
Modelling radiation damage in TCAD

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Outline

- ✓ Motivations and background.
- ✓ TCAD radiation damage modelling: discussion.
- ✓ Simulation results and comparison with experimental data:
 - DC (steady-state) -> Diodes / Gate Controlled Diodes.
 - AC (small-signals) -> MOS Capacitors.
 - Time (transient) -> Multi-strip structures.
- ✓ Conclusions.

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Motivations

- ✓ Modern TCAD tools⁽¹⁾ offer a wide variety of approaches, characterized by different combinations among physical accuracy and comprehensiveness, application versatility and computational demand -> **mixed-mode** approaches can be efficiently followed.
- ✓ A number of different physical damage mechanisms actually may interact in a non-trivial way. Deep understanding of physical device behavior therefore has the utmost importance, and device analysis tools may help to this purpose.
- ✓ **Bulk** and **surface** radiation damage have been taken into account by means of the introduction of deep level radiation induced traps whose parameters are physically meaningful and whose experimental characterization is feasible.
- ✓ Within a **hierarchical approach**, increasingly complex models have been considered, aiming at balancing complexity and comprehensiveness.

(1) Sentaurus Device **SYNOPSYS**[®]

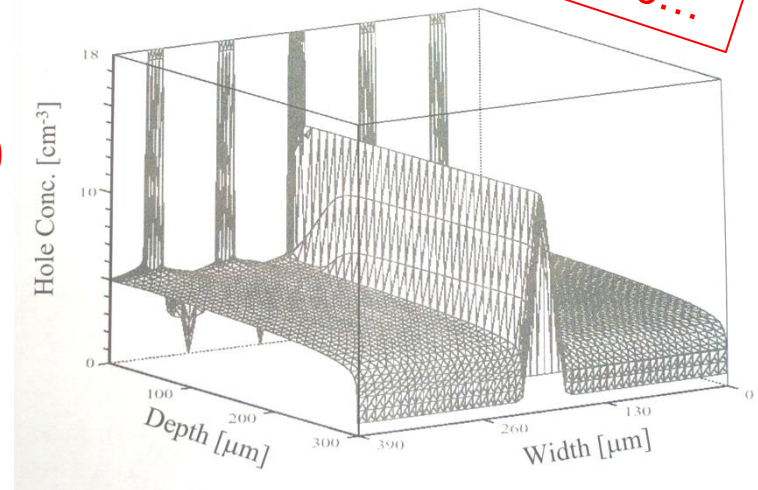
Once upon a time... (1996)

- ✓ Numerical analysis and physical modelling of semiconductor devices
-> application in High Energy Physics domain...
- ✓ Modelling of the interaction between ionizing particle / silicon substrate compatible with Box Integration Method simulation scheme.

$$\left\{ \begin{array}{l} \nabla \cdot (-\epsilon_s \nabla \varphi) = q (N_D^+ - N_A^- + p - n) \\ \frac{\partial n}{\partial t} - \frac{1}{q} \nabla \cdot \vec{J}_n = G - R + G^{rad} \\ \frac{\partial p}{\partial t} + \frac{1}{q} \nabla \cdot \vec{J}_p = G - R + G^{rad} \end{array} \right.$$

- ✓ G^{rad} can be distributed in time and space according to the numerical spatial and time discretization algorithms.

TCAD applications in HEP in 1996...



Radiation damage modelling

- ✓ Numerical modelling of radiation damage effects in semiconductor devices.
- ✓ Deep-level recombination centres / traps radiation induced.
- ✓ Explicit contribution of the trapped charges to the charge density (modified Poisson equation):

$$\nabla \cdot (-\varepsilon_s \nabla \varphi) = q (N_D^+ - N_A^- + p - n + p_d - n_a)$$

- ✓ Continuity equation for both free and trapped carriers:

$$\frac{\partial n}{\partial t} - \frac{1}{q} \nabla \cdot \vec{J}_n = -U_n$$

$$\frac{\partial p}{\partial t} + \frac{1}{q} \nabla \cdot \vec{J}_p = -U_p$$

$$\frac{\partial n_a}{\partial t} - \frac{1}{q} \nabla \cdot \vec{J}_{na} = -U_{na}$$

$$\frac{\partial p_d}{\partial t} + \frac{1}{q} \nabla \cdot \vec{J}_{pd} = -U_{pd}$$

"University of Perugia" model

1688

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 48, NO. 5, OCTOBER 2001

More than 20 specific journal papers on TCAD radiation damage modelling

Compreh

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 53, NO. 5, OCTOBER 2006

2971

Numerical Simulation of Radiation Damage Effects in p-Type and n-Type FZ Silicon Detectors

M. Petasecca, F. Moscatelli

THE RADIATION DAMAGE MODEL FOR P-TYPE

Level	Ass.	$\sigma_{n,p}$ (cm ²) Exp.[2]	σ_n (cm ²)	σ_p (cm ²)	η (cm ⁻¹)
Ec-0.42eV	VV ^(-/0)	2·10 ⁻¹⁵	2x10 ⁻¹⁵	2x10 ⁻¹⁴	1.613
Ec-0.46eV	VVV ^(-/0)	5·10 ⁻¹⁵	5x10 ⁻¹⁵	5x10 ⁻¹⁴	0.9
Ev+0.36eV	CiOi	2.5x10 ⁻¹⁵	2.5x10 ⁻¹⁴	2.5x10 ⁻¹⁵	0.9

TABLE II

THE THREE LEVELS RADIATION DAMAGE MODEL FOR N-TYPE

Level	Ass.	$\sigma_{n,p}$ (cm ²) Exp.[2,9]	σ_n (cm ²)	σ_p (cm ²)	η (cm ⁻¹)
Ec-0.42eV	VV ^(-/0)	2x10 ⁻¹⁵	2x10 ⁻¹⁵	1.2x10 ⁻¹⁴	13
Ec-0.50eV	VVO(?)	5x10 ⁻¹⁵	5x10 ⁻¹⁵	3.5x10 ⁻¹⁴	0.08
Ev+0.36eV	C _i O _i	2.5x10 ⁻¹⁵	2x10 ⁻¹⁸	2.5x10 ⁻¹⁵	1.1

I. INTRODUCTION

IN RECENT years there has been much effort to improve the radiation tolerance of detectors to be used in high energy physics (HEP) experiments, owing to the continuous increase of accelerators energy and efficiency. As a reference the Large Hadron Collider (LHC) at CERN is planned to be upgraded to a luminosity of 10³⁵ cm⁻² s⁻¹. Under these conditions the expected radiation fluence at the micro-vertex tracking distance (R = 4 cm) from the impact point is expected to be less than 10¹⁶ 1 MeV neutron equivalent per square centimetre. This will require more radiation-tolerant detectors.

Abstract—In this paper radiation-damaged silicon detectors employed the actual physical picture at a first-principle (i.e., understood, a hierarchical suitable approximation of behavior of silicon device in a three deep-level trapping of Shockley–Read–Hall the radiation is considered.

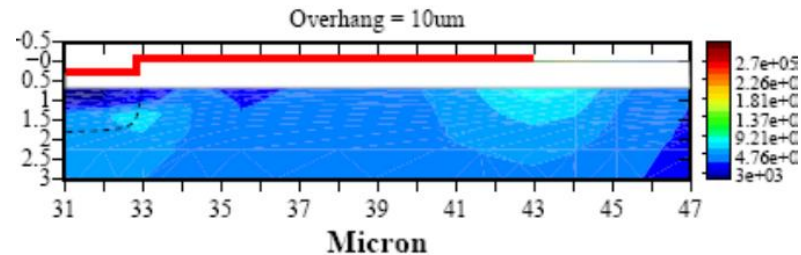
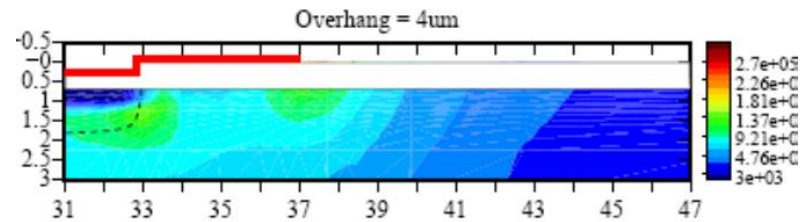
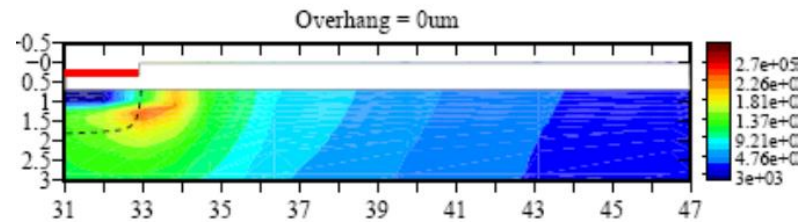
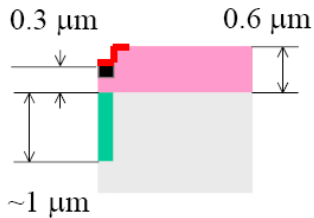
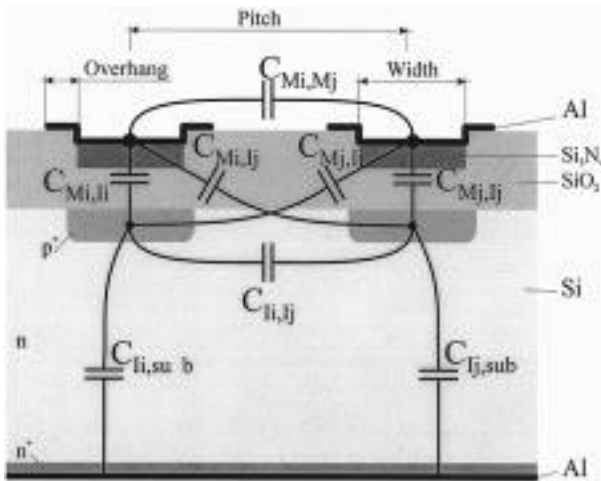
Index Terms—Radiation

SOLID-STATE semiconductor devices are widely used in the detectors, due to a number of more conventional conventional fabrication technology, can be integrated on a fine spatial resolution, noisy operating environment depends on a number of request for a satisfactory kept under strict control a full depletion of the raises significant concentration and to occur reliability is an issue induced by the incoming. Hence, despite their

- [1] D. Passeri, I. Radiation D
- [2] M. Petasecca, F. Moscatelli, D. Passeri, and G. Type and n-Type FZ Silicon Detectors, IEEE Tr

LHC CMS Si Tracker design

- ✓ Choice of the Si-Strip detector substrate resistivity.
- ✓ Strip geometry optimization (w/p, metal overhang).



