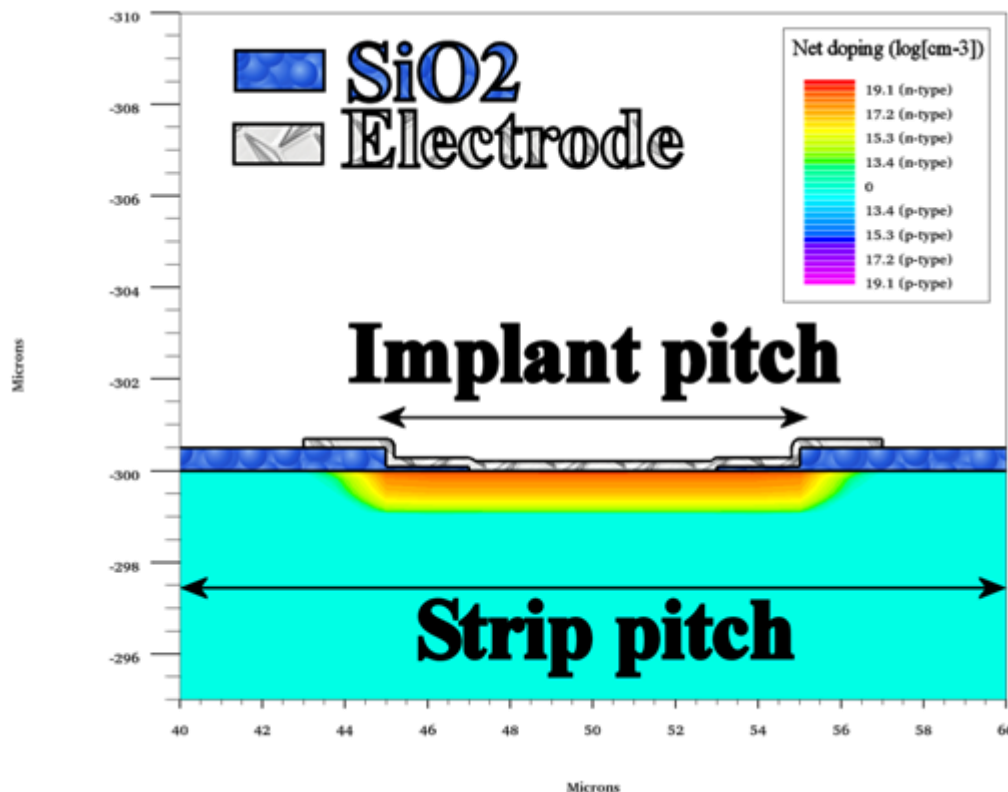
In IEEE Nuclear Science Symposium & Medical Imaging Conference (October 2010), pp. 612-616, doi:10.1109/NSSMIC.2010.5873832

