Improving TCAD simulation of 4H-SiC particle detectors

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Introduction

Measure and verify material and model parameters from prototype 4H-SiC samples and adapt parameter files and models accordingly

→

SYNOPSYS Sentaurus

Utilize TCAD simulations

Global TCAD Solutions (GTS)

→

Design and production of 4H-SiC particle detectors

Introduction

SYNOPSYS Sentaurus [1]

- One of the two big players in semiconductor TCAD software
- Widely used within the HEP community
- Access via Europractice [3]
- Extensive material and model database
- Provides all tools necessary for a full simulation workflow (e.g. process simulation, meshing, electrical simulation, post processing, optimization,…

Global TCAD Solutions (GTS) [2]

- Vienna-based TCAD provider
- Focusing on micro,- and nanoelectronics devices (only device simulations)
- Collaboration with HEPHY since 2023
- Investigating 4H-SiC samples and implementing the material in GTS
- Single-event-upsets using GEANT4
- Direct contact with developers

Introduction

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- Collaboration with HEPHY since 2023
- Investigating 4H-SiC samples and implementing the material in GTS
- Adapting the software to efficiently model silicon carbide (QFT-solver)
- Custom user support

Parameters

- Constant improvement of literature values due to better processing techniques
- Especially in the last six years, SYNOPSYS continuously improved their SiC parameters
- Consider anisotropy of SiC (marked with *) → Be aware of the implemented orientation

Most important parameters and models to include for 4H-SiC

Band structure	Charge carriers	Recombination
– Permittivity* – BG-narrowing (SB) – Incomplete ionization Al (p) and N (n) doping – Split energy levels (N)	– Mobility: Temperature dep.* Doping dep.* High field saturation* – Impact ionization*	– SRH – Surface-SRH – Auger – Traps ($Z_{1/2}$-defect)

Parameters

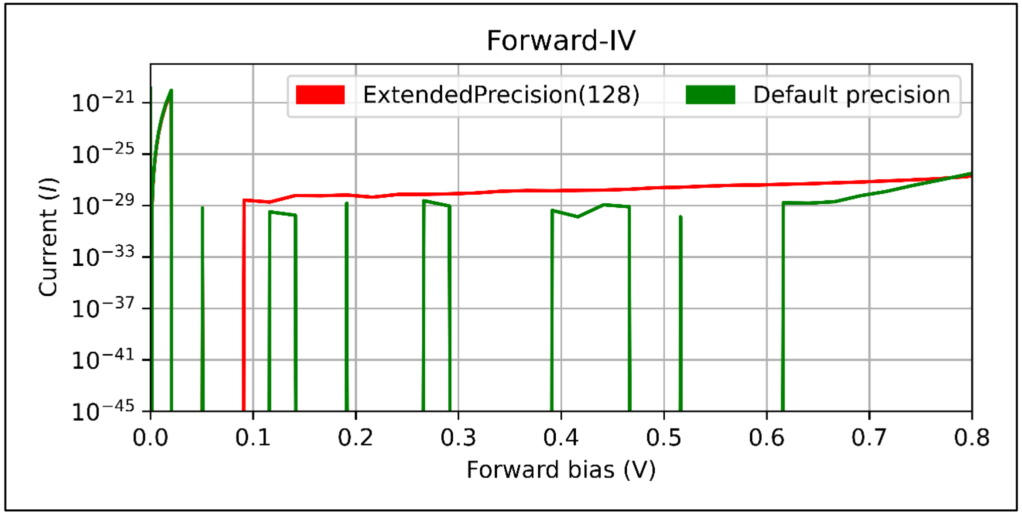
- Constant improvement of literature values due to better processing techniques
- Especially in the last six years, SYNOPSYS continuously improved their SiC parameters
- The anisotropic nature of SiC-polytypes should be considered (marked with *)

Some things to consider when using the default *4H-SiC.par*

Recombination	Mobility	Impact ionization
– Model parameters for Shockley-Read-Hall *(Scharfetter)*, *Auger* (and traps) are very process dependent – No *SurfaceRecombination*	– No anisotropy for holes in *ConstantMobility* – No anisotropy for *EnormalDependence* – Equal saturation velocity for e^- & h^+	– Only *OkutoCrowell* includes anisotropy

Tackling convergence issues

- The wide bandgap of 4H-SiC leads to very low intrinsic charge carrier densities
- Usually, a much higher numeric accuracy than the default settings are required
- This can partially be mitigated by finer meshing
- Tuning error & convergence criteria and solver settings can improve convergence drastically