Critical Electric Fields (within Si) reduction

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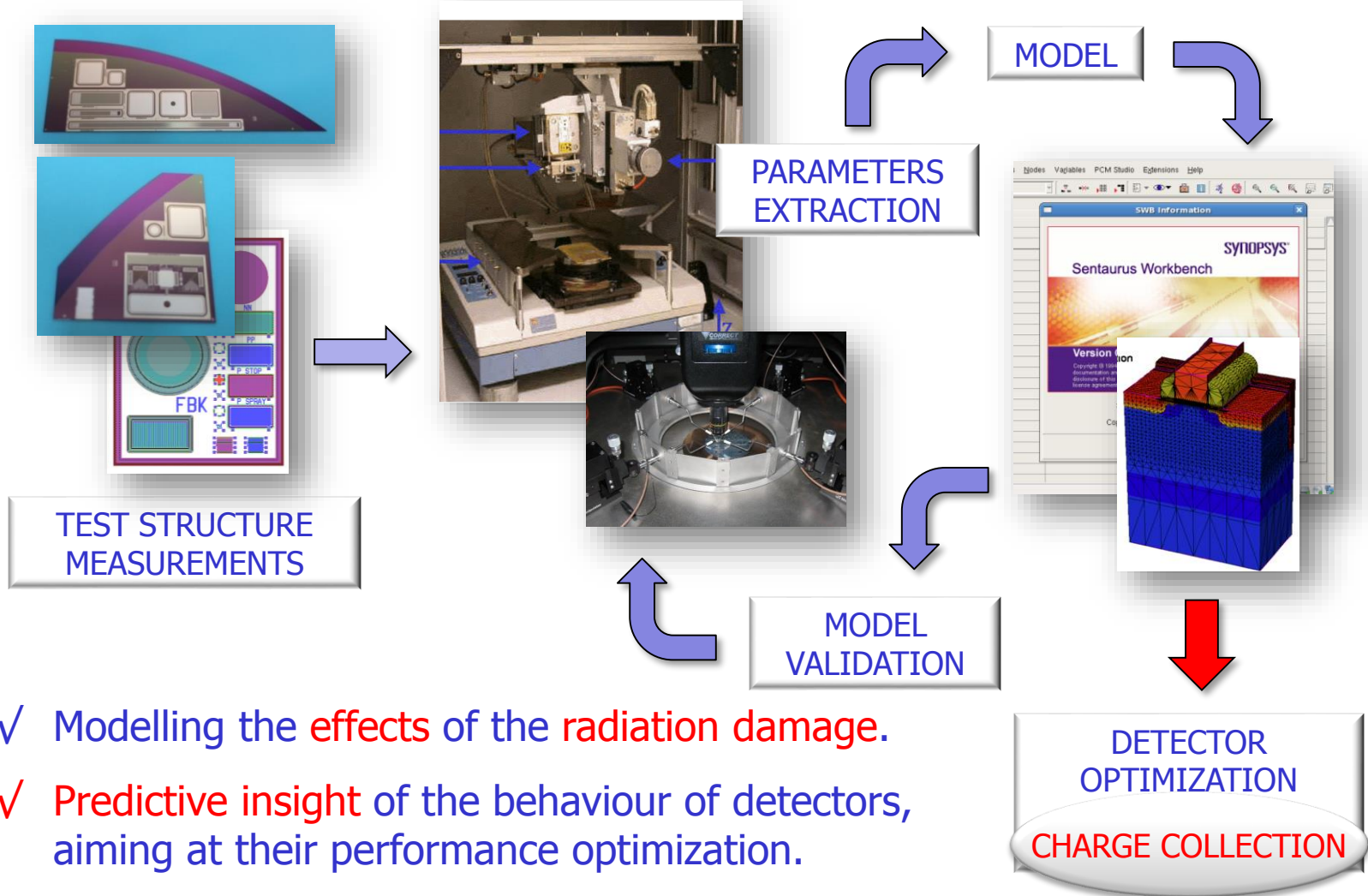
TCAD radiation damage models

- √ Pennicard et al., *Simulations of radiation-damaged 3D detectors for the Super-LHC*, NIM A 592 (2008) 16–25 .
 - 3 levels, increased capture cross-sections σ_n , σ_p .
- √ E. Verbitskaya et al., *Operational voltage of silicon heavily irradiated strip detectors utilizing avalanche multiplication effect*, JINST 7 C02061, 2012.
 - 2 levels, avalanche multiplication, 1D “analytical” approach.
- √ Delhi University (R. Dalal et al., Vertex - 2014, 23rd RD50 CERN, Nov. 2013)
 - 5 levels + Q_F / 2 levels + Q_F + Q_{it} .
- √ RD50 Collaboration (T. Peltola PSD2014 / RESMDD2014)
 - defect models tuned by R. Eber from V. Eremin et al., *Avalanche effect in Si heavily irradiated detectors: Physical model and perspectives for application*, NIM A 658 (2011) for $\Phi_{eq}=1.0\times 10^{14}$ - 1.5×10^{15} cm⁻² at fixed T=253 K;
 - 3-level model within 2 μ m of device surface + proton model in bulk.
- √ Hamburg model J. Schwandt, R. Klanner – Global parameter optimization (27th RD50 Workshop, December 2-4, 2015).

New “University of Perugia” model

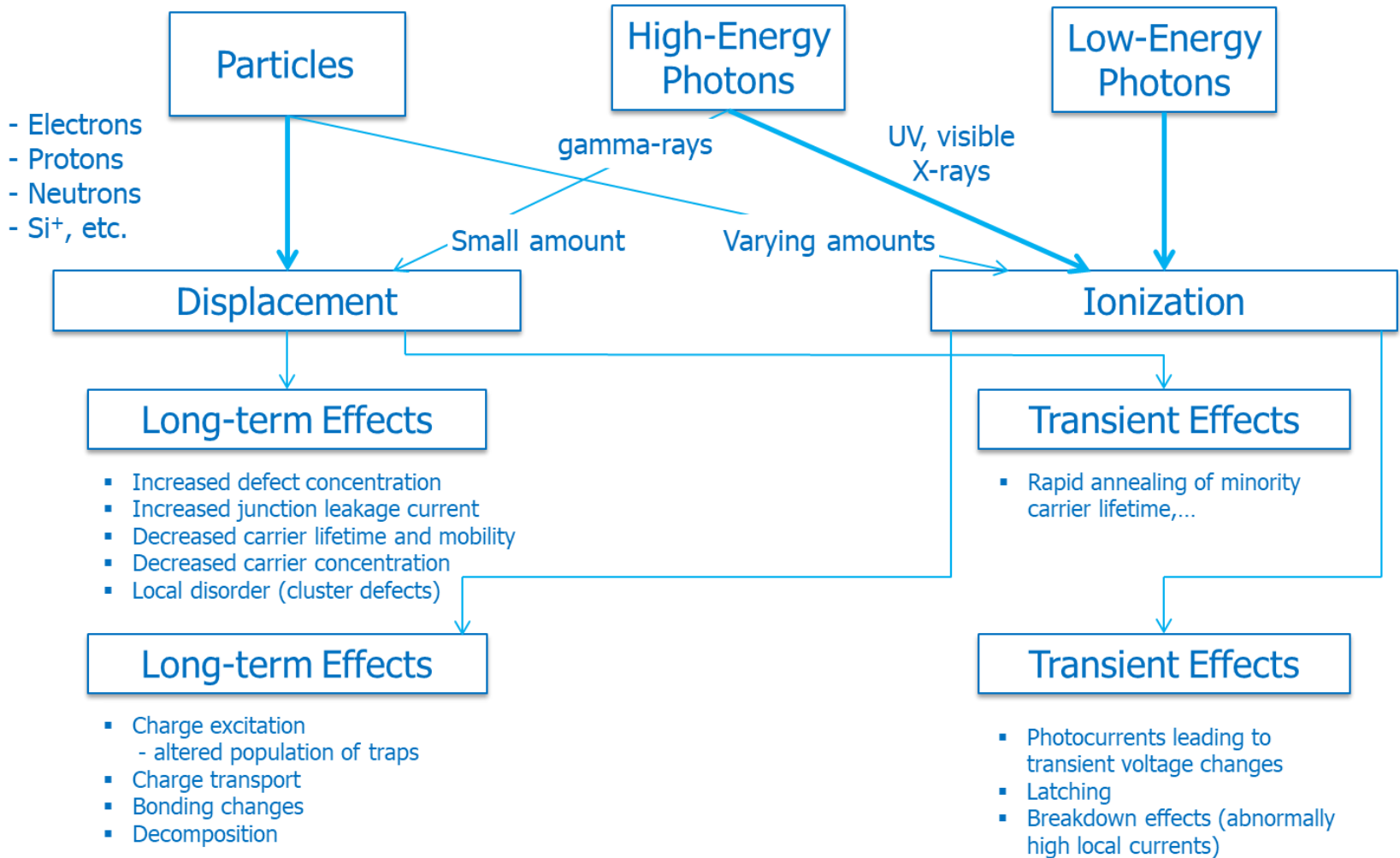
- ✓ Extend the predictive capabilities to HL-LHC radiation damage levels (e.g. fluences $> 2.0 \times 10^{16} \text{ cm}^{-2}$ 1 MeV neutrons).
- ✓ Keep low the number of traps (e.g. fitting parameters).
- ✓ New effects (e.g. charge multiplication \leftarrow avalanche effects).
- ✓ Physically grounded approach.
- ✓ No over-specific modelling (one model fits all...).
- ✓ Predictive capabilities @ Φ , @ T , @ V_{bias} ...

New "University of Perugia" model



- ✓ Modelling the **effects** of the **radiation damage**.
- ✓ **Predictive insight** of the behaviour of detectors, aiming at their performance optimization.

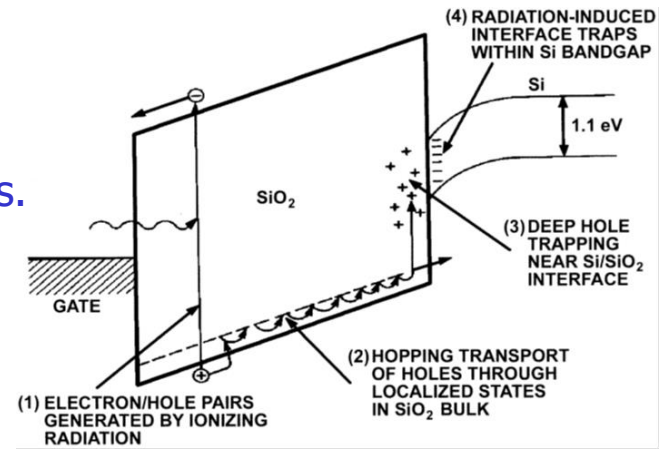
Radiation damage effects



Radiation damage effects (2)

✓ Ionization -> SURFACE damage

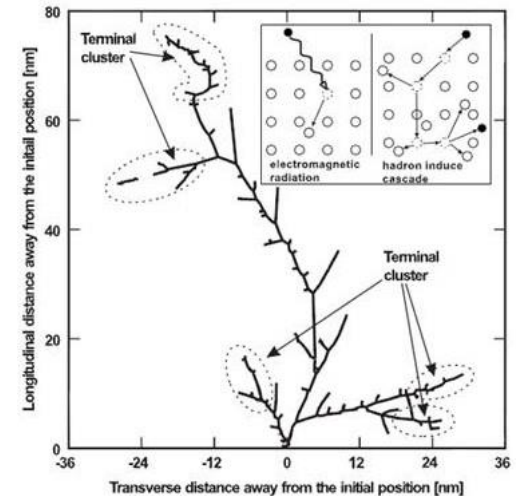
- build-up of trapped charge in the oxide;
- increase in the number of bulk oxide traps.
- increase in the number of interface traps;
- Q_{OX} , N_{IT}