Charge multiplication in silicon planar sensors



2D simulation : Strips with various doping profile and geometry

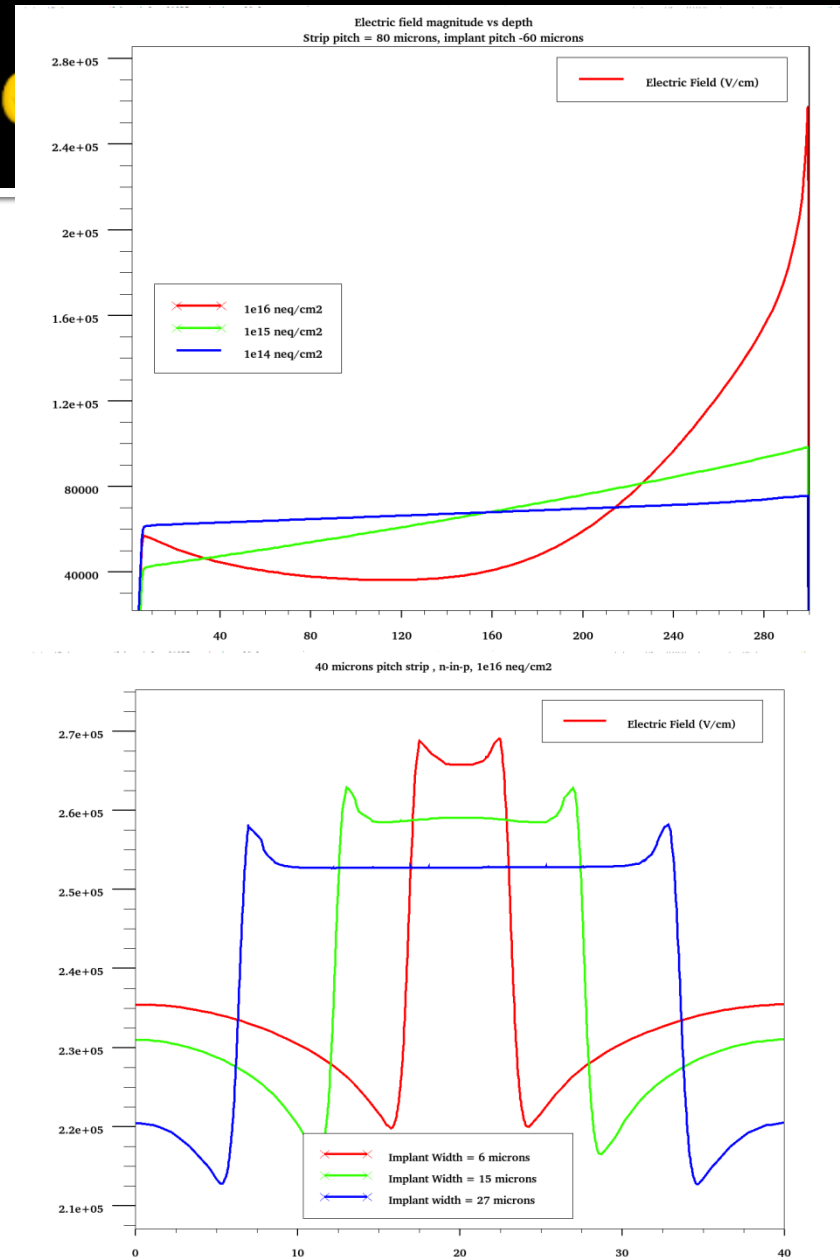
- A set of n-in-p strip sensor with different strip and implant pitch, and with different intermediate strip pitch was studied



Strip pitch (μm)	Implant width (μm)
80	60
80	25
80	6
100	70
100	33
100	10
40	27
40	15
40	6

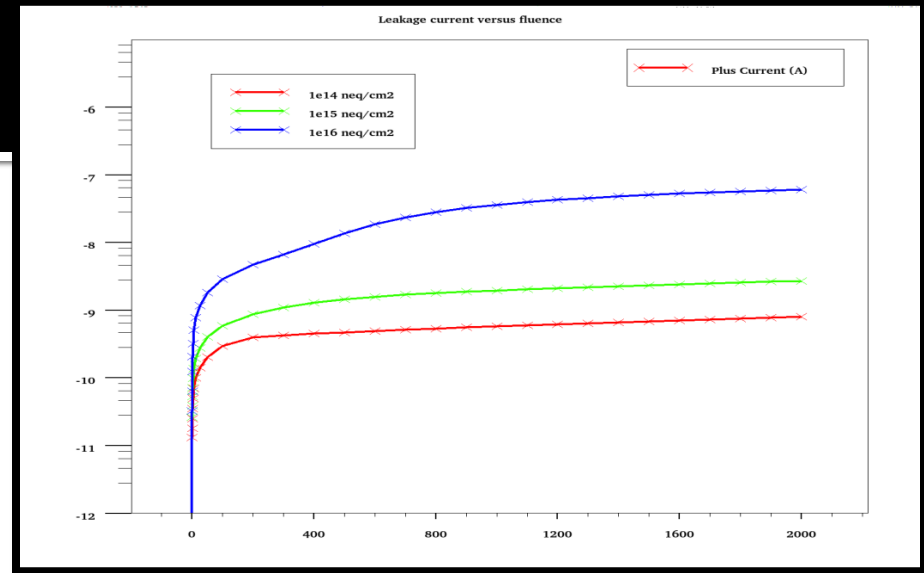
2D simulation : Strips with various doping profile and geometry

- Each sensor was biased at 2000V, and simulated for a fluence of $10^{14,15,16}$ n_{eq}/cm^2
- Moderate p-spray insulation between strips
- Classical implantation for n strip implant
- Drive-in 100 min @ 900C