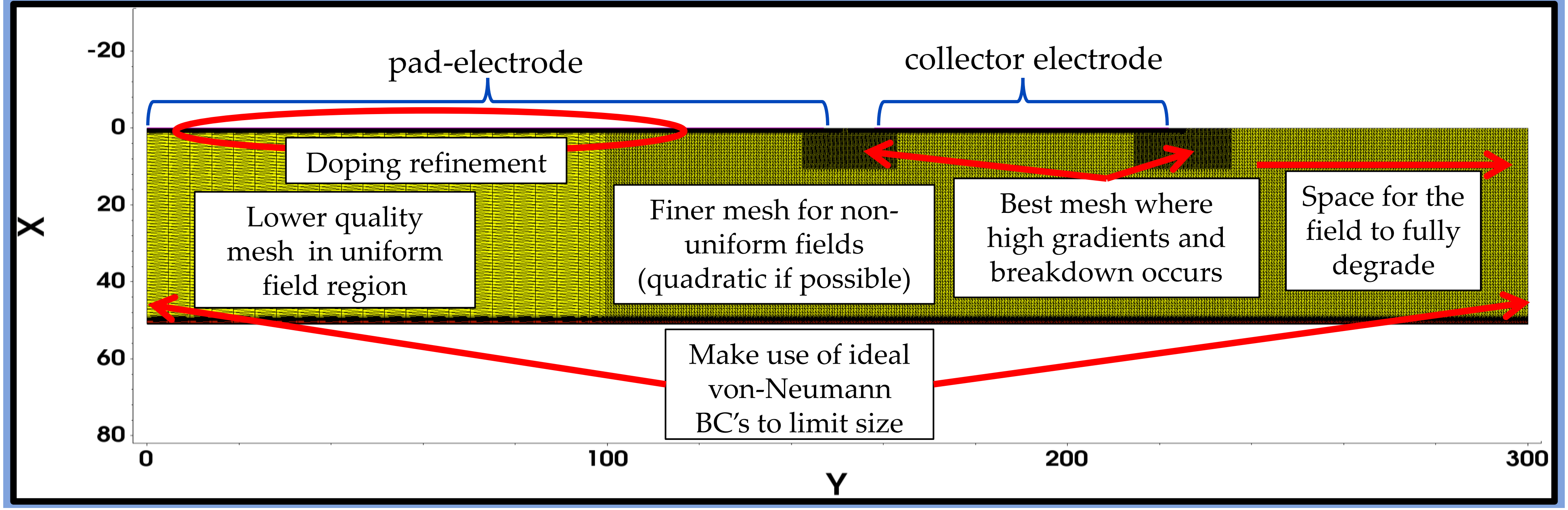


Numerical instability on the example of a forward-IV (transient) simulation

Tackling convergence issues

- Due to the low wafer quality (compared to Si), the Debye length is very small
- $\lambda = \sqrt{\frac{k_B T \varepsilon}{q^2 N_{Doping}}} \approx 0.3\ \mu m$ for $N_{Doping} = 1.5 \cdot 10^{14}\ cm^{-3}$ → large computation times [4]

Efficient meshing strategy



Tackling convergence issues

Floating-point accuracy

- Drift diffusion PDE'S subtract almost equal charge carrier concentrations
- Sentaurus allows for dynamically changing the floating-point accuracy
- *ExtendedPrecision(128)* usually sufficient (minimum 80!)
- Only compatible with *SUPER, PARDISO* and *ILS* solvers

```
***** Floating point accuracy *****
ExtendedPrecision(128)
****
```

Tackling convergence issues

Error and convergence criteria

- Tightening the accuracy and error criteria (*Digits, RHSmin)*
- High *RHSFactor* and *RHSmax* allows for solutions to "bounce back"
- Stating reference values for low charge carrier densities

```
***** Error and convergence criteria *****
Digits = 15
RelErrControl
ErrEff(electron) = 1e-2
ErrEff(hole) = 1e-2
RhsAndUpdateConvergence
RHSmax = 1e30
RhsFactor = 1e120
RHSmin = 1e-10
CdensityMin = 1e-20
RefDens_eGradQuasiFermi_ElectricField_HFS = 1e14
RefDens_hGradQuasiFermi_ElectricField_HFS = 1e14
*****
```

Tackling convergence issues

Solver settings

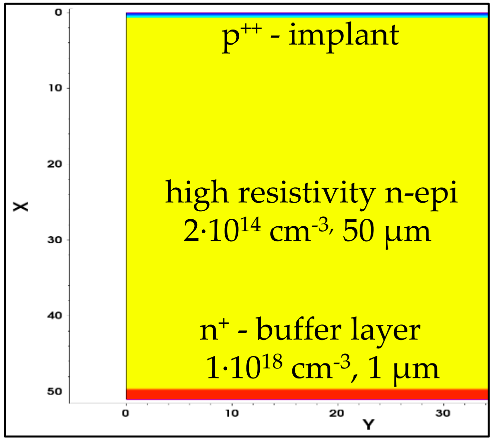
– *ILS* and *SUPER* solver more robust for wide bandgaps

– Use Backwards Euler method (BE) for transient simulations

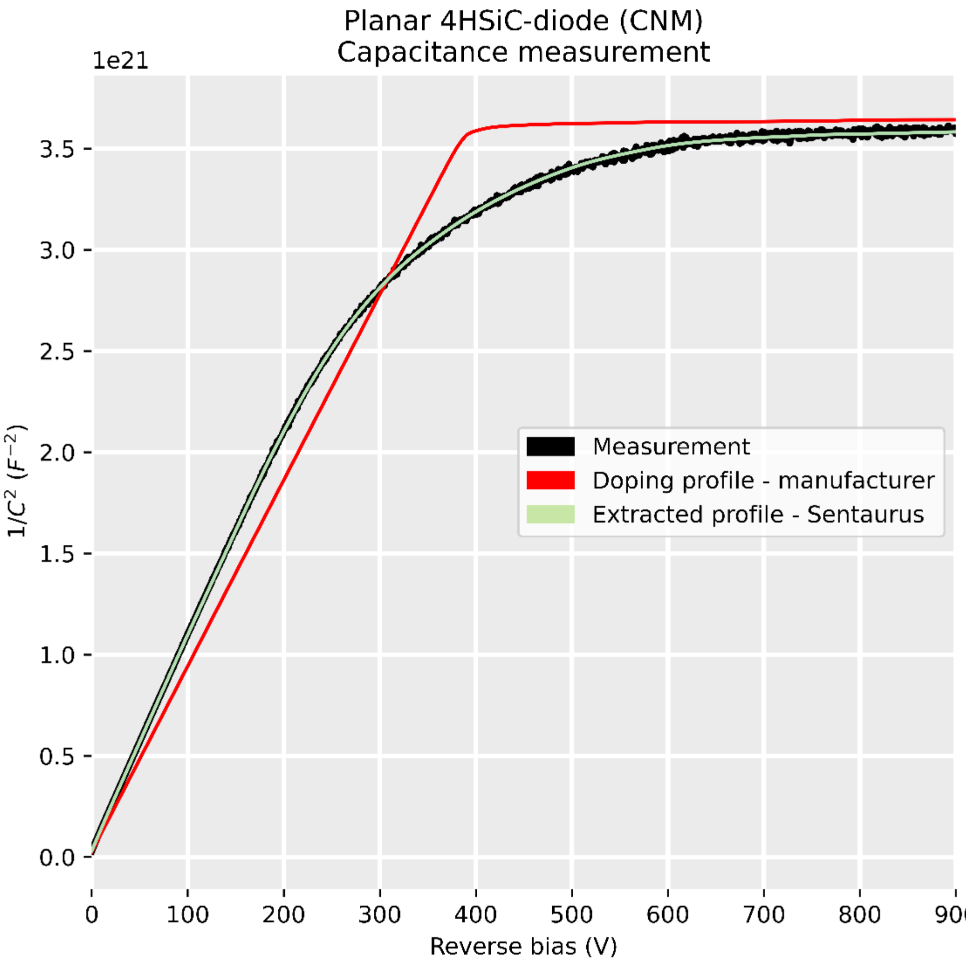
```
***** Individual solver settings *****
Method = Blocked
SubMethod = ILS(set=25)
ACMethod = Blocked
ACSubMethod = ILS(set=25)
ILSrc= "set (25) {
        iterative(gmres(100), tolrel=1e-10, tolunprec=1e-4, tolabs=0, maxit=200);
        preconditioning(ilut(1.5e-6,-1), right);
        ordering(symmetric=nd, nonsymmetric=mpsilst);
        options(compact=yes, linscale=0, refineresidual=10, verbose=0);
};"
Transient = BE
****
```