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

✓ Atomic Displacement -> BULK damage

- silicon lattice defect generations;
- point and cluster defects;
- increase of deep-level trap states;
- N_T



Traps characteristics

- ✓ Traps provide allowed energy states within the band-gap, affecting the device behavior to many respects, e.g. by altering the effective doping, by enhancing recombination, by increasing leakage...
- ✓ Several models, e.g. Shockley–Read–Hall recombination, depend on traps implicitly

$$R_{net}^{SRH} = \frac{np - n_{i,eff}^2}{\tau_p(n + n_1) + \tau_n(p + p_1)}$$

$$p_1 = n_{i,eff} e^{\left(\frac{-E_{trap}}{kT}\right)}$$

$$n_1 = n_{i,eff} e^{\left(\frac{E_{trap}}{kT}\right)}$$

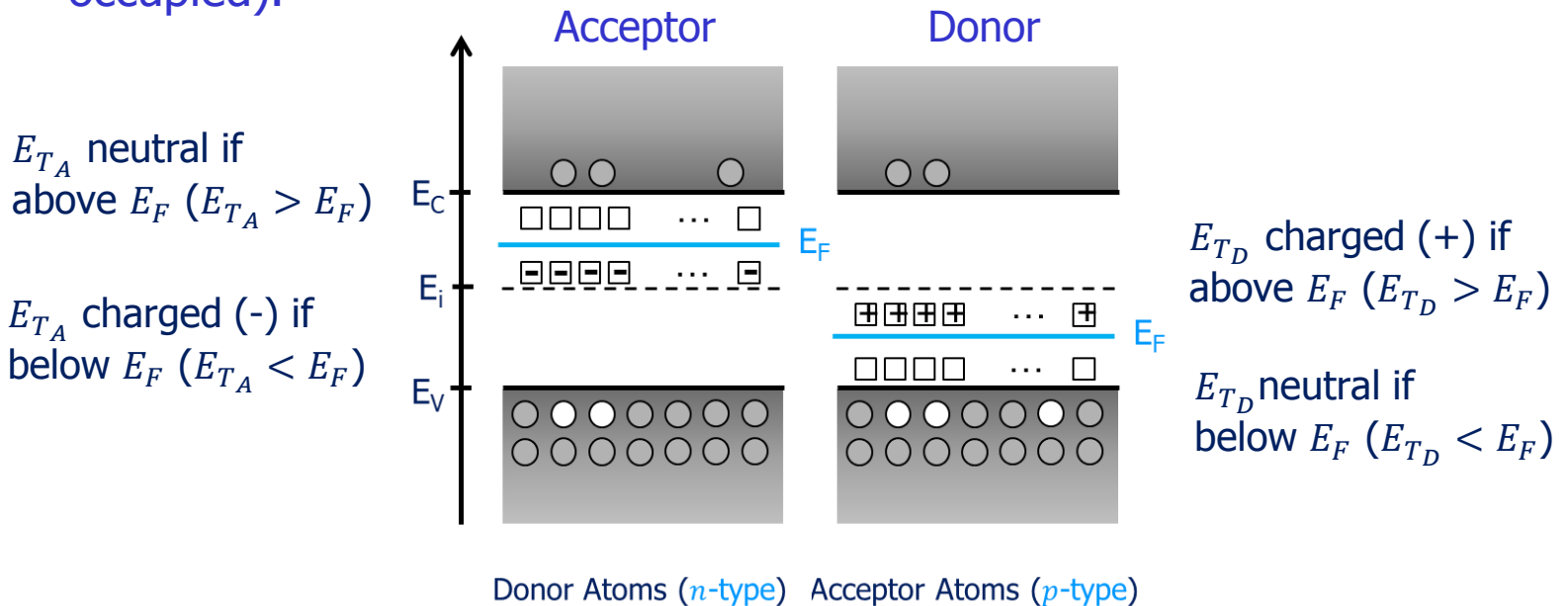
- ✓ Traps can be specified in terms of:

- ✓ **Type** (Acceptor, Donor)
- ✓ **Energy Distribution** (Level, Gaussian, Uniform, ...)
- ✓ Capture cross-sections (electrons, holes)
- ✓ Concentration / Spatial distributions

$$\tau_{n,p} = \tau_{dop} \frac{f(T)}{1 + g_{n,p}(F)}$$

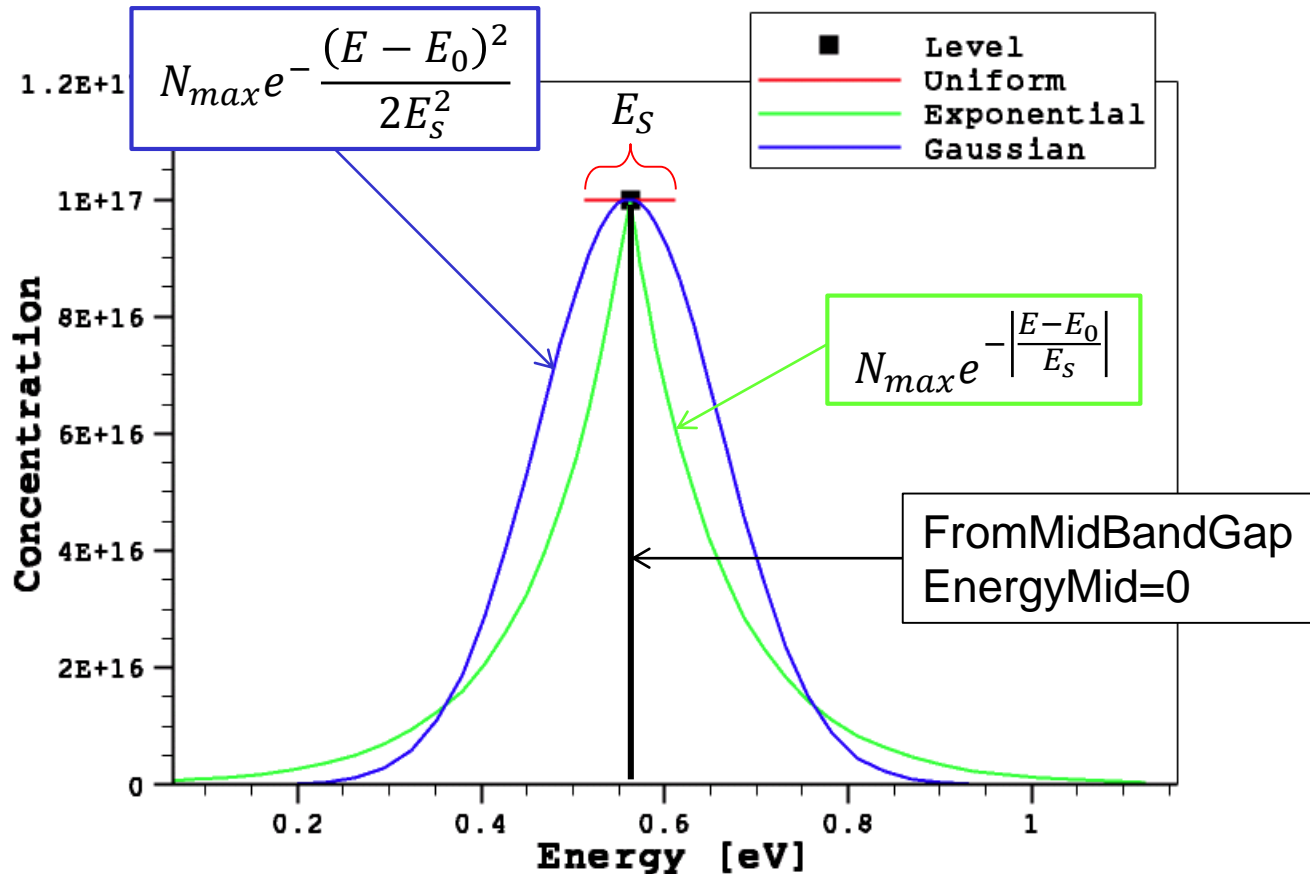
Traps type

- ✓ **Acceptor** traps are uncharged when unoccupied (empty) / negatively charged when occupied (they carry the charge of one electron when fully occupied).
- ✓ **Donor** traps are uncharged when unoccupied (empty) / positively charged when occupied (they carry the charge of one hole when fully occupied).



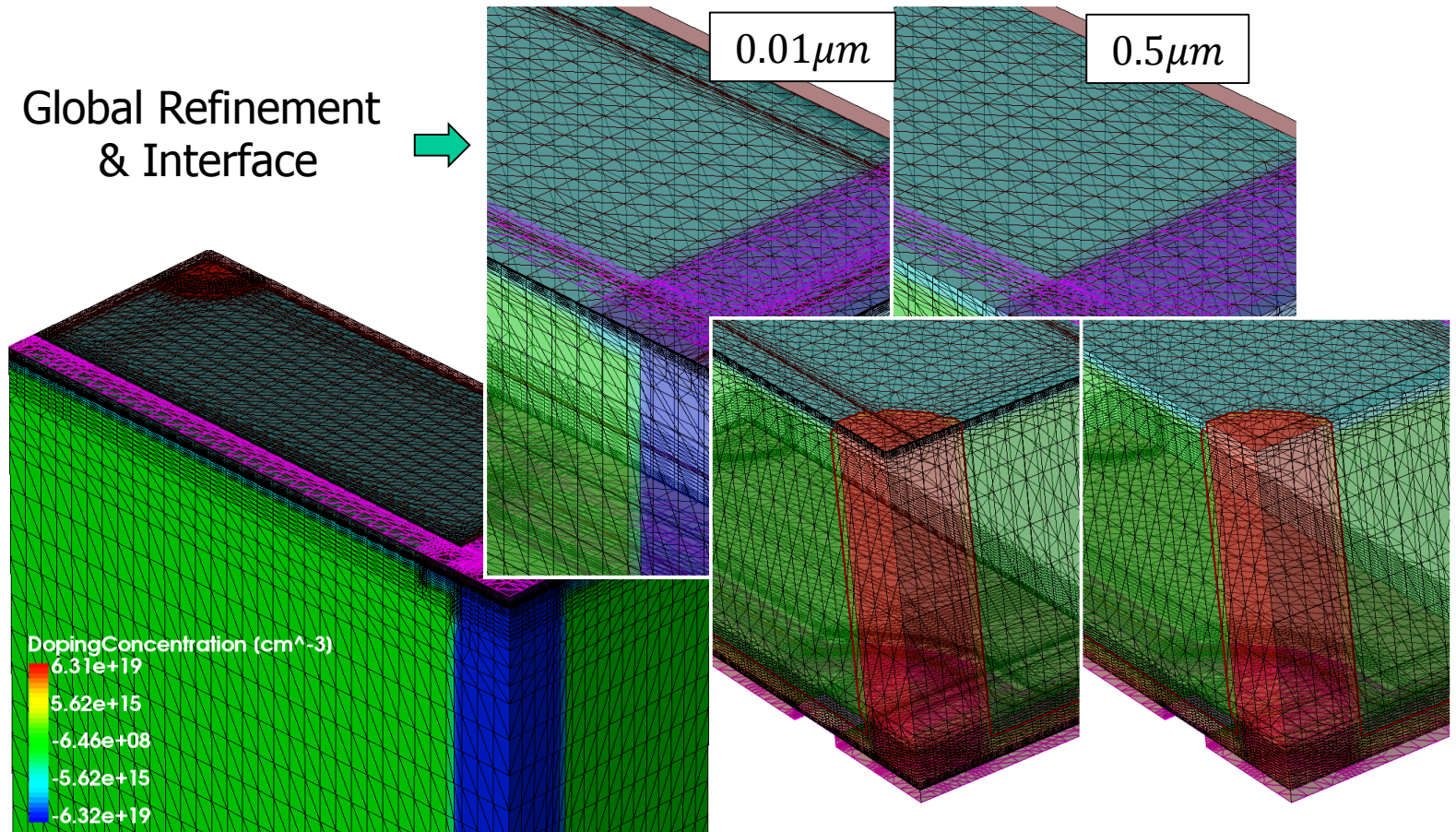
Traps energy distribution

✓ Traps energetic parametrization.