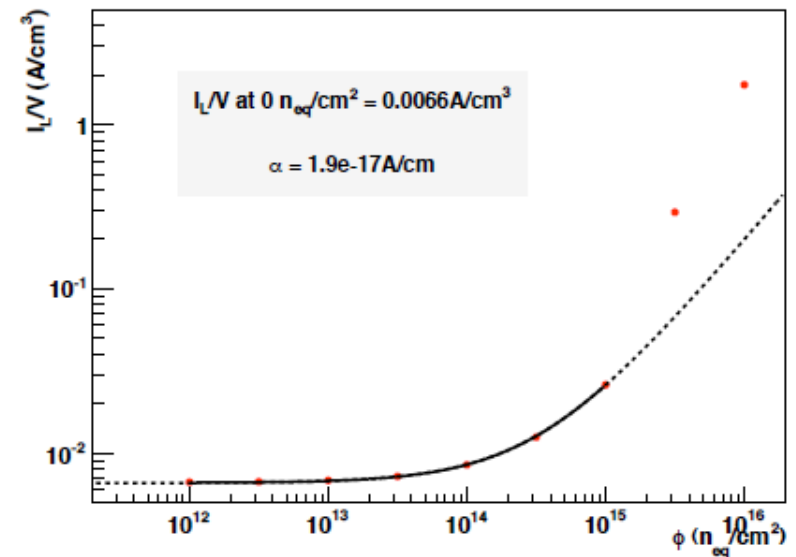


2D simulation : Leakage current

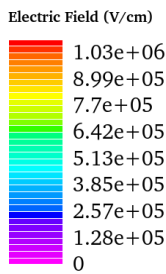
- Leakage from different strip pitch not influenced by the pitch
- Hard breakdown of the junction at the strip extremity lower for small implant pitch/strip pitch ratio
- $\alpha = 1.9\text{e-}17\text{A/cm}$
- Contribution from Trap-to-band tunnelling and impact ionization visible in leakage current about $1\text{e}15\text{ n}_{\text{eq}}/\text{cm}^2$



I_L vs ϕ at 2400V. Thickness = 300.00 μm



2D simulation : Electric field (at $10^{14} \text{ n}_{\text{eq}}/\text{cm}^2$)



Strip
pitch

40 μm

Implant
width = 6 μm

30 μm depth represented

15 μm

27 μm

80 μm

6 μm

25 μm

60 μm

100 μm

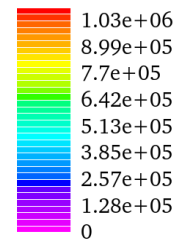
10 μm

33 μm

70 μm

2D simulation : Electric field (at $10^{15} n_{eq}/cm^2$)

Electric Field (V/cm)



Strip
pitch

40 μm

Implant
width = 6 μm

30 μm depth represented

15 μm

27 μm

80 μm

6 μm

25 μm

60 μm

100 μm

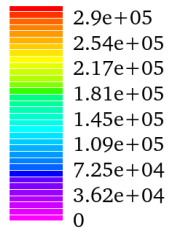
10 μm

33 μm

70 μm

2D simulation : Electric field (at $10^{16} \text{ n}_{eq}/\text{cm}^2$)

Electric Field (V/cm)



Strip
pitch

40 μm

Implant
width = 6 μm

30 μm depth represented

15 μm

27 μm

80 μm

6 μm

25 μm

60 μm

100 μm

10 μm

33 μm

70 μm

From measurements to prediction

- TCAD softwares offer a large parameter space to fit RD50 measurements
- Optimization packages are available within the software to fit data to simulation by varying a few parameters
- Knowing well the characteristics of the simulated structures is very helpful to produce quantitative results
 - Doping/Active dopant profile
 - Mask design and processing parameters

Conclusion

- TCAD simulation proves to be a powerful tool for studying the behavior of rather complex semiconductor structure
 - Qualitative results reproducing main aspects of radiation damage can be performed easily
 - Further work with test structure and extensive characterization is needed to produce more quantitative results
- Commercial TCAD software are mature products that have proven the usefulness
 - Large user base
 - Fast, well coded software, ready to use by a non-programmer
 - Careful and detailed tuning of radiation damage model by the RD50 collaboration would be a wonderful addition to the TCAD toolbox

Thank you !

