TCAD Models/Parameters and Tool Fusion

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Simulations @ HEPHY

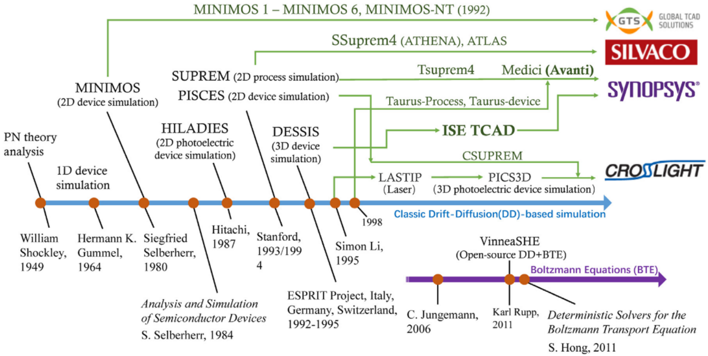
TCAD
- 4H-SiC
- LGADs
- radiation damage
- GEANT4 integration

Allpix^2, GATE
- time of flight
- medical applications

SPICE
- readout electronics
- chip layout

TCAD Frameworks

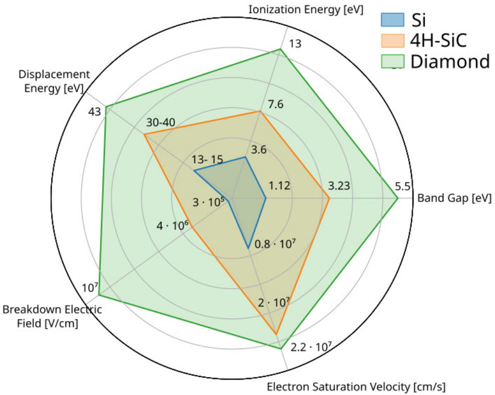
- Global TCAD solutions (GTS) [1]
  - spin-off of TU Wien
  - direct access to developers (in walking distance)
- Sentaurus Workbench [2]
  - access via Europractice



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

Silicon Carbide

- 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



Content

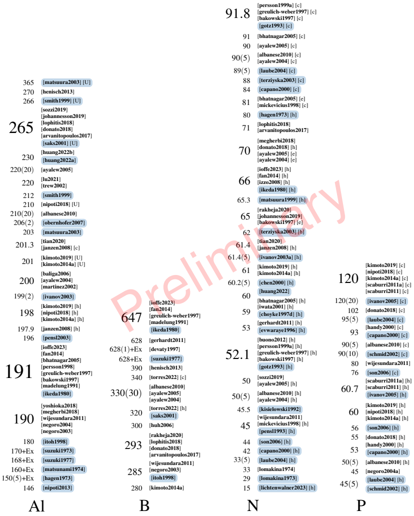
1. 4H-SiC TCAD Parameter Review
2. Radiation Damage Simulations in 4H-SiC
3. GEANT4 Integration in GTS
4. Conclusion

4H-SiC TCAD Parameter Review

Really? Use a chat bot ... ;)

4H-SiC TCAD Parameter Review

- state-of-the-art
  - lots of models and parameters available
  - origin/trustworthiness not clear
- methods
  - present published models/parameters
  - check consistency with references
  - identify key publications and values
  - distinguish hexagonal/cubic lattice sites and direction ⊥ / ∥ to c-axis
- goals
  - focus on bulk properties
  - provide entry point for newcomers
  - trigger critical evaluation in community



4H-SiC TCAD Parameter Review cont’d

Topics:

- relative permittivity
  - $\varepsilon^{\parallel}, \varepsilon^{\perp}, \varepsilon_{\infty}^{\parallel}, \varepsilon_{\infty}^{\perp}$
- (temperature dependent) bandgap
  - (exciton) bandgap energy
- mobility
  - low and high field, saturation velocity
- impact ionization
  - fitting and physics based models
- effective electron/hole masses
  - calculations and measurements
- incomplete ionization
  - doping and temp. dependency
- generation/recombination
  - SRH, bimolecular and Auger
- possible additions
  - thermal conductivity, electron affinity

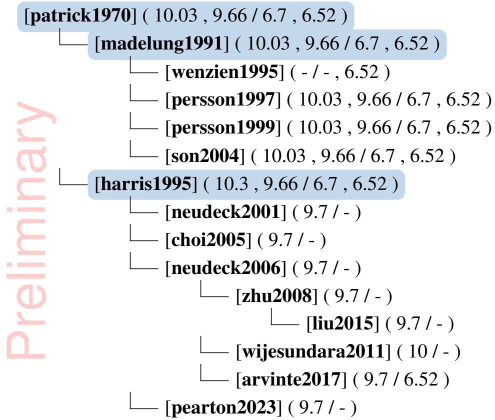
4H-SiC TCAD Parameter Review cont'd

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

relative permittivity $(\varepsilon^{\parallel}, \varepsilon^{\perp} / \varepsilon^{\parallel}_{\infty}, \varepsilon^{\perp}_{\infty})$

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)
    - **[pearton2023]** (9.7 / -)