Simulations – CV diode

- Planar 4H-SiC p-in-n diodes from CNM [5]
- Capacitance measurements show strong deviation from suggested doping profile
- Slower propagation of the depletion zone due to higher doping concentration at the back
- Most likely due to diffusion processes during growth

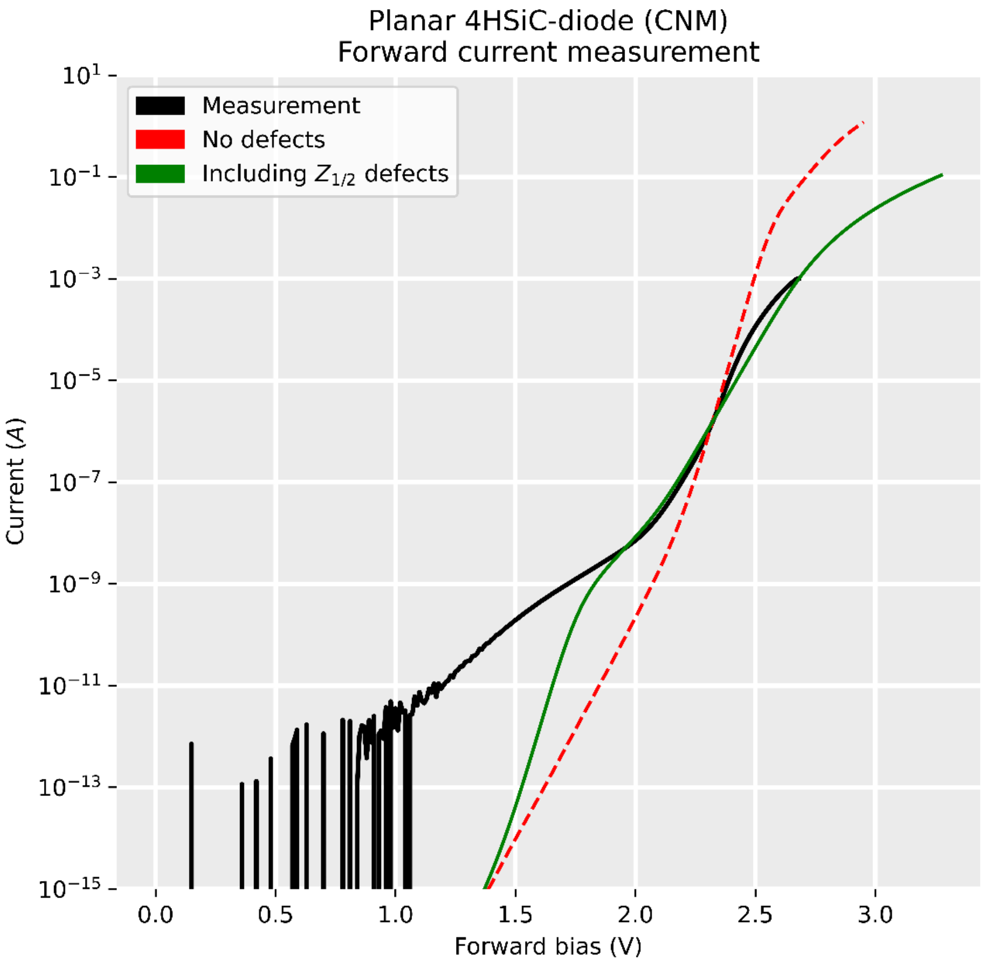


Initially modelled doping profile of the 4H-SiC planar diode [6]