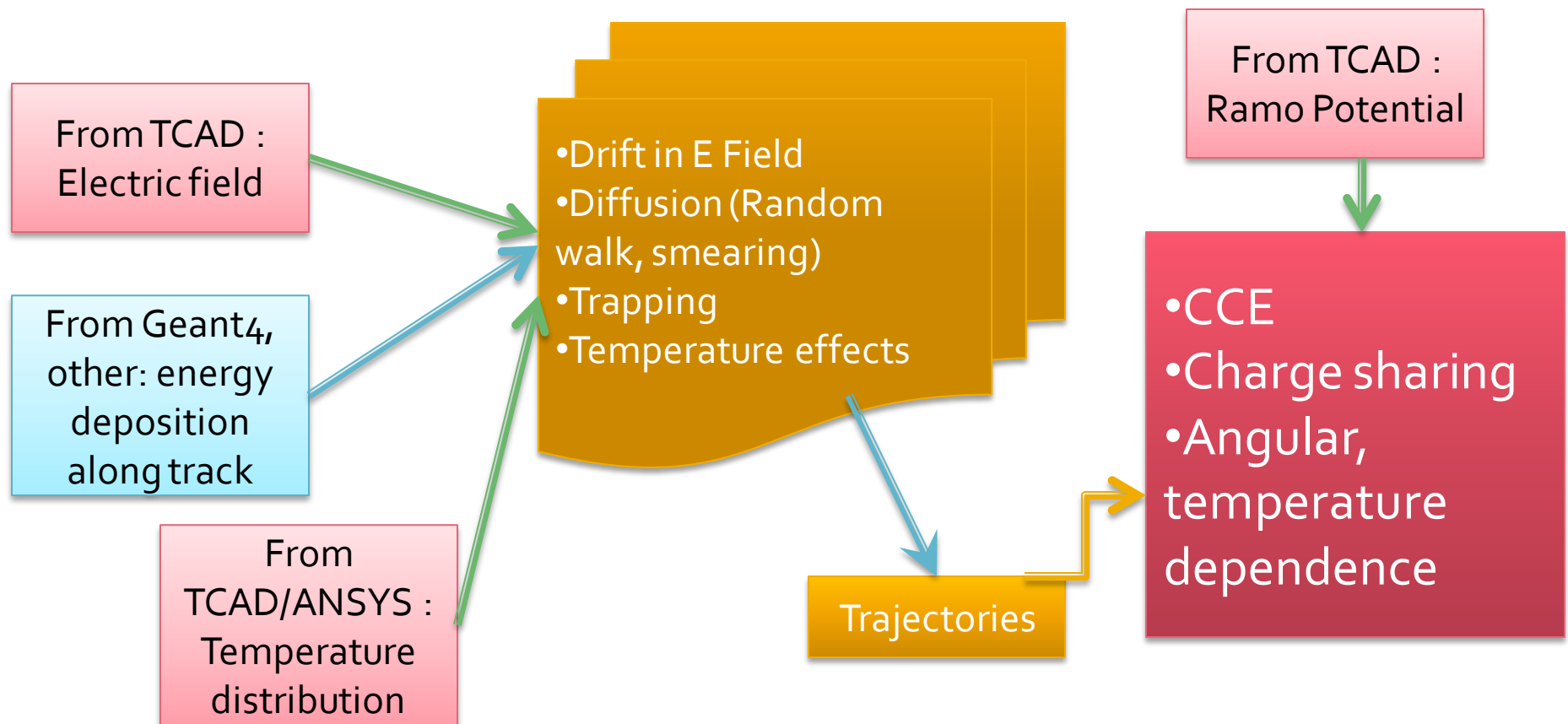
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Thesis (in english) : [Étude des détecteurs planaires pixels durcis aux radiations pour la mise à jour du détecteur de vertex d'ATLAS](#)

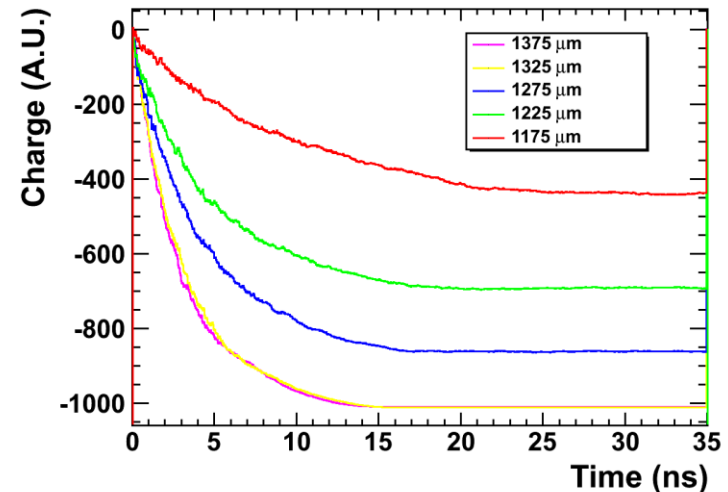
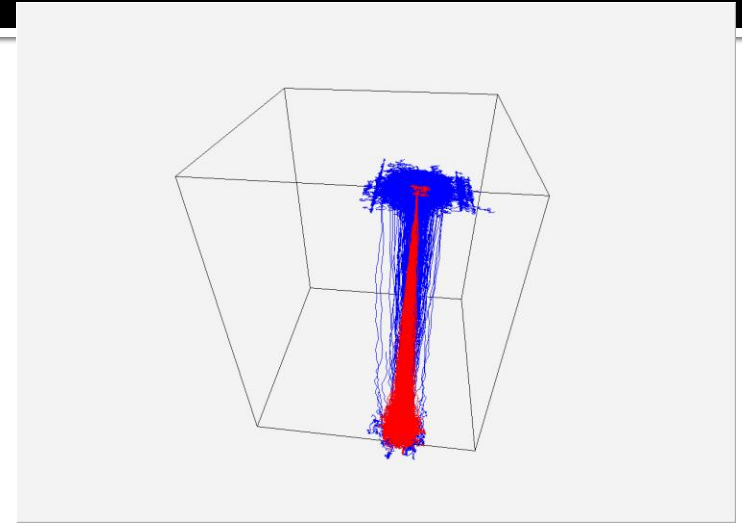
Simulation of detector behaviour : MC Charge Transport