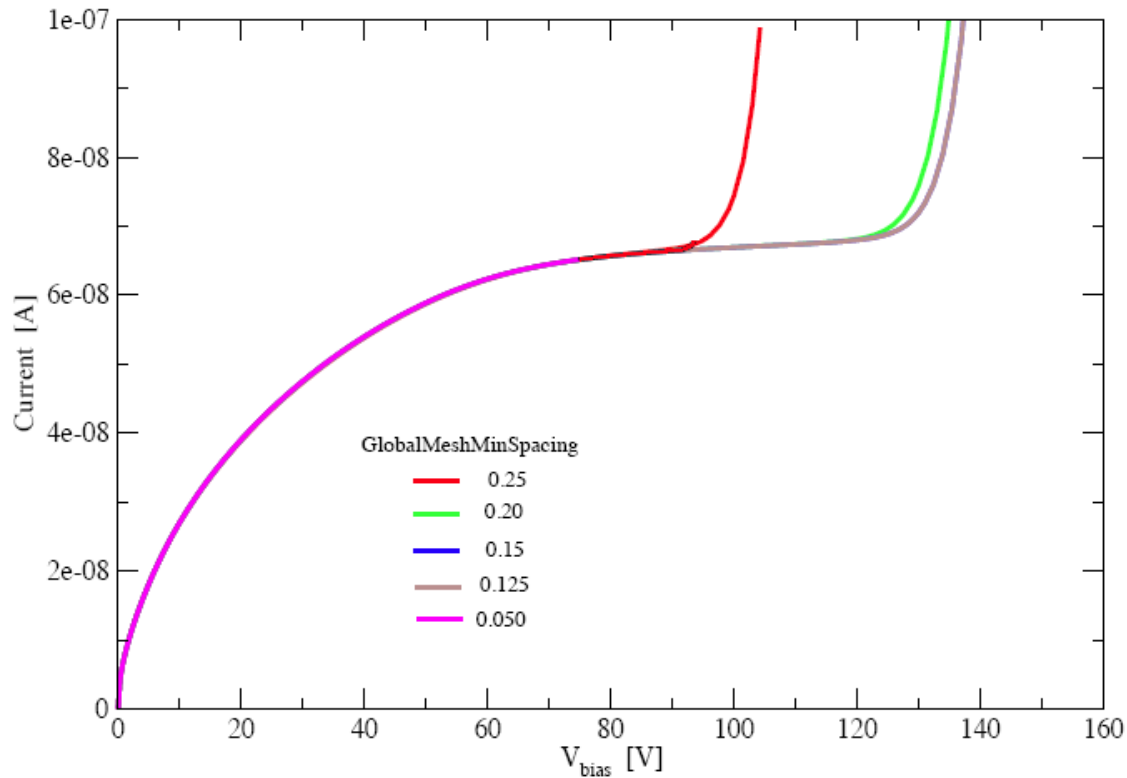
The space discretization issue

✓ Mesh (grid) definition is crucial for simulation accuracy.



The space discretization issue (2)

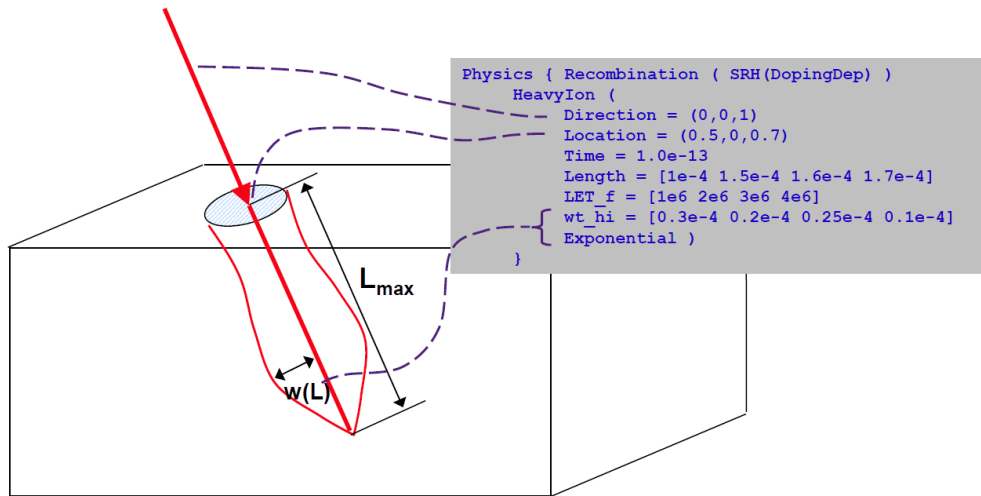
- ✓ Mesh (grid) definition is a crucial for simulation accuracy / simulation convergence.



G. Giugliarelli et al., "TCAD simulations of breakdown voltage and isolation properties of 3D sensors", 12th "Trento" Workshop on Advanced Silicon Radiation Detectors.

The time discretization issue

MIP DISCRETIZATION



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

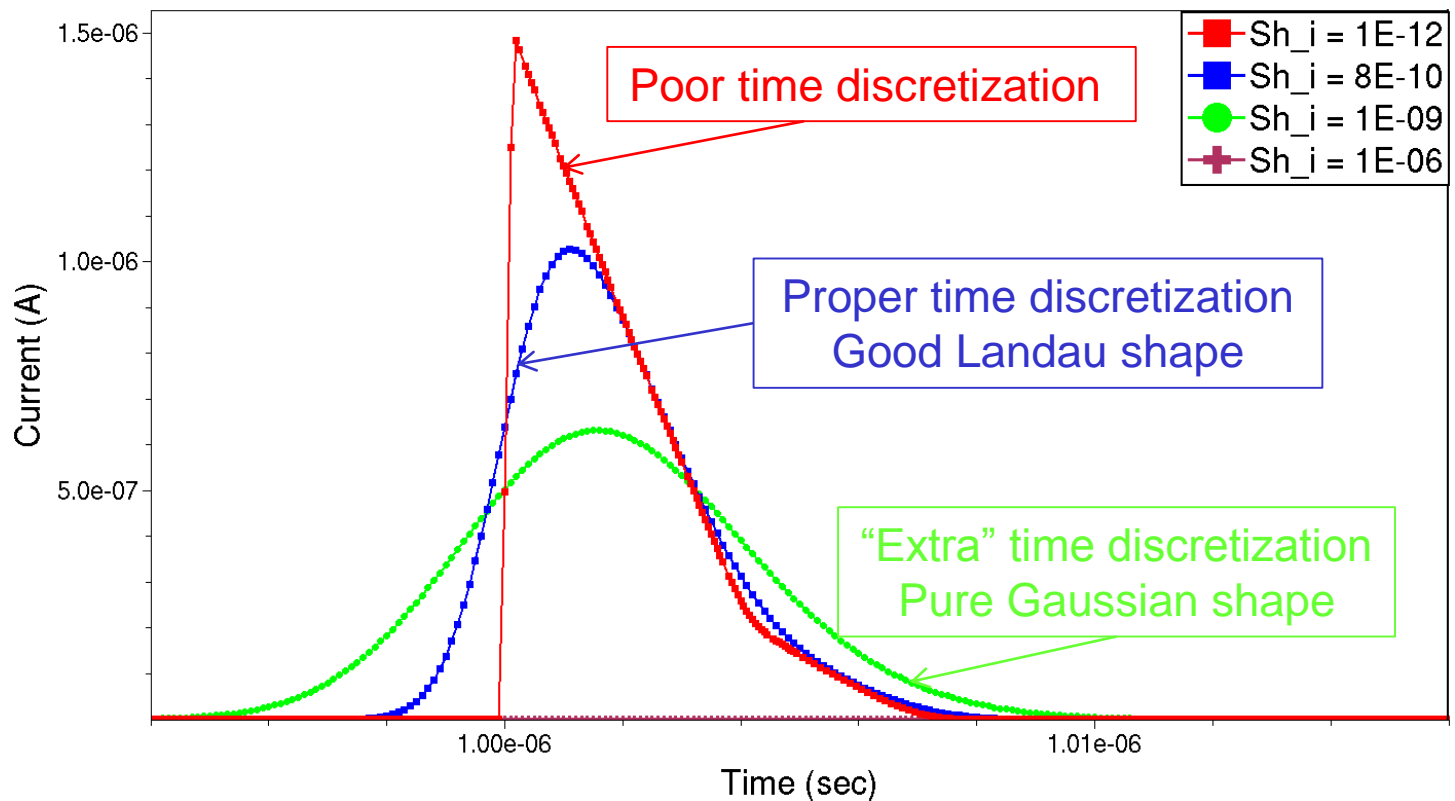
$$R(w, l) = \exp\left(-\frac{w}{w_t(l)}\right)$$

$$T(t) = \frac{2 \cdot \exp\left(-\left(\frac{t-t_0}{\sqrt{2} \cdot s_{\text{hi}}}\right)^2\right)}{\sqrt{2} \cdot s_{\text{hi}} \sqrt{\pi} \left(1 + \operatorname{erf}\left(\frac{t_0}{\sqrt{2} \cdot s_{\text{hi}}}\right)\right)}$$

The time discretization issue (2)

✓ Time discretization of the charge generation...

✓ Numerical issues in charge generation -> charge collection evaluation.

