

Use of Silvaco

in HEP experiments

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versité

Outline

- Silvaco TCAD tool
- Example: edgeless detectors
- Radiation damage models
- From TCAD to Monte Carlo simulations
- 1D vs 2D vs 3D vs 4D simulations
- Conclusion & Outlook

SILVACO TCAD TOOL

TCAD simulations

- Technology Computer Aided Design TCAD
- Solve drift/diffusion & Poisson equations for electrons and holes:

$$J_n = qn\mu_n E + qD_n \frac{\partial n}{\partial x} \frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} + G_n - R_n$$
$$J_p = qn\mu_p E - qD_p \frac{\partial p}{\partial x} \frac{\partial p}{\partial t} = -\frac{1}{q} \frac{\partial J_p}{\partial x} + G_p - R_p$$
$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{q}{\epsilon_{Si}\epsilon_0} (N_D + p(x) - n(x) - N_A)$$



SILVACO

- taking into account boundary conditions
 - Electrodes' potentials, interface charges, etc
- on a grid of points

Normal work flow for a HEP silicon sensors



TCAD simulation work flow



So why bother with simulations?

• You repeat all the "steps" of real sensors...

So why bother with simulations?

- You repeat all the "steps" of real sensors...
- It is not true!

Possible work flow for real sensors



TCAD simulation work flow



TCAD simulation work flow



Simulations benefits

- Simulating sensors helps in saving:
- Development time
- Number of submissions
- Money
- You can learn a lot in terms of:
- Physics
 - Study quantities otherwise not accessible!
 - Examples:
 - Carrier distribution
 - Electric field distribution
 - Current densities
 - Etc....

EXAMPLE: EDGELESS DETECTORS

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Edgeless pixel detector



Simulation drive sensor design - Focus on breakdown (BD) voltage

DATA

SIMULATIONS



BD Voltage: Agreement within 20% or better

Hit efficiency at sensor edge JINST 12 P05006 (2017)



Pixel detector efficient beyond pixels area: > 80% up to 75 μ m away from the last one Reason: electric field lines closing on pixels and not on GRs!

New edgeless production – staggered trenches



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Hit efficiency at sensor edge A. Ducourthial thesis https://indico.in2p3.fr/e/18186/



130 μm thick sensor with staggered trenches, no GRs, ~50 μm last pixel to last edge

The efficiency follows the edge pattern

The efficiency is higher than 50% up to 44 μ m from the last pixel

Simulations in 3D



Electric field at sensor edge



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Hit efficiency at sensor edge - projections

TCAD Simulations - Electric field

Simulation of the electric field for several depth z in the sensor:

- E drops at 0 when at edge position
- low E in the bottom corner close to the edge.





Edge Efficiency



Efficiency drop matches the Electric field drop in the vicinity of the edge

RADIATION DAMAGE MODELS

Radiation damage in silicon bulk



Radiation damage in silicon: microscopic level



Impact on detector properties can be calculated if all defect parameters are known: $\sigma_{n,p}$: cross sections ΔE : ionization energy N_t : concentration

TCAD – Radiation damage models

- Device simulation of irradiated sensors
 - Using: Custom made simulation software and Silvaco & Synopsis TCAD tools
 - Good progress in reproducing results on leakage current, space charge, E-Field, trapping
 - Enormous parameter space ranging from semiconductor physics parameters and models over device parameters towards defect parameters → Tools ready but need for proper input parameters!
 - ...simulations are getting predictive power.
- Working with "effective levels" for simulation of irradiated devices
 - Most often 2, 3 or 4 "effective levels" used to simulate detector behavior
 - Introduction rates and cross sections of defects tuned to match experimental data



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Radiation damage models: history