- Monte-Carlo approach to simulation of charge transport of e/h in Silicon (Home code)



Simulation of detector behaviour : MC Charge Transport

- MC Charge transport act as a **middle man** between TCAD simulation and simple digitisation.
- It provides a **“fast” method** to obtain important value regarding the sensor, **taking advantage of TCAD data**
- The MC should be use as a **basis to provide data on expected shape of parameterization functions** used in further digitization
- Another approach is to directly use MC parameters and fit them to experimental data
(More time consuming)

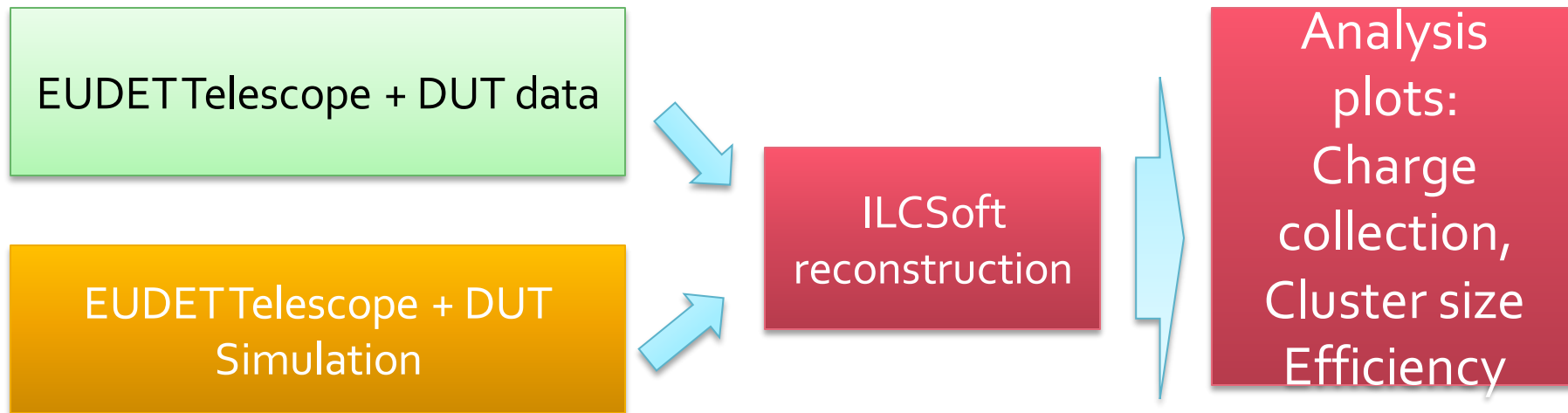


Simulation of detector behaviour : GEANT4 simulation and digitization calibration

- The final goal of the simulation is **to produce a fast digitizer reproducing well the behaviour of prototypes**, usable in full detector simulation
- Use Test Beam telescope data to **compare real DUT and Simulated DUT** to validate the digitizer
- **Incorporate chip effects into the simulation** at this level
 - Counter accuracy
 - timing accuracy
 - Noise, jitter of the DAC
 - Threshold
 - Crosstalk
 - Non-linearity in the analog acquisition chain
 - Inefficiency in the Digital buffers etc
 - SEE susceptibility
- Telescope (sim and data) are a good benchmark **for clustering algorithm**

Simulation of detector behaviour : GEANT4 simulation and digitization calibration

- Using a detailed GEANT4 framework **reproducing a well know telescope setup (EUNET)**, we can **compare and tune the digitizer** to represent well prototype behaviour by comparing real data and simulation in the reconstruction and analysis framework of the telescope



Example