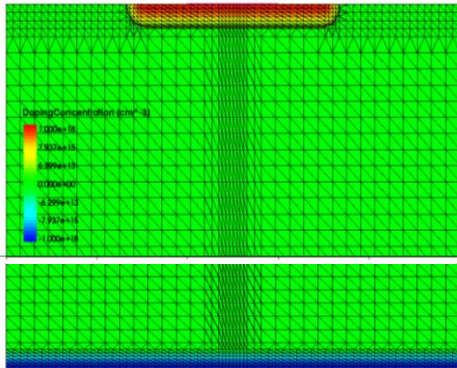


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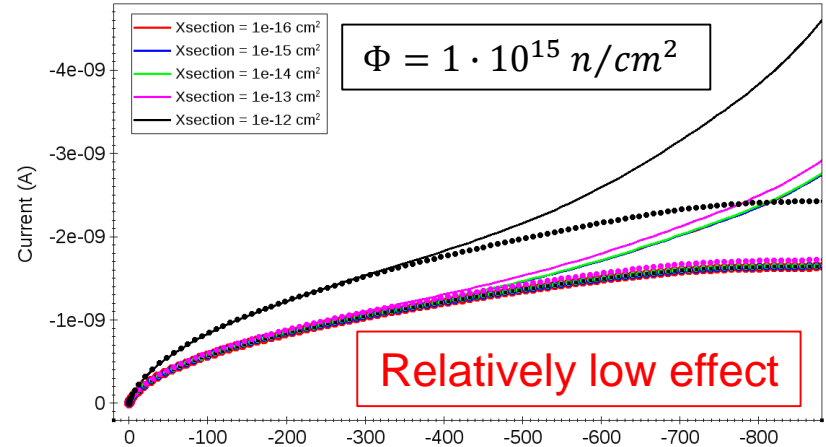
Diode simulation: leakage current

- ✓ Effect of the capture cross-sections variation combined with impact ionization (simplified n-on-p single strip structure).

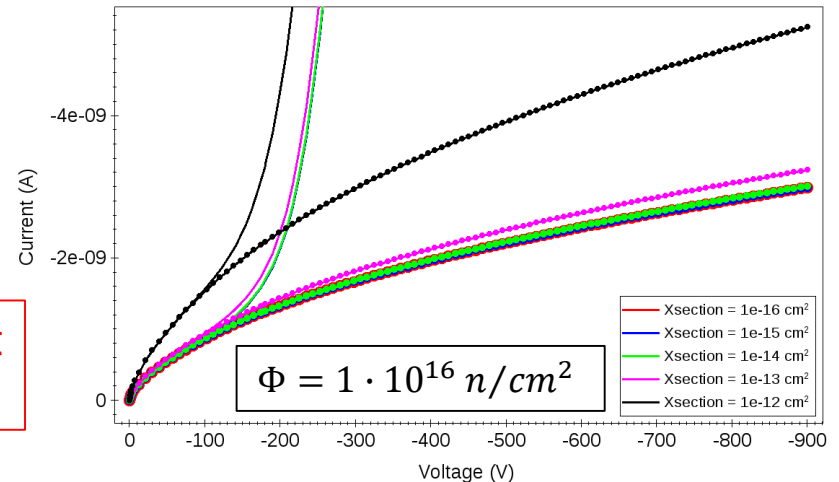


Significant effect of the impact ionization at high fluences

Avalanche ON (line), Avalanche OFF (marker)

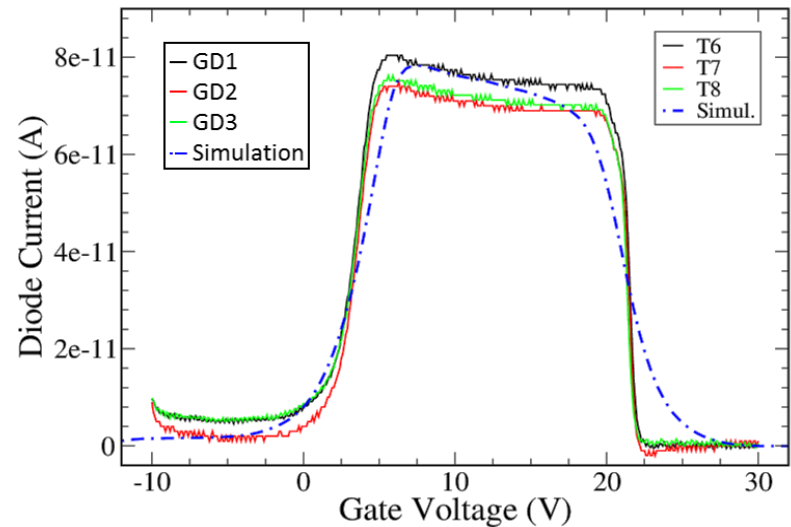
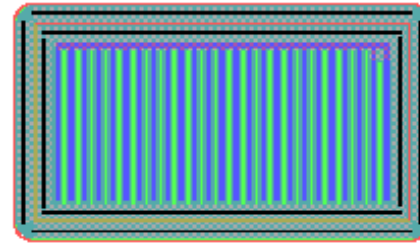
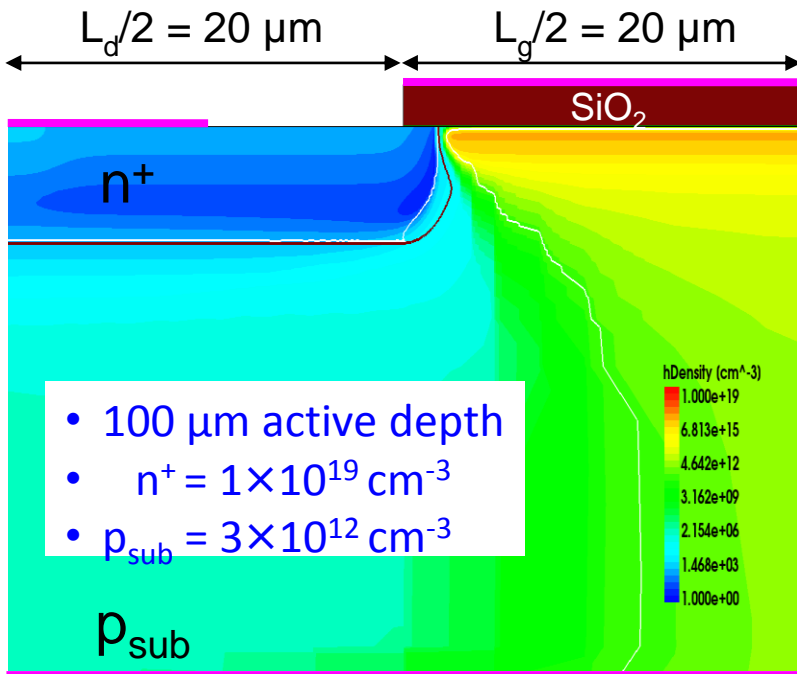


Avalanche ON (line), Avalanche OFF (marker)



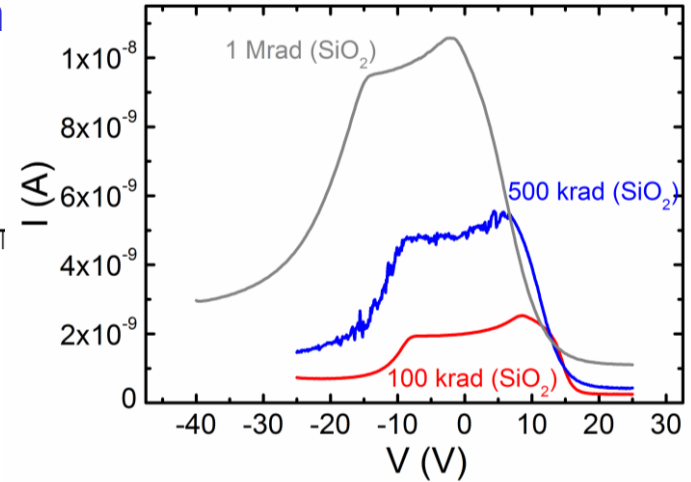
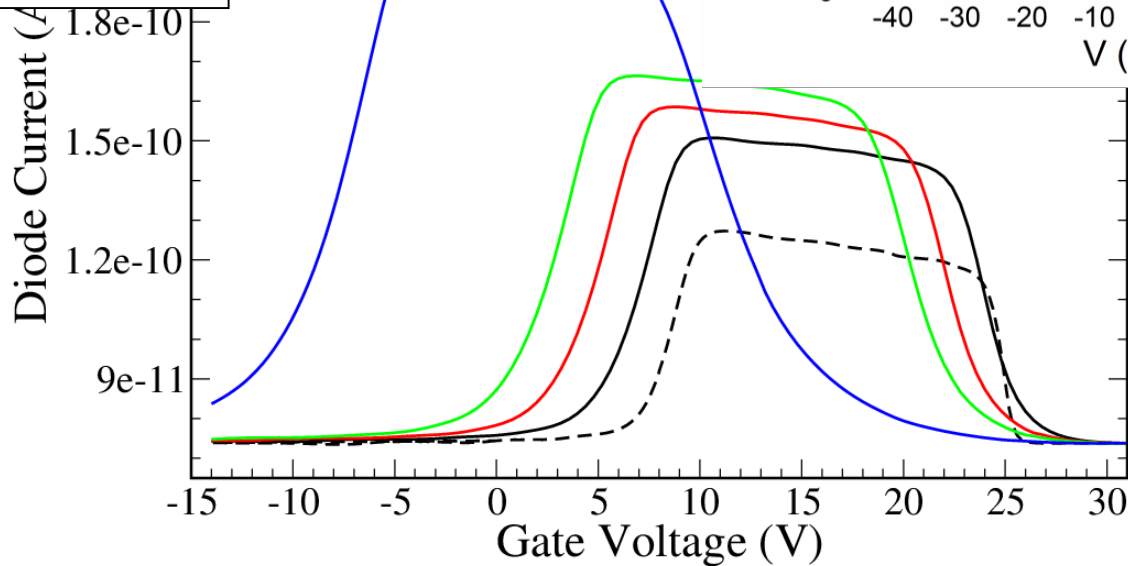
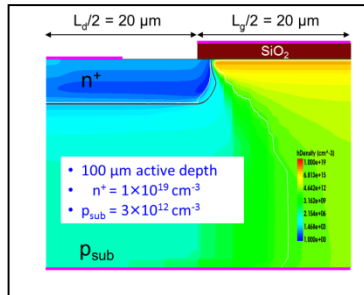
Gate Controlled Diode

✓ Non-irradiated structures.