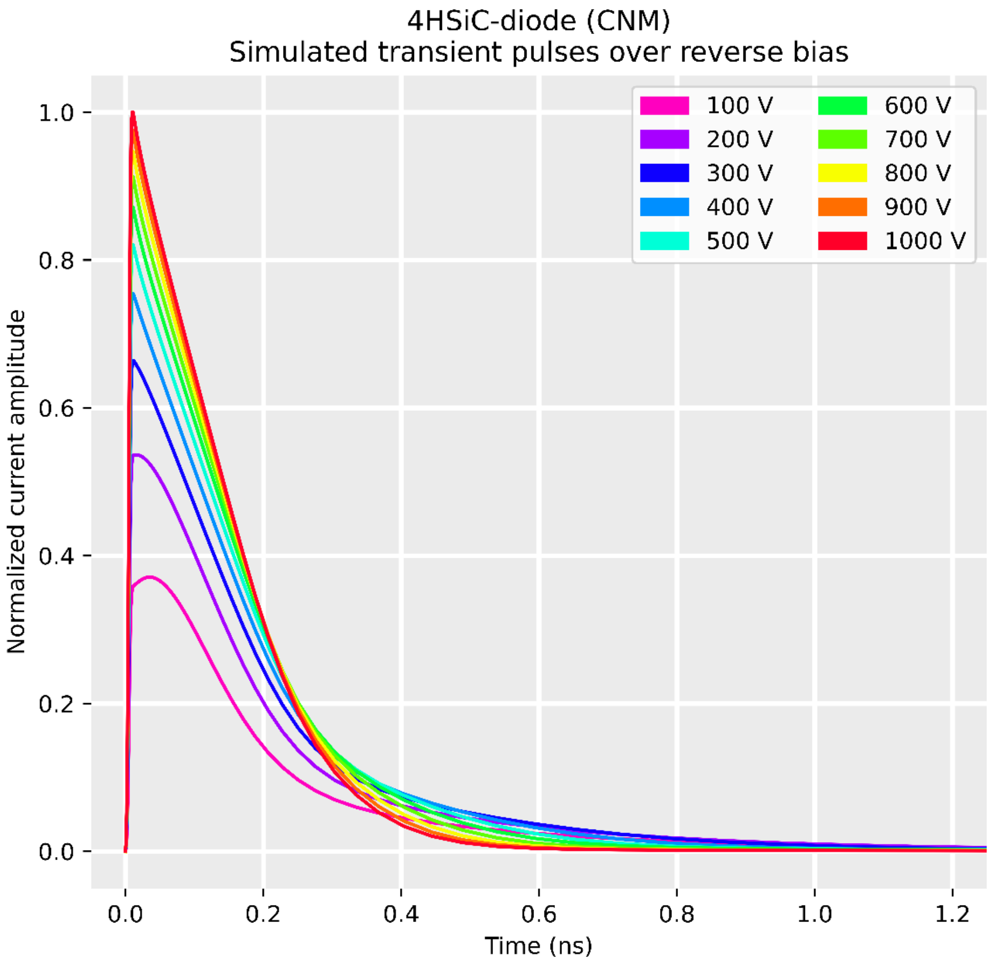
Simulations – Forward-IV

- Below detection limit at low bias
- Initial transient simulations agree decently
- Including the $Z_{1/2}$ **defect**:
  - Dominant deep level defect in 4H-SiC [7-11]
  - 0.63 eV - 0.68 eV below E_c [7-11]
  - Acceptor type, origin from C-Vacancy[7-9, 10, 11]
  - Thermally stable [8]
  - Strong dependence on Si and C environment during epitaxial growth [8]
  - **Best fit → $N_{Z1/2} \approx 10^{15} cm^{-3}$** (**assumed** cross section of $\sigma = 10^{-15}\ cm^2$)
- Reverse-IV: Waiting for more precise setup



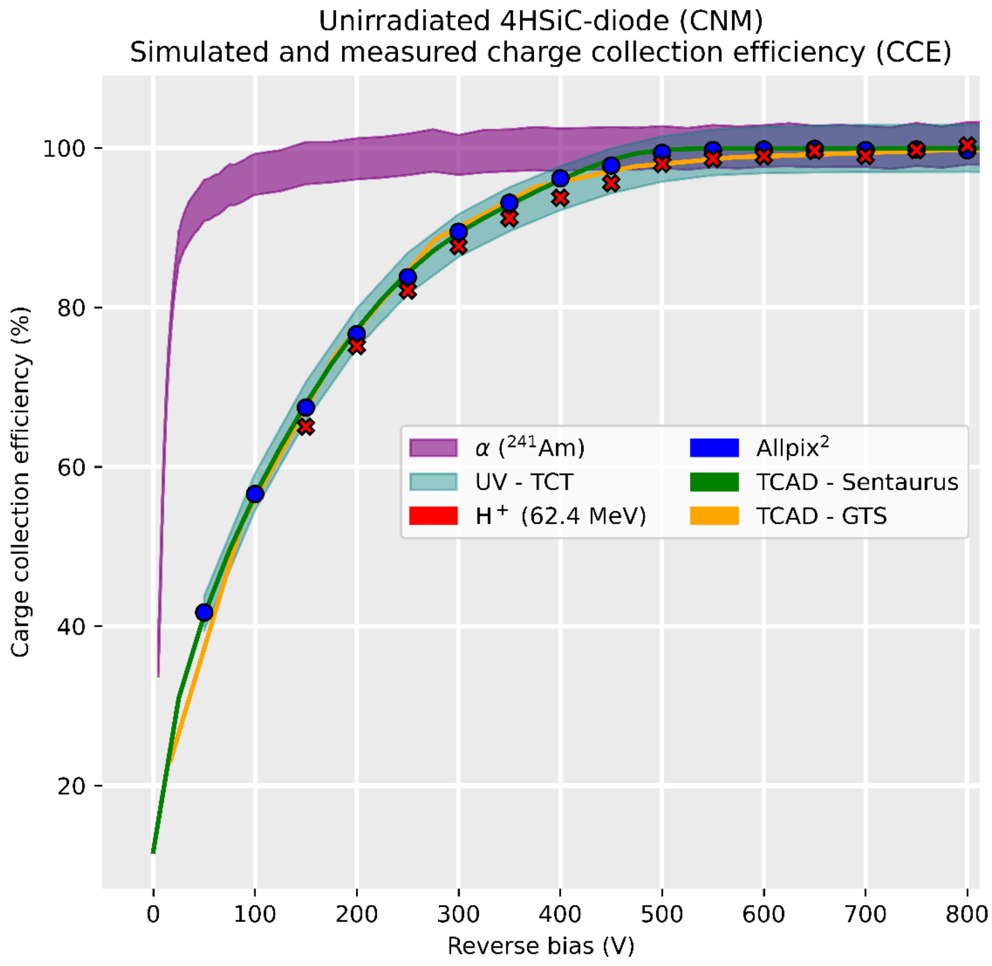
Simulations – Transient pulses

- Transient pulse simulations crucial to model and compare detector response
- *HeavyIon* model in SENTAURUS Device [12]
- Energy deposition across given particle path
- Not instantly, but over very short time (≈ 5 ps)
- Load fields from quasistationary simulation over reverse bias
- "Empty" transient simulation before energy deposition necessary to numerically stabilize the current



