

# TCAD Models/Parameters and Tool Fusion

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# Simulations @ HEPHY

## TCAD

- 4H-SiC
- LGADs
- radiation damage
- GEANT4 integration

## Allpix<sup>2</sup>, GATE

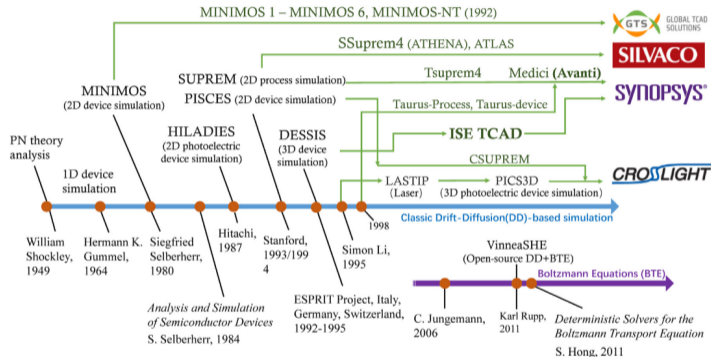
- time of flight
- medical applications

## SPICE

- readout electronics
- chip layout

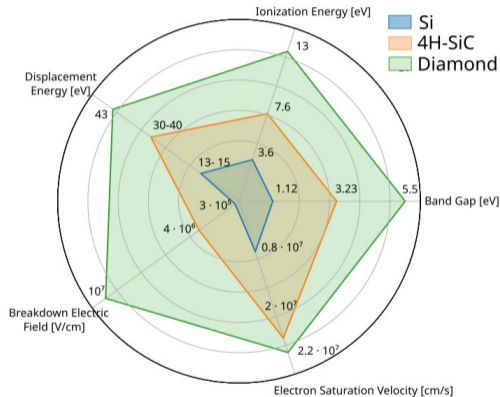
# TCAD Frameworks

- Global TCAD solutions (GTS) [1]
  - spin-off of TU Wien
  - direct access to developers (in walking distance)
- Sentaurus Workbench [2]
  - access via Europractice



Li et al. (2024) doi:10.1016/j.fmre.2024.01.010

- wide bandgap material (WBM)
  - one of first investigated semiconductors
  - used in power electronics
  - polytype 4H commonly used
- features high
  - charge carrier mobilities
  - breakdown field
  - thermal conductance
- utilization @ HEPHY
  - low noise particle detector
  - medical and HEP applications



1. 4H-SiC TCAD Parameter Review
2. Radiation Damage Simulations in 4H-SiC
3. GEANT4 Integration in GTS
4. Conclusion

## *4H-SiC TCAD Parameter Review*

*Really? Use a chat bot ... ;)*



## Topics:

- relative permittivity
- (temperature dependent) band gap
- low- and high-field mobility
- impact ionization
- effective electron/hole masses
- incomplete ionization
- generation/recombination





relative permittivity ( $\epsilon^{\parallel}, \epsilon^{\perp} / \epsilon_{\infty}^{\parallel}, \epsilon_{\infty}^{\perp}$ )

## Preliminary Results:

- many investigations available
  - > 800 publications analysed
- mixing of polytypes
  - many 6H values used
  - not properly labeled
- long citation chains
  - values may date back several decades
- active field of research

Patrick *et al.*

[patrick1970] ( 10.03 , 9.66 / 6.7 , 6.52 )

[madelung1991] ( 10.03 , 9.66 / 6.7 , 6.52 )

[wenzien1995] ( - / - , 6.52 )

[persson1997] ( 10.03 , 9.66 / 6.7 , 6.52 )

[persson1999] ( 10.03 , 9.66 / 6.7 , 6.52 )

[son2004] ( 10.03 , 9.66 / 6.7 , 6.52 )

[harris1995] ( 10.3 , 9.66 / 6.7 , 6.52 )

[neudeck2001] ( 9.7 / - )