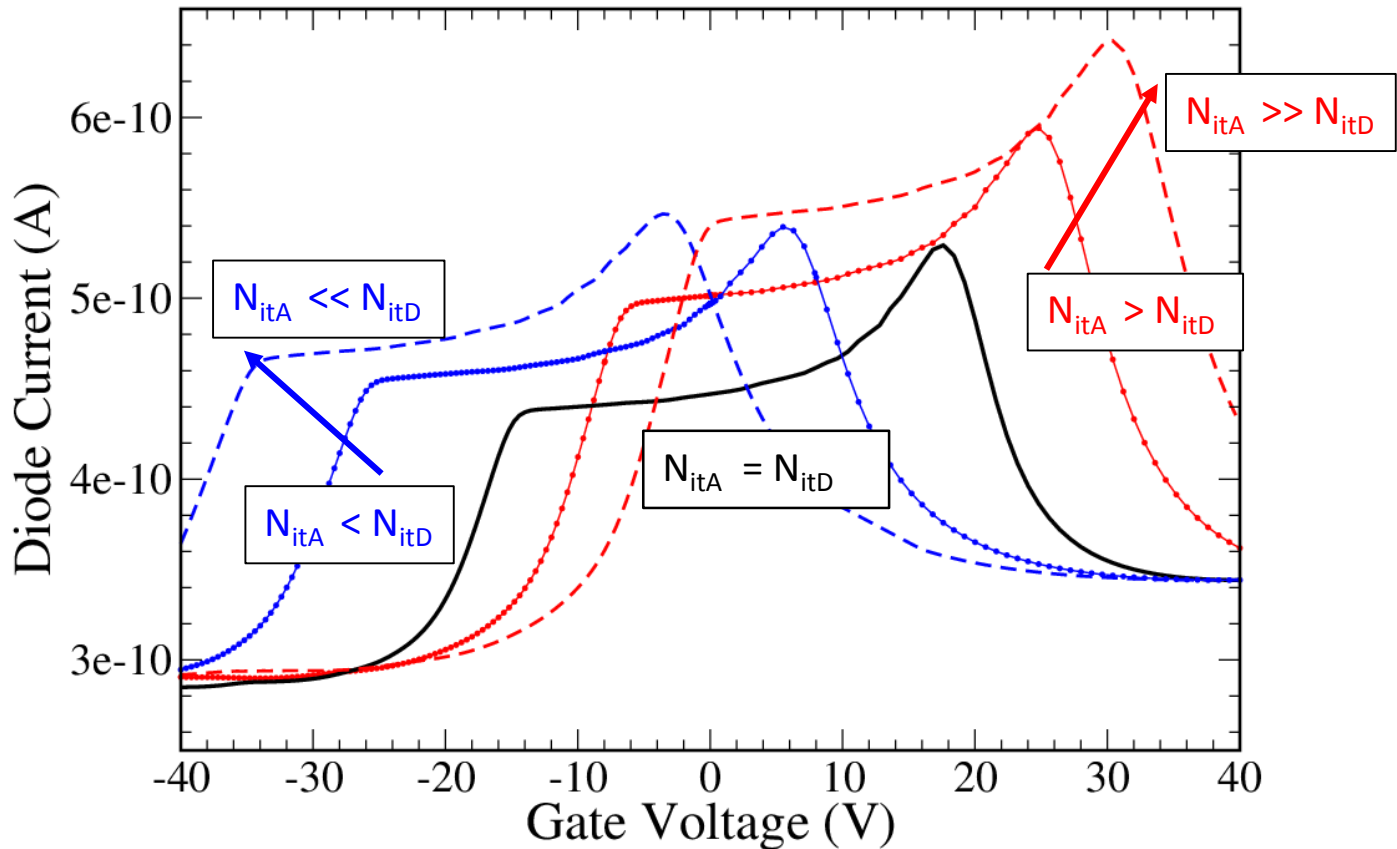
Sensitivity analysis: $Q_{OX} + N_{IT}$

- ✓ Combined effect of fixed charge (Q_{OX}) a states/trapped charge (N_{IT}) increase.



Effect of Interface Trap type

✓ N_{ITA} acceptor type traps, N_{ITD} donor type traps.



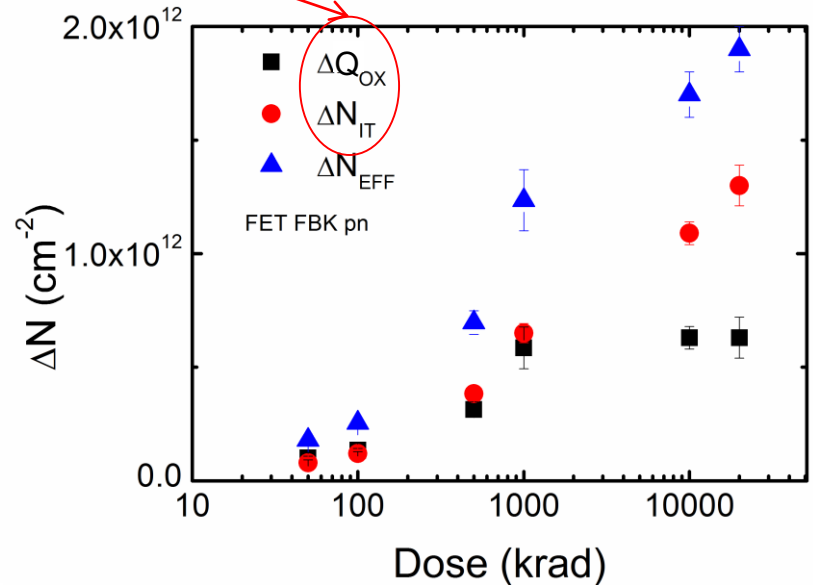
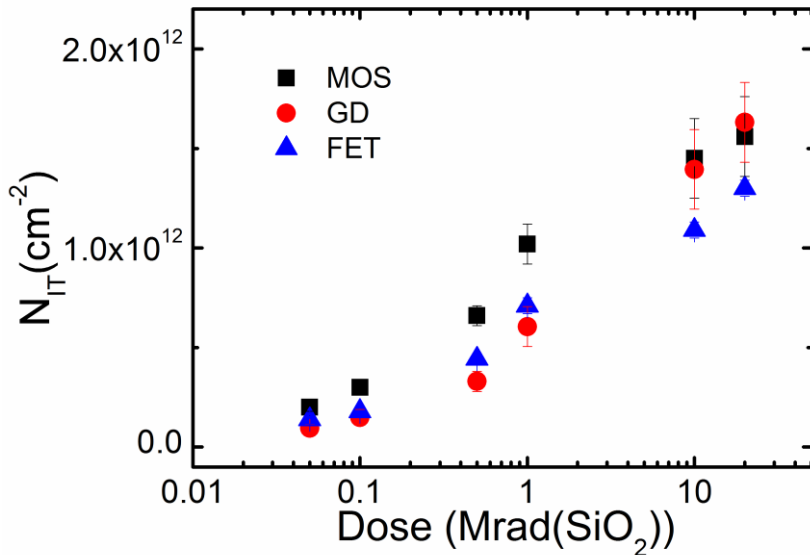
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MOS Capacitor measurements

- ✓ Q_{OX} and N_{IT} evaluation (from $C_{HF} - C_{QS}$ measurements).
- ✓ N_{IT} evaluation from **p-type** substrate (MOS C, GD) and **pMOSFET**.

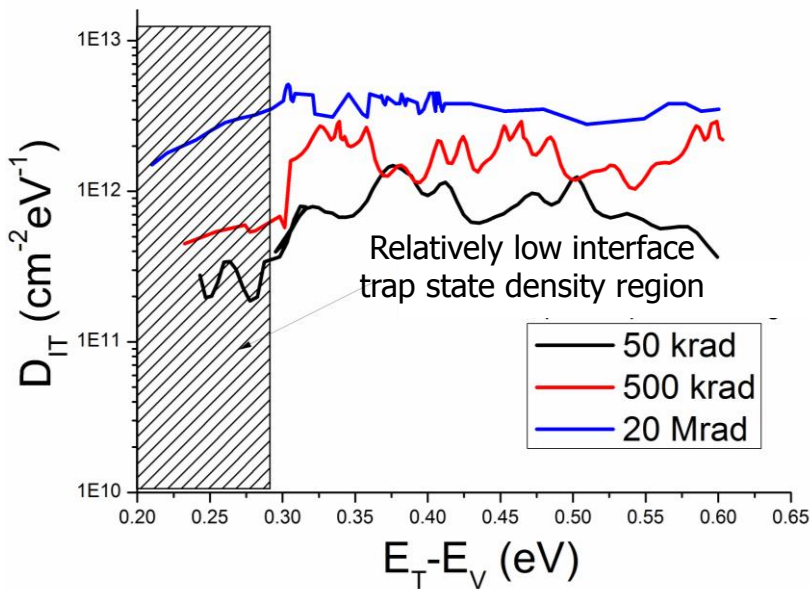
Following the method proposed in P. J. McWhorter and P. S. Winokur in Applied Physics Letters 48, 133 (1986), it is possible to separate the two contributions of Q_{OX} and N_{IT} .



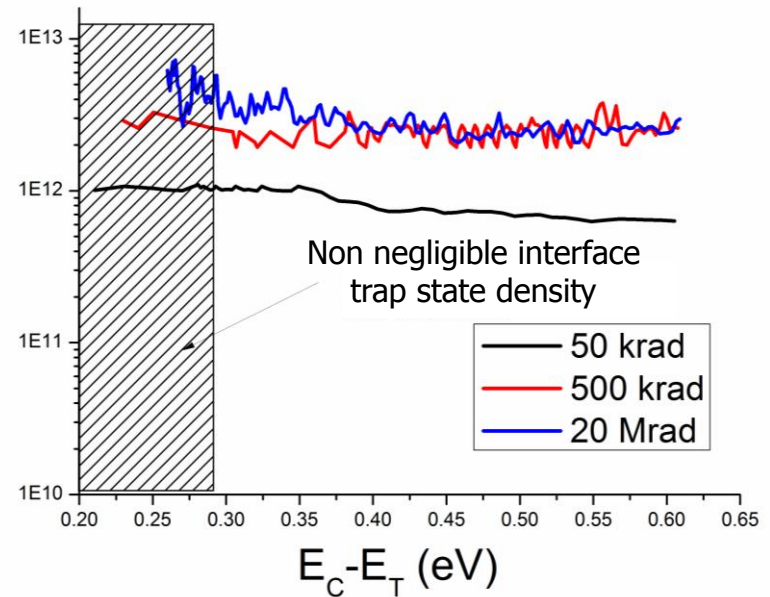
Interface Trap density measurements

✓ N_{IT}/D_{IT} evaluation (from $C_{HF} - C_{QS}$ measurements).