Simulations – Transient pulses

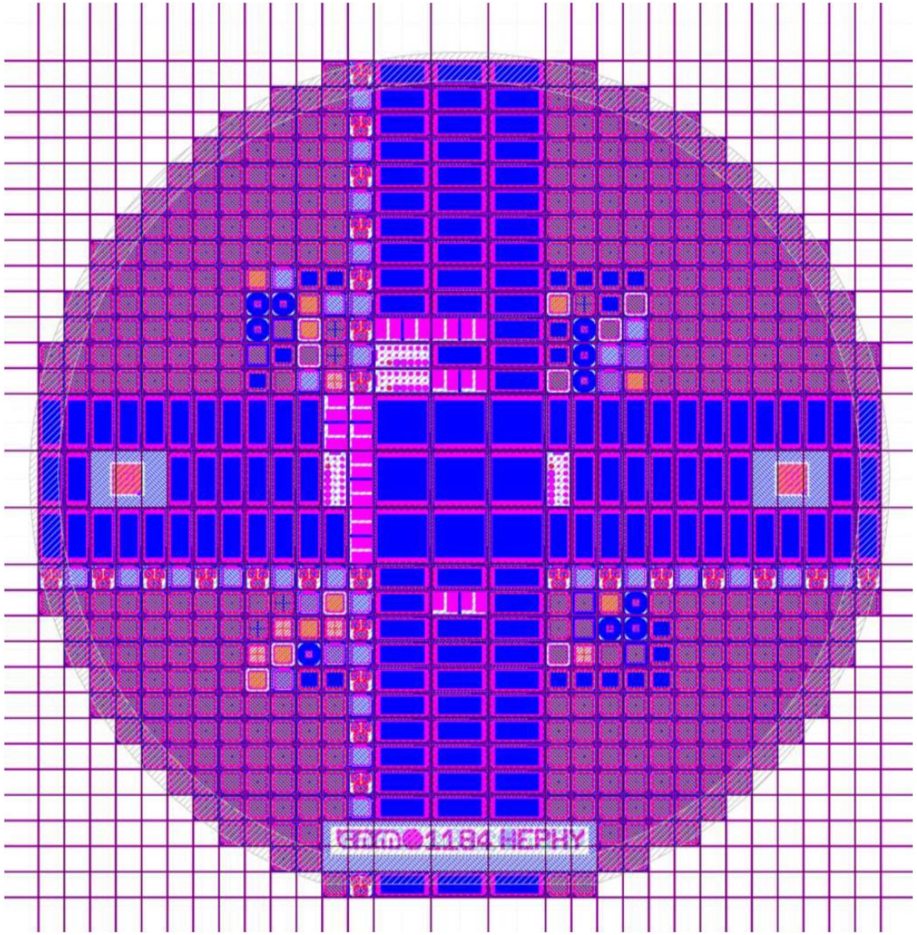
- Performed charge collection measurements using multiple signal sources
- α – particles (^{241}Am) [13]
  Proton beam (62.4 MeV) [6]
  UV-Laser (TCT) [14]
- Comparison with several simulation software for cross-checking
- Simulation results agree very well (for the unirradiated case)
- Next step:
  Reproduce measurements of neutron irradiated samples [13, 14]



Simulations – Breakdown

4H-SiC wafer-run

- In collaboration with CNM [5]
- 3 x 50 µm & 2 x 100 µm (epitaxial layer)
- Design at HEPHY, processing at CNM
- First measurements by the end of 2023
- For 100 µm, $V_{depl} \approx 1300\ V$
- Simulations to optimize guard structure
  → Maximize breakdown (BD) voltage
  → Minimize guard structure size



Final design of the 4H-SiC wafer layout

Simulations – Breakdown

4H-SiC wafer-run

- In collaboration with CNM [5]
- 3 x 50 µm & 2 x 100 µm (epitaxial layer)
- Design at HEPHY, processing at CNM
- First measurements by the end of 2023
- For 100 µm, $V_{depl} > 1300\ V$ (unirradiated)
- Simulations to optimize guard structure
  → Maximize breakdown (BD) voltage
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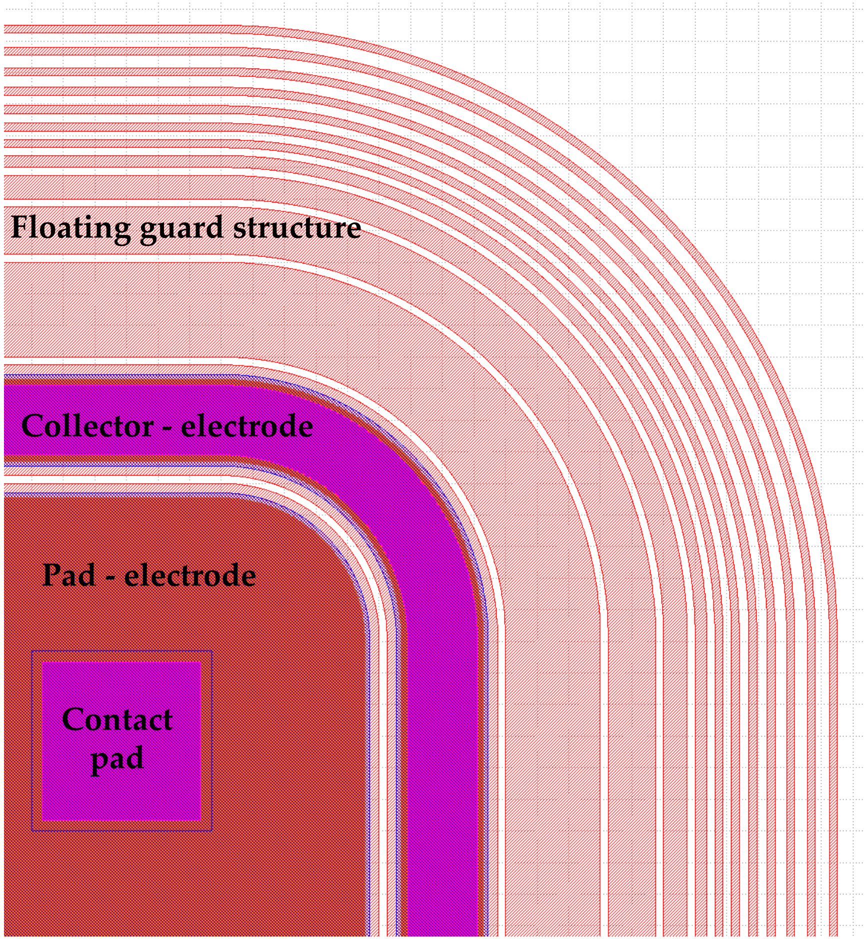
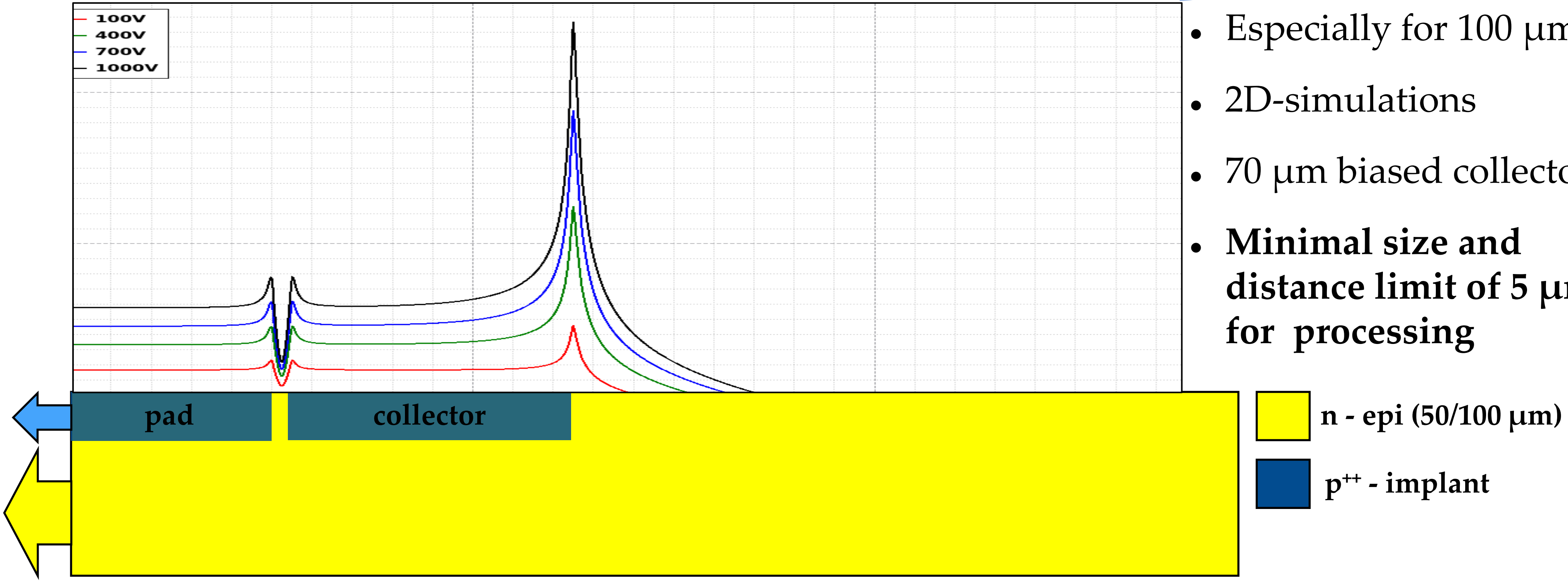