[choi2005] ( 9.7 / - )

[neudeck2006] ( 9.7 / - )

[zhu2008] ( 9.7 / - )

[liu2015] ( 9.7 / - )

[wijesundara2011] ( 10 / - )

[arvinte2017] ( 9.7 / 6.52 )

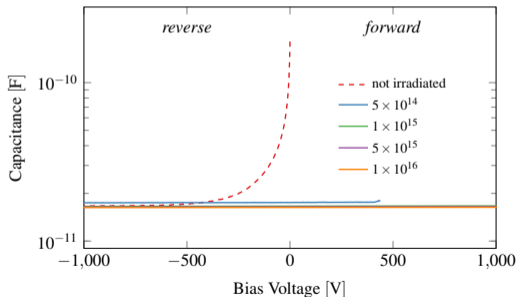
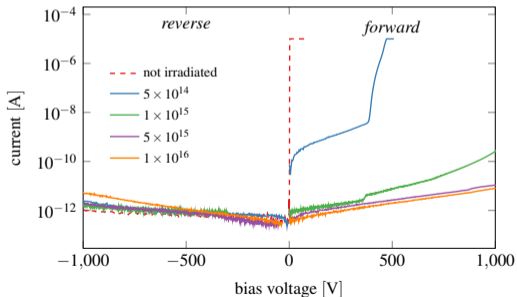
[pearnton2023] ( 9.7 / - )

Preliminary

## *4H-SiC Radiation Damage*

*Aah, all that luminosity ...*

- 4H-SiC planar diodes
  - run 13575 IMB-CNM-CSIC [3]
- neutron irradiation at ATI Vienna [4]
  - 1 MeV equivalent neutron fluences
- published by Gsponer *et al.* [5]
  - negligible conductance for forward bias
  - capacitance constant with varying bias voltage



# TCAD Radiation Damage Model

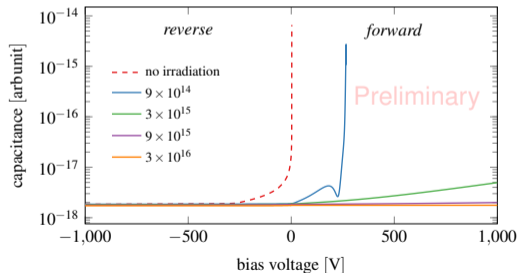
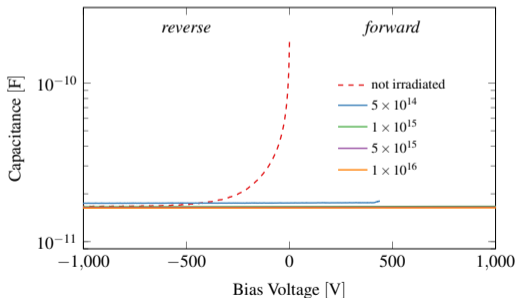
- trap information deviate in literature
  - energy level and type
  - capture cross sections  $\sigma_{e,h}$
  - introduction rate  $g_{int}$
- model by Gaggl *et al.* [6]
  - details in [talk by Philipp Gaggl](#)
  - actual trap levels utilized
  - subset used in this work

Defect	Type	Energy	$g_{int}$ [cm <sup>-1</sup> ]	$\sigma_e$ [cm <sup>2</sup> ]	$\sigma_h$ [cm <sup>2</sup> ]
Z <sub>1,2</sub>	Acceptor	$E_C - 0.67 \text{ eV}^a$	5.0 <sup>b</sup>	2e-14 <sup>a</sup>	3.5e-14 <sup>a</sup>
EH <sub>6,7</sub>	Donor <sup>c</sup>	$E_C - 1.6 \text{ eV}^{d,e}$	1.6 <sup>b</sup>	9e-12 <sup>e</sup>	3.8e-14 <sup>d,e</sup>
EH <sub>4</sub>	Acceptor	$E_C - 1.03 \text{ eV}^{f,g}$	2.4 <sup>b</sup>	5e-13 <sup>g</sup>	5.0e-14 <sup>g</sup>