Donor interface trap states
from p -type substrates

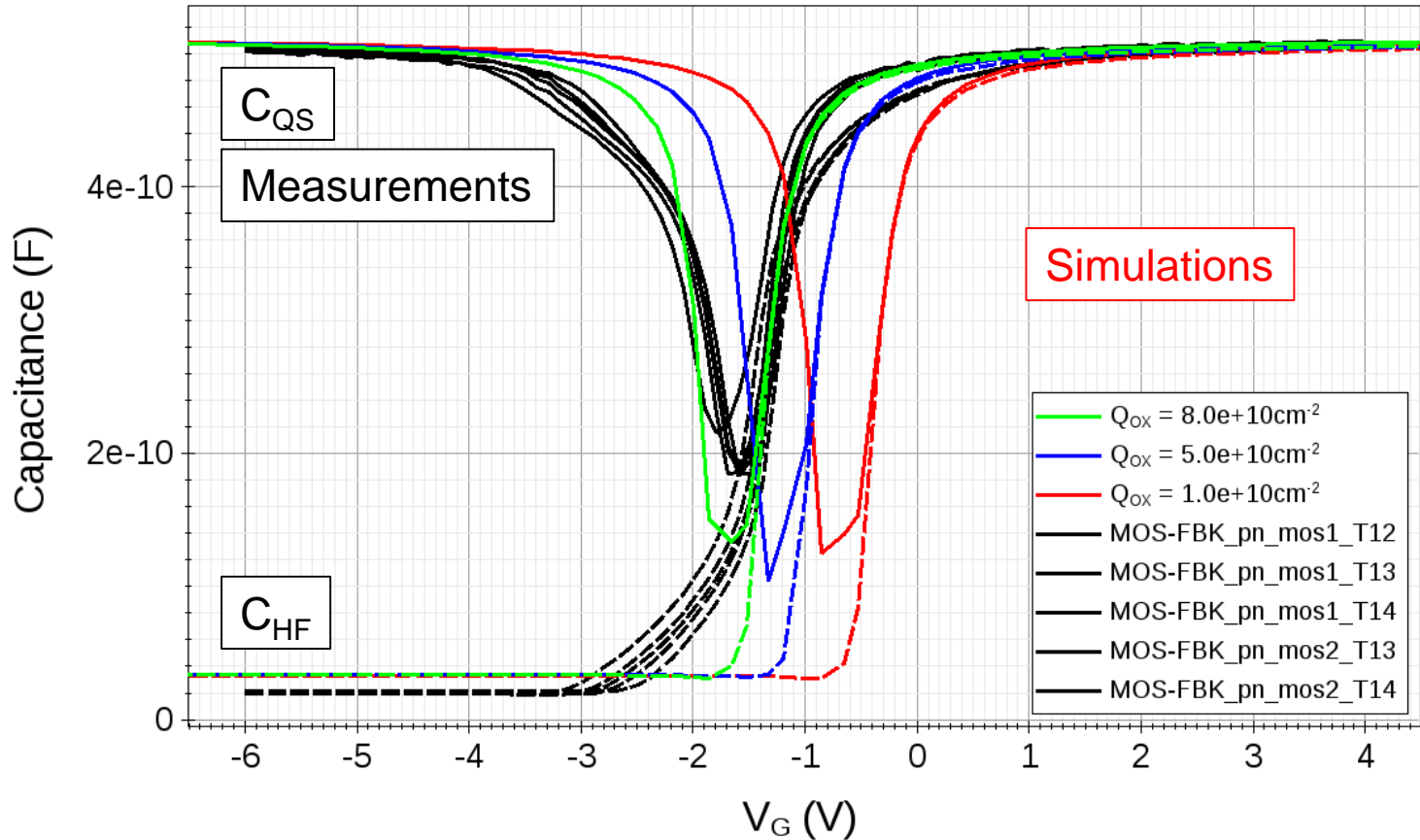


Acceptor interface trap states
from n -type substrates



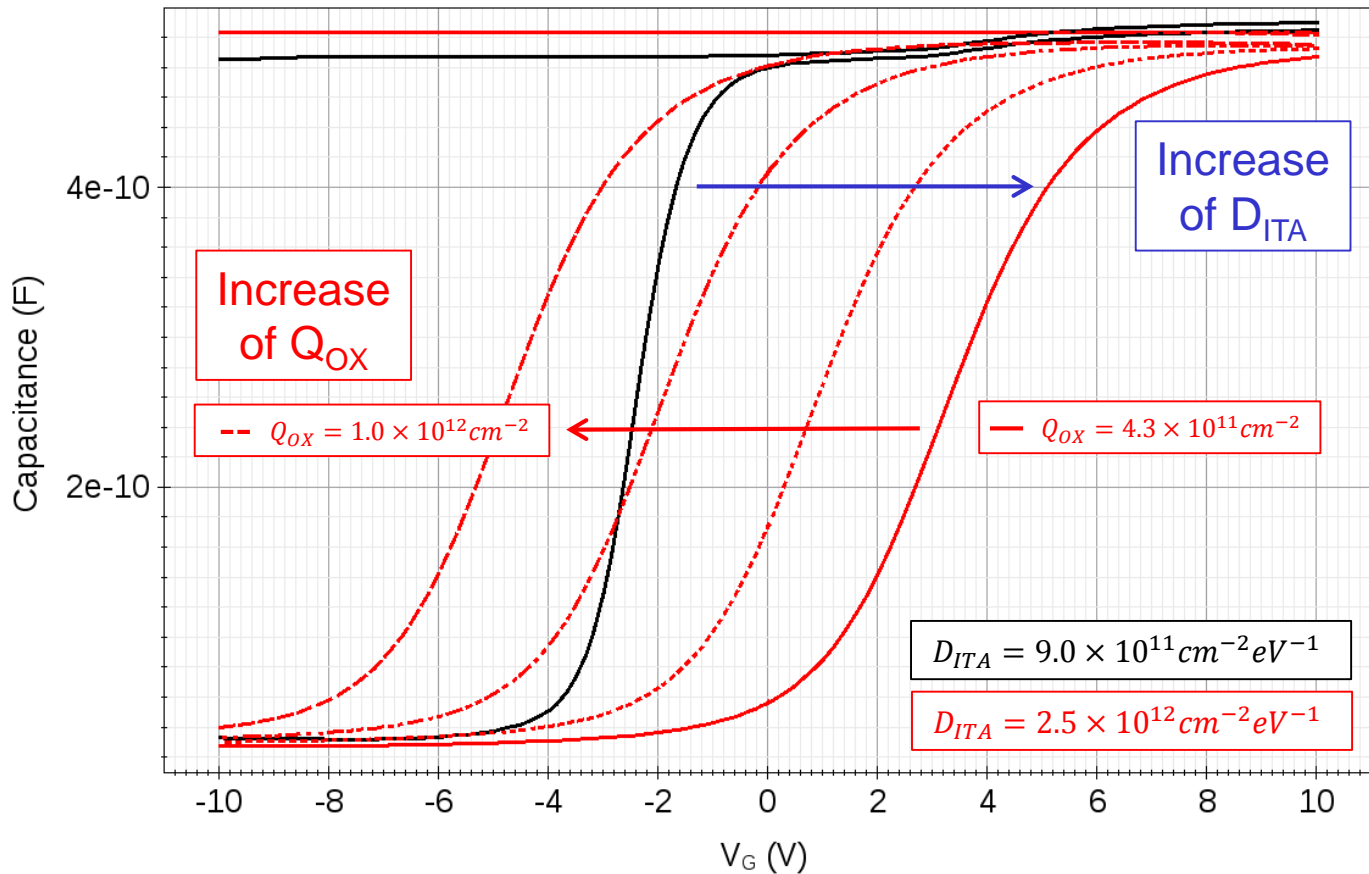
MOS Capacitor simulations

✓ Non-Irradiated structures.



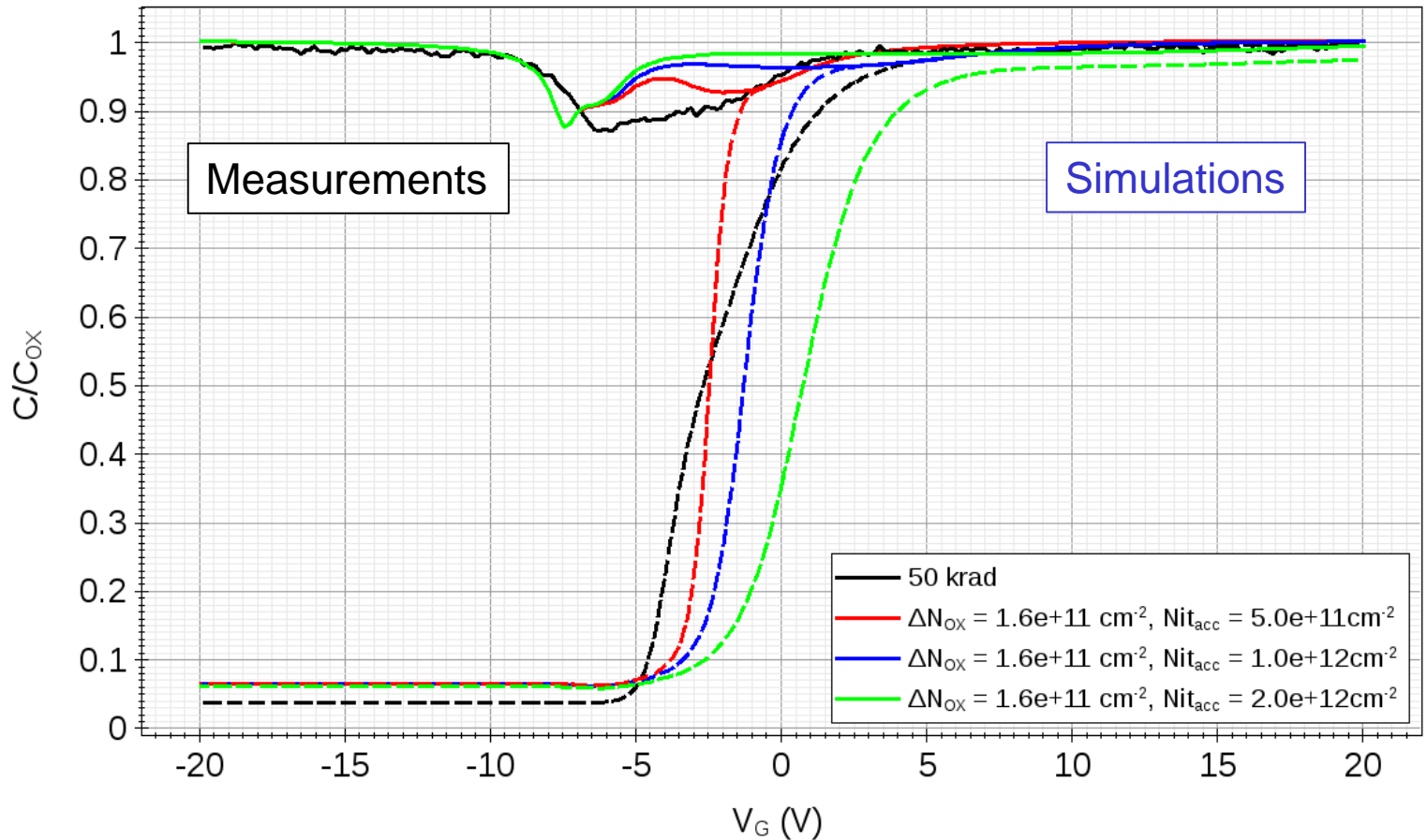
MOS Capacitor simulations

✓ Sensitivity analysis: effect of Q_{OX} and D_{IT} .



MOS Capacitor simulations

✓ Irradiated structures.