Guard structure design after optmimization

Simulations – Breakdown

Sensor thickness	Collector biased	Collector floating
50 µm	1007 V	1184 V
100 µm	1029 V	1191 V

Additional floating guards necessary to increase BD-voltage

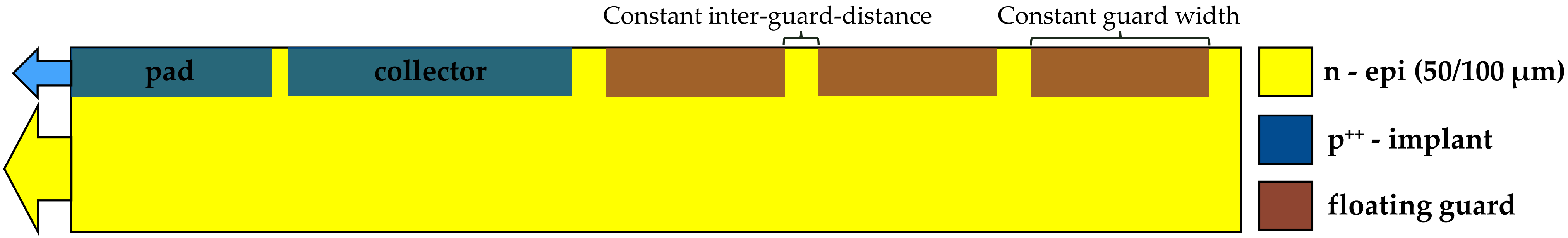


- Especially for 100 µm
- 2D-simulations
- 70 µm biased collector
- **Minimal size and distance limit of 5 µm for processing**

Simulations – Breakdown

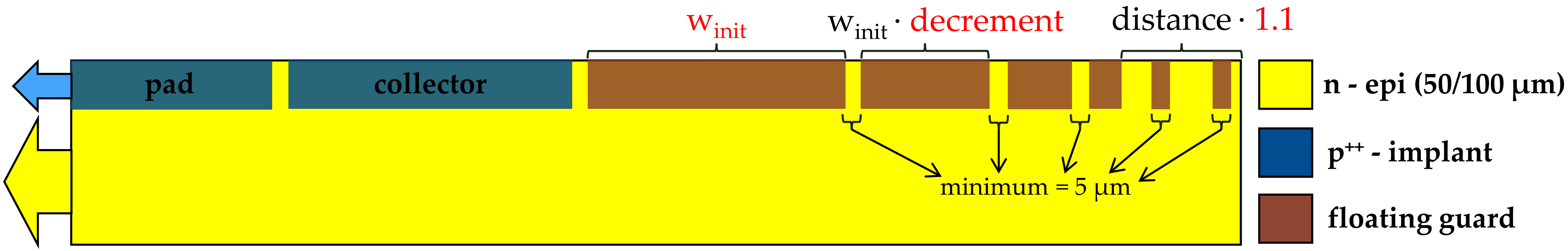
Uniform guards:

- Wider guards with small distances yield the best BD-behaviour
- BD occurs after the collector, where the field peak is highest
- Further optimization after collector required