<sup>a</sup> [7]   <sup>b</sup> [8]   <sup>c</sup> [9]   <sup>d</sup> [10]   <sup>e</sup> [11]   <sup>f</sup> [12]   <sup>g</sup> [13]

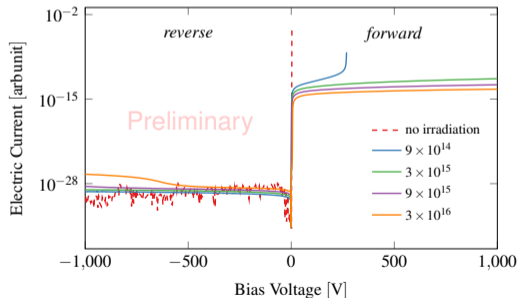
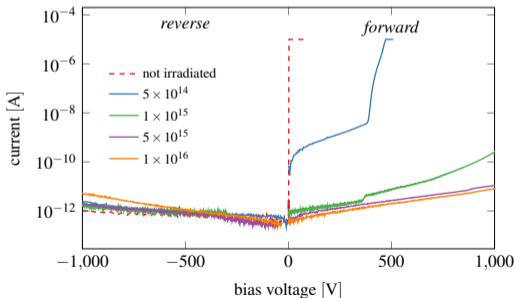
- convergence hard to achieve
  - necessary to deactivate some modelling
- qualitative match with measurements

- explanation for low forward current
  - trapped charge carriers form space charge
- simulations need to be improved

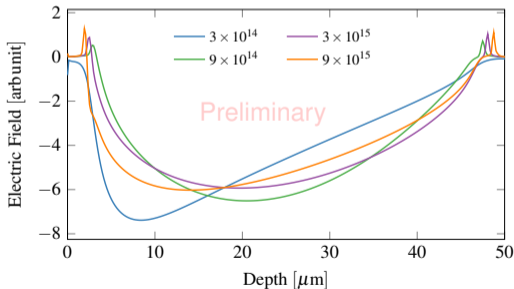


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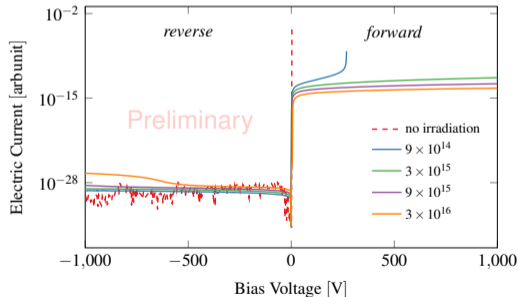
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## *GEANT4 Integration in GTS*

*Combine those tools!*



- utilize particle traces for realistic charge deposition
- workflow
  1. create structure in GTS framework
  2. define GEANT4 commands in .mac file
  3. run precompiled GEANT4 binary
  4. load structure in GTS and run simulations
- goals
  - get it going
  - add statistics to simulations
  - retrace measurement effects, e.g., gain suppression and energy distribution



GLOBAL TCAD  
SOLUTIONS

- simulations utilized at various occasions @ HEPHY
- TCAD parameter review of 4H-SiC
  - overview and critical evaluation
  - ongoing research
- simulation of radiation damage in 4H-SiC
  - first steps towards a TCAD model
  - project “TCAD Radiation Model for 4H-SiC” proposed in [WG3](#)
- integration of GEANT4 in GTS
  - tight interleaving of tools

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Thank you for your attention.