- Modelling all known defects in silicon in TCAD is (still) computationally prohibitive
 - Plus: how to model defects clusters?
- Hence only a certain number of "effective states" are modelled
- a. 1 acceptor-like state (q=-/0)
 - e.g. D. Passeri et al., IEEE TNS 45 (1998) 602-608
- b. 2 states, 1 acceptor- and 1 donor-like (q=+/0)
 - e.g. V. Eremin et al., NIM A476 (2002) 556-564, aka EVL
- c. 3 states, adding 1 acceptor wrt b., very close to mid-gap, to better control type inversion and leakage current increase rate
 - e.g. M. Petasecca et al., IEEE TNS 53 (2006) 2971-2976
- d. 4 states, adding 1 acceptor more (rather unique example)
 - e.g. F. Moscatelli et al., NIM B186 (2002) 171

Radiation damage models for HL-LHC

- "Perugia" model: IEEE TNS 64 (2017) 2259-2267
 - Two acceptors and one donor
 - Interface damage modelled too (2 acc. and 1 don. again)
 - Valid up to $2.2 \times 10^{16} n_{eq}/cm^2$
- "3D" model: Pennicard et al., NIM A592 (2008) 16-25
 - Two acceptors and one donor as in Perugia model but larger cross sections wrt Petasecca et al. 2006
 - Used recently in M. Baselga et al. "Simulations of 3D-Si sensors for the innermost layer of the ATLAS pixel upgrade" NIM A847 (2017) 67-76
 - Valid up to $1 \times 10^{16} n_{eq}/cm^2$
- "LHCb model": NIM A874 (2017) 94-102
 - Two acceptors and one donor
 - One acceptor and one donor as in EVL plus one acceptor close to the valence band

- Valid up to $8 \times 10^{15} n_{eq}/cm^2$

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Result of tuning: Hamburg Penta Trap Model (HPTM)

Defect	Туре	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	Newl
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	

ΗΡΤΜ

- Trap concentration of defects: $N = g_{int} \cdot \Phi_{neq}$
- Simulations for the optimization have been performed at T= -20 °C with:
 - 1. Slotboom band gap narrowing
 - 2.Impact ionisation (van Overstaeten-de Man)
 - 3. TAT Hurkx with tunnel mass = $0.25 m_e$ (default value: 0.5 m_e) in case of the I_p 4. Relative permittivity of silicon = 11.9 (default value : 11.9)
- Both cross section for the E30K and the electron cross section for the C_iO_i were fixed
 → 12 free parameter
- Optimization done with the nonlinear simplex method





Simulated E-field as function of position for different fluences at 1000V



E-field vs position

- Double peak structure for fluences $\geq 3 \cdot 10^{15} n_{eq}/cm^2$ clearly visible
- Peak field of $\approx 2 \cdot 10^5$ V/cm at the highest fluence \rightarrow impact ionisation



Compatibility across TCAD softwares

- Most used TCAD tools in HEP are:
 - Silvaco ATLAS
 - Synospys SENTAURUS
- And that the two do not agree on some fundamental aspects \bigcirc
 - AIDA 2020 WP7 meeting (Paris, 2/2016): https://indico.cern.ch/event/477003/contributions/1155199/attachments/1234150/1811069/bomben_comparison_160225.pdf
 - 28th RD50 WS (Torino, 6/2016): <u>https://agenda.infn.it/getFile.py/access?</u> <u>contribId=3&sessionId=1&resId=0&materialId=slides&confId=11109</u>
 - 31st RD50 WS (Geneva, 11/2017):

https://indico.cern.ch/event/663851/contributions/2788159/ attachments/1562199/2460062/bomben_silvaco_simulations.pdf

Cross-validation of radiation damage models is mandatory!