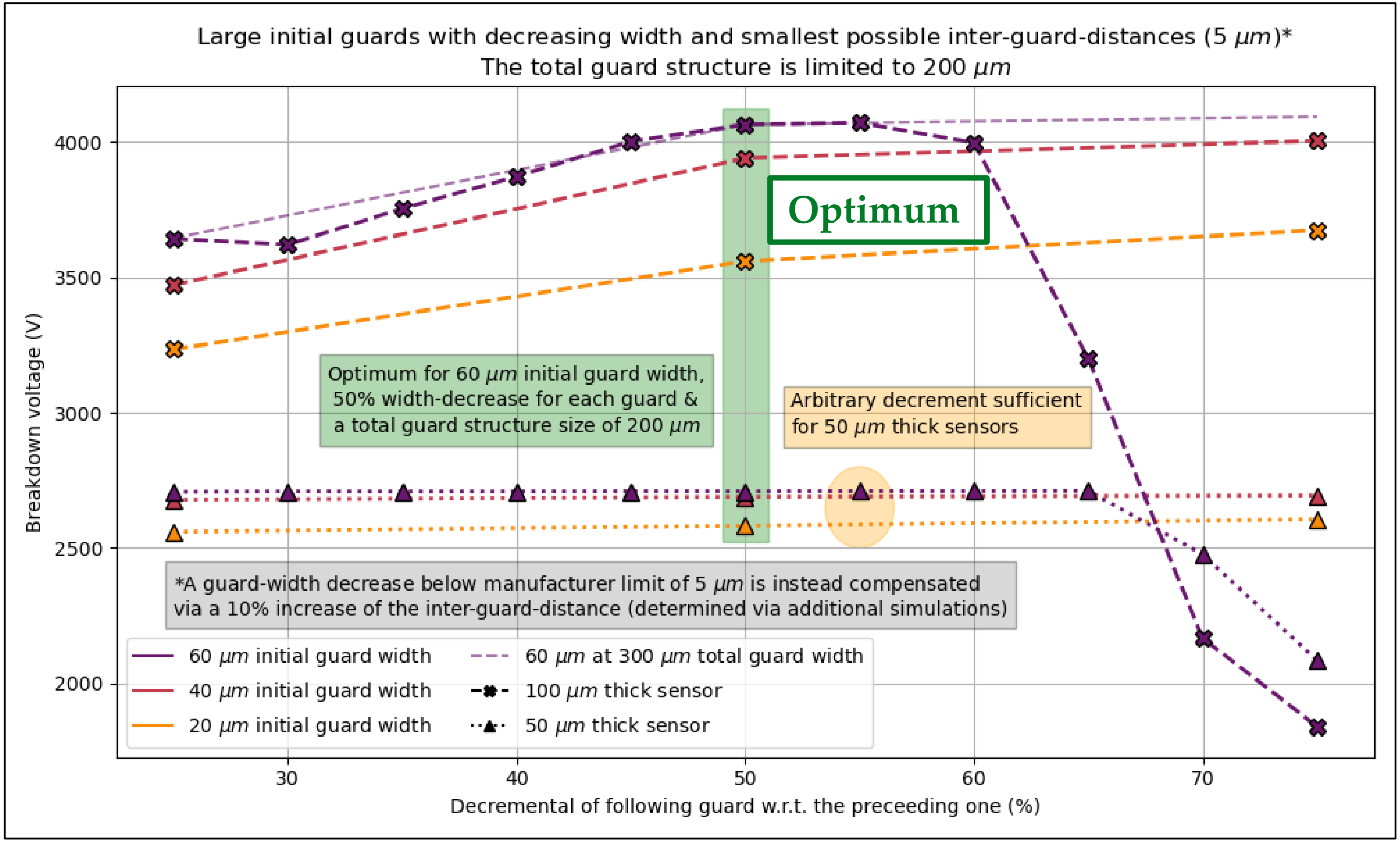
Simulations – Breakdown

- Use limit of 5 µm for the distance between guards
- Starting with a wide initial guard reduces field peak right after collector
  → w_{init}
- Decrease guard width by some factor with every step to save space
  → decrement
- As soon as limitation is reached (w_{guard} < 5 µm), increase the distance between the guards by an increment (highest BD for 6%-12%)
- Multiple parameter sweeps (50 µm & 100 µm) to find an optimum



Simulations – Breakdown

Parameter	Value
w_{init}	60 µm
distance	5 µm
decrement	50%
increment	10%
total	200 µm



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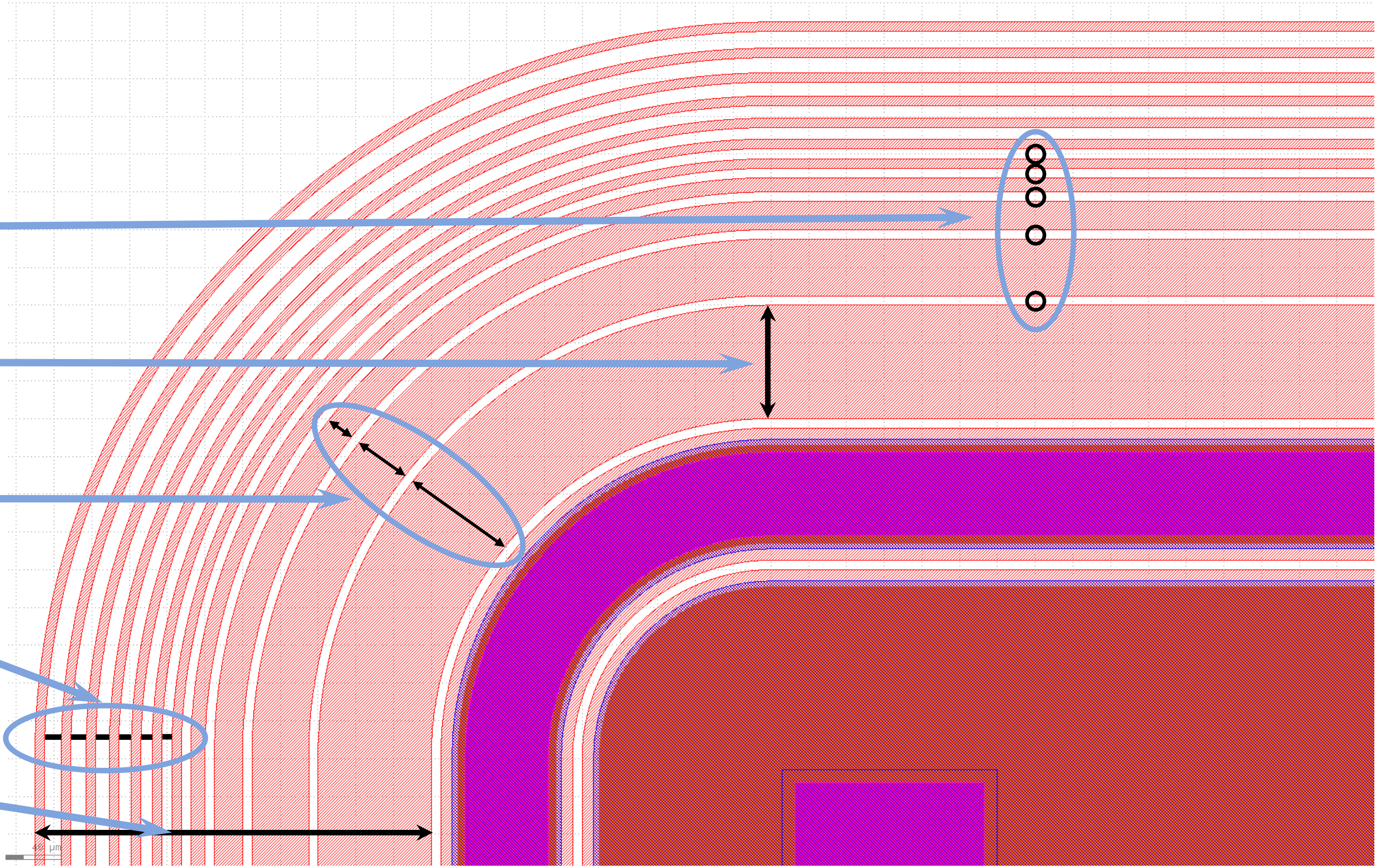