- [1] *GTS Framework*. URL: <https://www.globaltcad.com/products/gts-framework/>.
- [2] *Synopsys Sentaurus TCAD Framework*. URL: <https://www.synopsys.com/manufacturing/tcad/framework.html>.
- [3] Joan Marc Rafí et al. “Electron, Neutron, and Proton Irradiation Effects on SiC Radiation Detectors”. In: *IEEE Transactions on Nuclear Science* 67.12 (2020). DOI: [10.1109/TNS.2020.3029730](https://doi.org/10.1109/TNS.2020.3029730).
- [4] Peter Salajka. *Irradiation of silicon detectors for HEP experiments in the Triga Mark II reactor of ATI*. 2021. DOI: [10.34726/hss.2021.92420](https://doi.org/10.34726/hss.2021.92420).
- [5] Andreas Gsponer et al. “Neutron radiation induced effects in 4H-SiC PiN diodes”. In: *Journal of Instrumentation* 18.11 (Nov. 2023). DOI: [10.1088/1748-0221/18/11/C11027](https://doi.org/10.1088/1748-0221/18/11/C11027).
- [6] Philipp Gaggl et al. “TCAD modeling of radiation induced defects in 4H-SiC diodes and LGADs”. Poster at the 16th Pisa Meeting on Advanced Detectors. 2024.
- [7] P. B. Klein. “Identification and Carrier Dynamics of the Dominant Lifetime Limiting Defect in n<sup>-</sup> 4H-SiC Epitaxial Layers: Dominant Lifetime Limiting Defect in n<sup>-</sup> 4H-SiC Epitaxial Layers”. In: *physica status solidi (a)* 206.10 (Oct. 2009). ISSN: 18626300. DOI: [10.1002/pssa.200925155](https://doi.org/10.1002/pssa.200925155).
- [8] Pavel Hazdra, Vít Záhlava, and Jan Vobecký. “Point Defects in 4H–SiC Epilayers Introduced by Neutron Irradiation”. In: *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* 327 (May 2014). ISSN: 0168583X. DOI: [10.1016/j.nimb.2013.09.051](https://doi.org/10.1016/j.nimb.2013.09.051).
- [9] Tamas Hornos, Adam Gali, and Bengt Gunnar Svensson. “Large-Scale Electronic Structure Calculations of Vacancies in 4H-SiC Using the Heyd-Scuseria-Ernzerhof Screened Hybrid Density Functional”. In: *Materials Science Forum* 679–680 (Mar. 2011). ISSN: 1662-9752. DOI: [10.4028/www.scientific.net/MSF.679-680.261](https://doi.org/10.4028/www.scientific.net/MSF.679-680.261).

- [10] M. L. Megherbi et al. "Analysis of the Forward I–V Characteristics of Al-Implanted 4H-SiC p-i-n Diodes with Modeling of Recombination and Trapping Effects Due to Intrinsic and Doping-Induced Defect States". In: *Journal of Electronic Materials* 47.2 (Feb. 2018). ISSN: 0361-5235, 1543-186X. DOI: [10.1007/s11664-017-5916-8](https://doi.org/10.1007/s11664-017-5916-8).
- [11] J. Zhang et al. "Electrically Active Defects in *n*-Type 4H–Silicon Carbide Grown in a Vertical Hot-Wall Reactor". In: *Journal of Applied Physics* 93.8 (Apr. 15, 2003). ISSN: 0021-8979, 1089-7550. DOI: [10.1063/1.1543240](https://doi.org/10.1063/1.1543240).
- [12] C. Hemmingsson et al. "Deep Level Defects in Electron-Irradiated 4H SiC Epitaxial Layers". In: *Journal of Applied Physics* 81.9 (May 1, 1997). ISSN: 0021-8979, 1089-7550. DOI: [10.1063/1.364397](https://doi.org/10.1063/1.364397).
- [13] G. Alfieri et al. "Annealing Behavior between Room Temperature and 2000 °C of Deep Level Defects in Electron-Irradiated *n*-Type 4H Silicon Carbide". In: *Journal of Applied Physics* 98.4 (Aug. 15, 2005). ISSN: 0021-8979, 1089-7550. DOI: [10.1063/1.2009816](https://doi.org/10.1063/1.2009816).