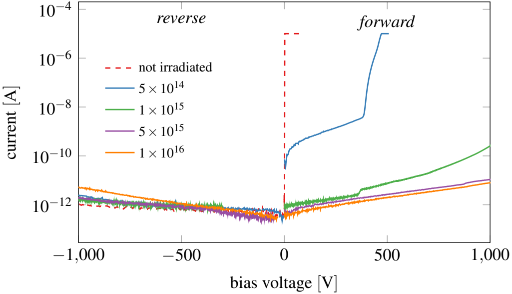
4H-SiC Radiation Damage

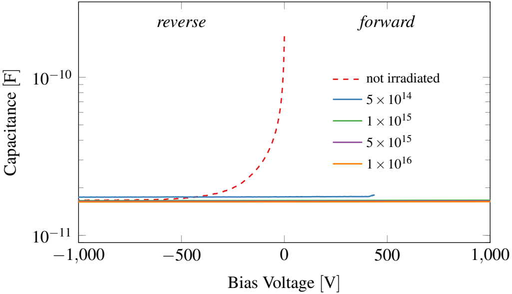
Aah, all that luminosity ...

Measurements

- 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

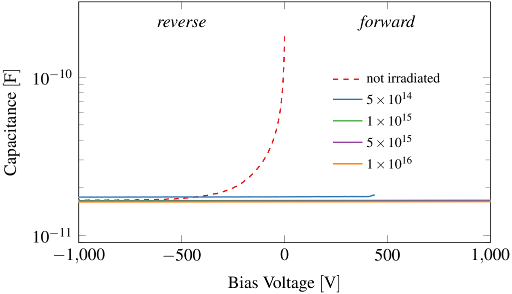
Defect	Type	Energy	g_{int} [cm^{-1}]	σ_e [cm^2]	σ_h [cm^2]
$Z_{1,2}$	Acceptor	$E_C - 0.67\,\text{eV}$ [a]	5.0 [b]	$2e{-}14$ [a]	$3.5e{-}14$ [a]
$EH_{6,7}$	Donor [c]	$E_C - 1.6\,\text{eV}$ [d,e]	1.6 [b]	$9e{-}12$ [e]	$3.8e{-}14$ [d,e]
EH_4	Acceptor	$E_C - 1.03\,\text{eV}$ [f,g]	2.4 [b]	$5e{-}13$ [g]	$5.0e{-}14$ [g]

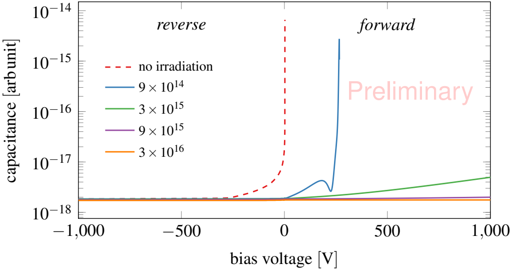
[a] [7] [b] [8] [c] [9] [d] [10] [e] [11] [f] [12] [g] [13]

Simulations in GTS

- 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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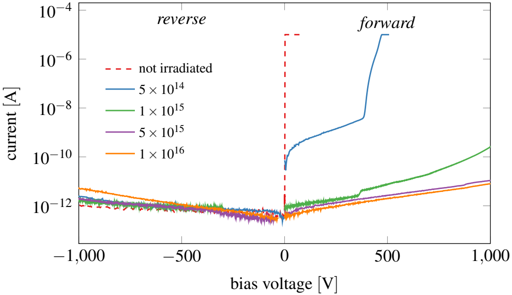

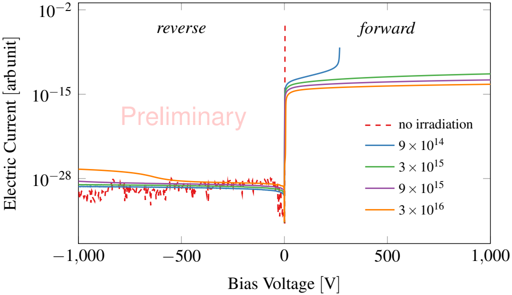

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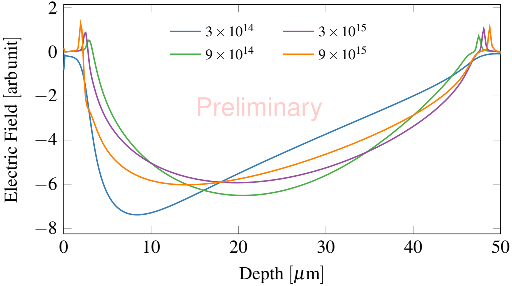

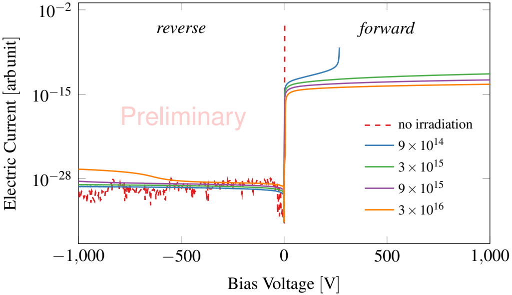

GEANT4 Integration in GTS

Combine those tools!

GEANT4 in GTS

- 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 supression and energy distribution

GEANT4
A SIMULATION TOOLKIT

GTS
GLOBAL TCAD SOLUTIONS

Conclusion

- 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.

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