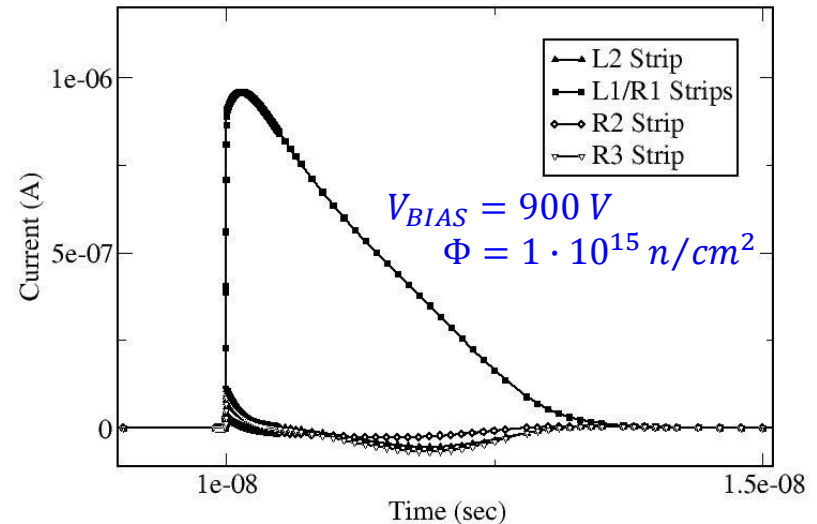
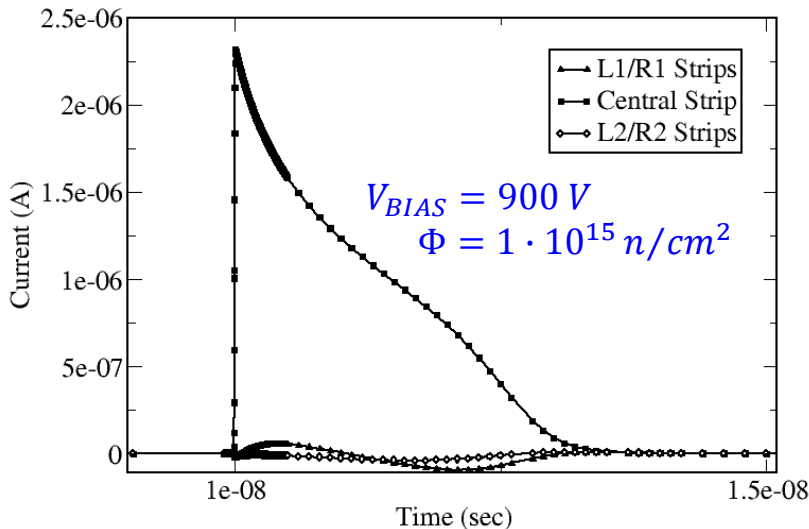
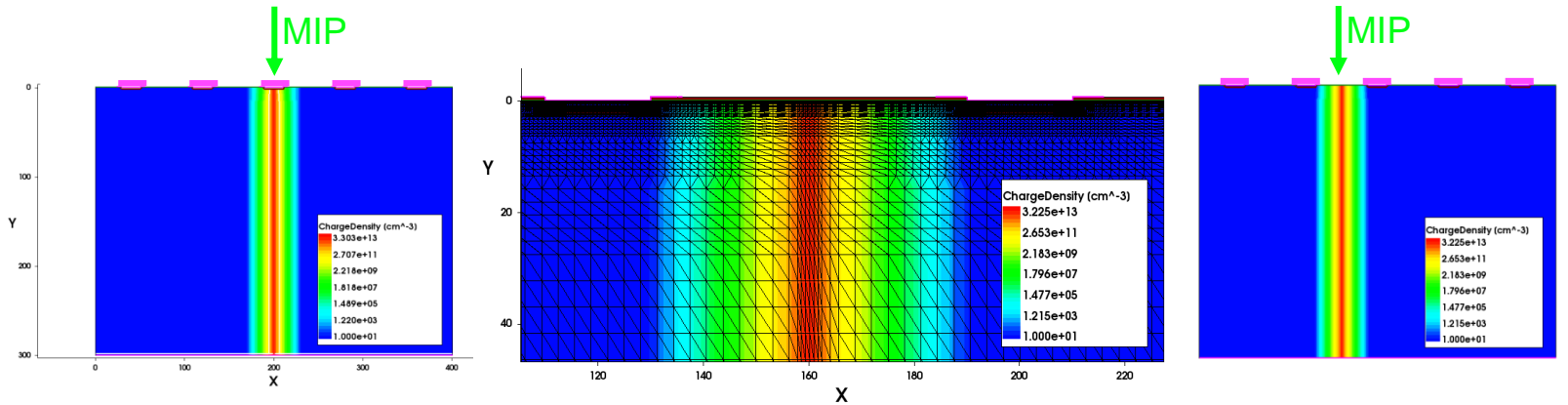


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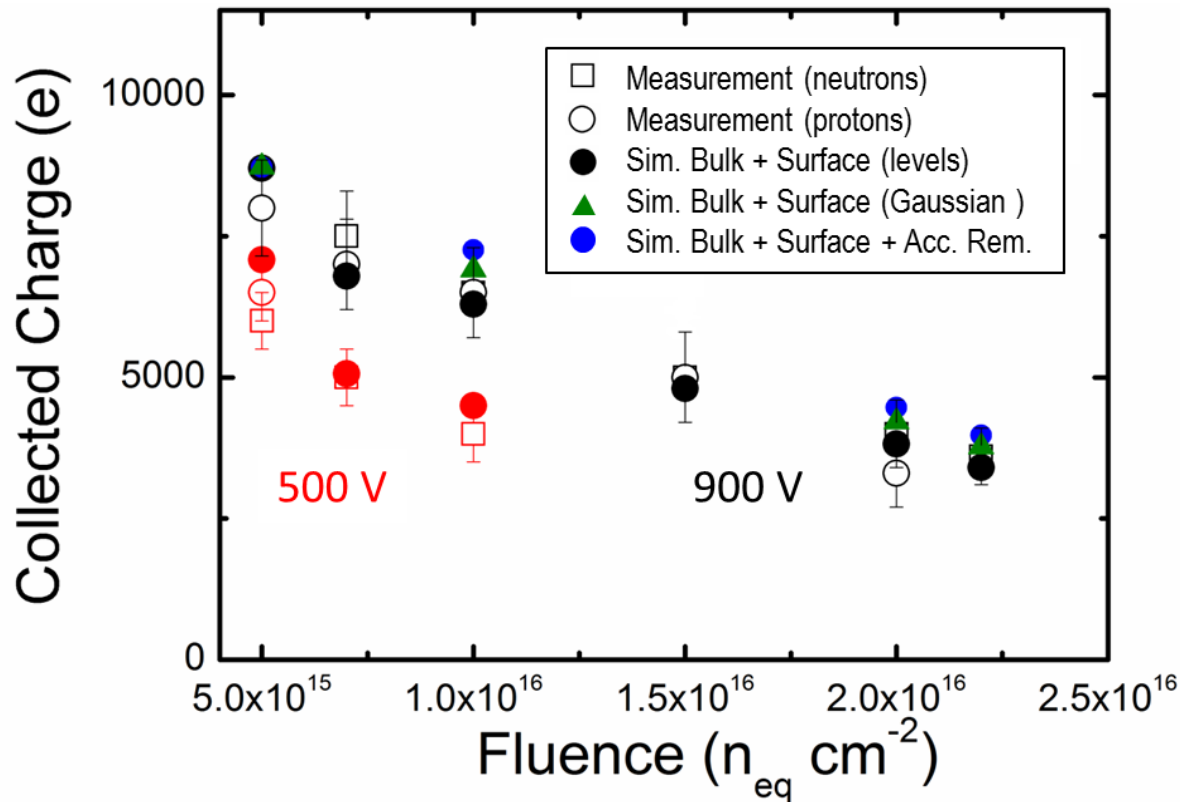
MultiStrips simulation: MIP response

✓ Current responses to different impact locations.



Transient analysis: Charge Collection

- ✓ Charge collection: simulations vs. measurements at different biasing voltages (T = 248 K)



Measurements from Affolder et al., "Collected charge of planar silicon detectors ..." NIM A, Vol. 623 (2010), pp. 177-179.

Outline

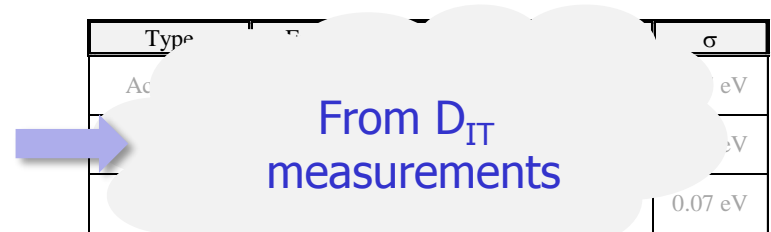
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The model

✓ Surface damage (+ Q_{OX})

F. Moscatelli; D. Passeri; A. Morozzi; S. Mattiazzo; G. -F. Dalla Betta; M. Dragicevic; G. M. Bilei, *Effects of Interface Donor Trap States on Isolation Properties of Detectors Operating at High-Luminosity LHC*, IEEE Transactions on Nuclear Science, 2017, Vol. 64, Issue: 8, 2259 - 2267

Type	Energy	Concentration	σ
Acceptor	$E_C - 0.4$ eV	40% of acceptor N_{IT} ($N_{IT} = 0.85 \cdot N_{OX}$)	0.07 eV
Acceptor	$E_C - 0.6$ eV	60% of acceptor N_{IT} ($N_{IT} = 0.85 \cdot N_{OX}$)	0.07 eV
Donor	$E_V + 0.7$ eV	100% of donor N_{IT} ($N_{IT} = 0.85 \cdot N_{OX}$)	0.07 eV



✓ Bulk damage

Type	E (eV)	σ_e (cm ²)	σ_h (cm ²)	η (cm ⁻¹)
Acceptor	$E_C - 0.42$	1.0×10^{-15}	1.0×10^{-14}	1.6
Acceptor	$E_C - 0.46$	7.0×10^{-15}	7.0×10^{-14}	0.9
Donor	$E_V + 0.36$	3.2×10^{-13}	3.2×10^{-14}	0.9

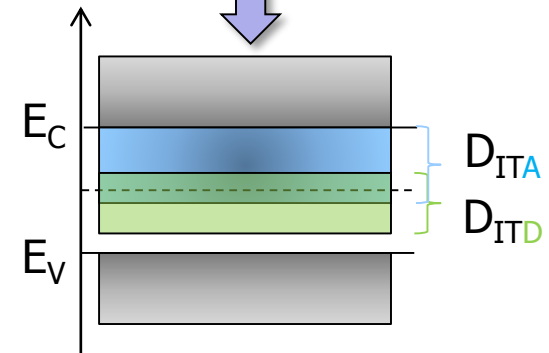
(up to 7.0×10^{15} n/cm²)

Type	E (eV)	σ_e (cm ²)	σ_h (cm ²)	η (cm ⁻¹)
Acceptor	$E_C - 0.42$	1.0×10^{-15}	1.0×10^{-14}	1.6
Acceptor	$E_C - 0.46$	3.0×10^{-15}	3.0×10^{-14}	0.9
Donor	$E_V + 0.36$	3.2×10^{-13}	3.2×10^{-14}	0.9

($7.0 \times 10^{15} \div 1.5 \times 10^{16}$ n/cm²)

Type	E (eV)	σ_e (cm ²)	σ_h (cm ²)	η (cm ⁻¹)
Acceptor	$E_C - 0.42$	1.0×10^{-15}	1.0×10^{-14}	1.6
Acceptor	$E_C - 0.46$	1.5×10^{-15}	1.5×10^{-14}	0.9
Donor	$E_V + 0.36$	3.2×10^{-13}	3.2×10^{-14}	0.9

($1.6 \times 10^{16} \div 2.2 \times 10^{16}$ n/cm²)



Conclusions

- ✓ Modelling radiation damage effects is a hard task!
- ✓ Radiation damage modelling scheme (bulk + surface), suitable for commercial TCAD tools (e.g. Synopsys Sentaurus).
- ✓ Predictive capabilities extended to HL-LHC radiation damage levels (e.g. fluences $> 2.0 \times 10^{16} \text{ cm}^{-2}$ 1 MeV neutrons).
- ✓ Further validation with experimental data comparisons -> model refinement.
- ✓ Application to the optimization of (pixel) detectors (3D detectors, 2D planar detectors, ...).