FROM TCAD TO MONTE CARLO SIMULATIONS

ATLAS Pixel Detector Digitizer

https://indico.cern.ch/event/666427/contributions/2881831/attachments/1603791/2543967/ TrentoWorkshop slides RadDamDig wl.pdf

Develop digitizer that model inside effects of radiation damage

"Chunks" of charges are drifted to the electrodes. Digitizer accounts for:

- Charges drift
- E/B Field effects
- Lorentz Angle (function of E/B fields and distance in the detector)
- Trapping probability
- Ramo potential to account for induced charge
- Charge conversion to ToT
- Pixel clustered



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Electric field - Chiochia model



Model prediction and data comparison

https://indico.cern.ch/event/666427/contributions/2881831/attachments/1603791/2543967/ TrentoWorkshop slides RadDamDig wl.pdf

Charge Collection Efficiency as a function of Luminosity for IBL with data from Run 2

Charge Collection Efficiency

- Simulation points error bars
 - x: 15 % on fluence-to-luminosity conversion
 - y: radiation damage parameter variations
- Data points error bars
 - x: ToT-charge calibration drift
 - y: 2% on luminosity



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Model prediction and data comparison

https://atlas.web.cern.ch/Atlas/GROUPS/PHYSICS/PLOTS/PIX-2017-004/



1D VS 2D VS 3D VS 4D SIMULATIONS

1D vs 2D simulations

1D simulations are OK for:

- Leakage current density
- Electrode to backside capacitance
- Charge collection efficiency
 - For pads
 - For strip detectors at low fluences

2D simulations are OK for:

- Interstrips capacitance
- Charge collection efficiency
 - For strip detectors
 - For pixels detectors at low fluences

2D vs 3D simulations

2D simulations are OK for: 3D simulations are perfect for:

- Interstrips capacitance
- Charge collection efficiency
 - For strip detectors
 - For pixels detectors at low fluences

- Interpixels capacitance
- Charge collection efficiency
 - For pixel detectors

Ramo Potential: 1D vs 2D



$3D 50x50 \ \mu m^2 \ structure$



Ramo Potential: 3D



Ramo potential: comparison



Charge Collection Efficiency: comparison



4D simulations?

- Time dependent simulations of segmented Low Gain Avalanche Diodes (LGADs)...
- Computational complexity might be prohibitive, though

CONCLUSIONS AND OUTLOOK

Conclusions

- TCAD is a very powerful tool for HEP silicon sensors
- You can reduce the number of submission, and so cutting time and money to get results
- Combining TCAD simulations, laboratory and testbeam data can probe fundamental quantities like electric field distribution, trapping, etc. and have radiation damage models based simulation making quantitative predictions
- A solid knowledge of semiconductor physics, and good data inputs are recommended to fully exploit TCAD simulations
- If you are interested in working with TCAD simulations, feel free to contact me: <u>marco.bomben@cern.ch</u>



Outlook

- To understand the performance of heavily irradiated segmented detectors the combination of:
- > TCT data and/or data from a grazing angle runs at testbeams
- Simulation of both bulk and surface damage is needed
- Validation of models across different TCAD softwares
- Larger and larger fluences demand for new parameterisation of fundamental silicon properties (*e.g.* mobilities)
- The new parameterisation can be added to TCAD simulation and quantitative predictions made
- Charge multiplication is exploited successfully in LGADs but the impact of radiation damage has to be understood
- A lot of simulation work is ongoing

https://indico.in2p3.fr/e/simdet2018



THANK YOU!

BACKUP MATERIAL



Protons with more "double junction", flatter field, less peaked at junction

TREDI, Paris, Feb 22, 2016 M. Bomben - SIMDET 2018 - LPNHE, Paris Marko Mikuž: E, μ and τ in irrad. Si

0

50

4 100

 $\times 150$

× 200

250

+300

350

- 400

450

500

<u>4</u> 550

 $\times 600$

× 650

0700

750 800



TREDI, Paris, Feb 22, 2016 M. Bomben - SIMDET 2018 - LPNHE, Paris Marko Mikuž: E, μ and τ in irrad. Si

Collected charge at ultra high fluences



How to model annealing?



TIME DEPENDENT SIMULATIONS

Chiochia model



Instantaneous current (Φ=1x10¹⁴ /cm²)



Instantaneous current (Φ=1x10¹⁴ /cm²)



Instantaneous current (Φ=1x10¹⁴ /cm²)