Open challenges

- Need some fixed 4H-SiC parameters to extract others from measurement
- Measurement accuracy
  - Dark current in pA - nA range even for irradiated samples
  - Low noise CSA or high bandwidth TIA required to accurately measure (MIP) signals
- Defects need to be better understood (densities, origin, cross sections)
- Same for interface traps
- Modeling of irradiation processes and damage
  → Reproduce measurements of neutron irradiated samples [13, 14]

Outlook

- First measurements of new wafer run by the end of 2023
  - Various devices (circular & rectangular pad & strip diodes, MOSFETs, GCDs, MOSCAPs, Pixel-detectors…)
  - 5 wafers → high statistic
- Investigate temperature dependency of model parameters
- Extensive irradiation studies of pad/strip-detectors and MOSFETs
- Updating TCAD-framework to simulate and design 4H-SiC-LGADs

References

[1] : https://www.synopsys.com/silicon/tcad.html

[2] : https://www.globaltcad.com/

[3] : https://europractice-ic.com/

[4] : Johnson et al., The Influence of Debye Length on the C-V Measurement of Doping Profiles, IEEE TRANSACTIONS ON ELECTRON DEVICES (1971)

[5] : https://www.imb-cnm.csic.es/en

[6] : Christanell et al., 4H-silicon carbide as particle detector for high-intensity ion beams. J. Inst. 17, C01060 (2022).

[7] : Brodar et al., Depth Profile Analysis of Deep Level Defects in 4H-SiC Introduced by Radiation, Crystals (2020), doi:10.3390/cryst10090845

[8] : Tsunenobu Kimoto, Fundamentals of Silicon Carbide Technology: Growth, Characterization, Devices and Applications, IEEE Press (2014)

[9] : Capan et al., Deep Level Defects in 4H-SiC Epitaxial Layers, Materials Science Forum, ISSN: 1662-9752, Vol. 924, pp 225-228 (2018)

[10] : Zippelius et al., Z1/2- and EH6-Center in 4H-SiC: Not Identical Defects?, Materials Science Forum, ISSN: 1662-9752, Vols. 717-720, pp 251-254 (2012)

[11] : Kawahara et al., Investigation on origin of Z1/2 center in SiC by deep level transient spectroscopy and electron paramagnetic resonance, American Institute of Physics (2013), doi: 10.1063/1.4796141

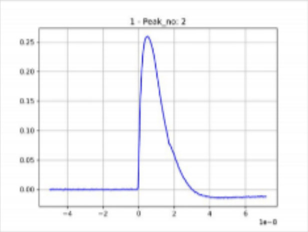
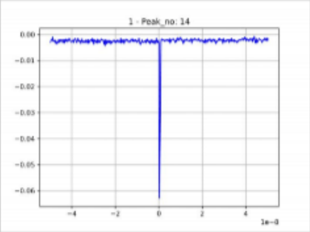
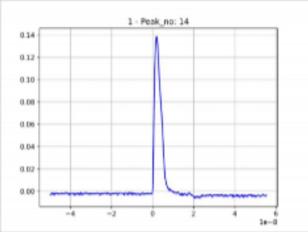
[12] : Sentaurus™ Device User Guide (Version: U-2022.12)

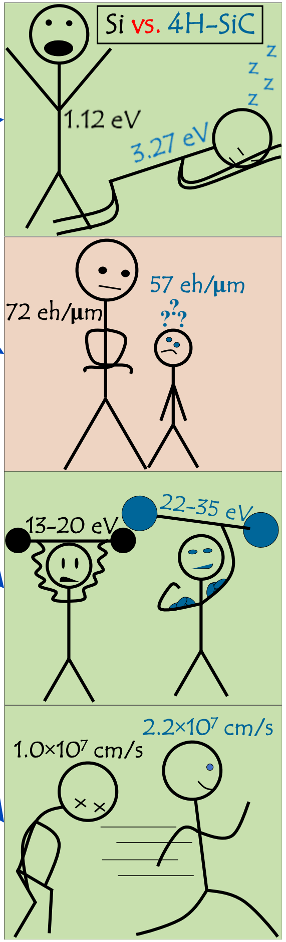
[13] : Gaggl et al.,, Charge collection efficiency study on neutron-irradiated planar silicon carbide diodes via UV-TCT, 10.1016/j.nima.2022.167218

[14] : Gaggl et al., Performance of neutron-irradiated 4H-silicon carbide diodes subjected to alpha radiation, J. Inst.18, C01042 (2023)

BACKUP

4H-SiC detector properties

	Silicon	4H-Silicon carbide	CVD Diamond
Band gap [eV]	1.1	3.26	5.5
Ionization energy [eV]	3.6	5 – 8	12.86
atomic displacement threshold	13-20 eV	20-35	43
Density [g/cm^3]	2.33	3.22	3.52
Electron Mobility [cm^2/Vs]	1430	⊥ c: 800; ∥ c: 900	1800-2200
Hole Mobility [cm^2/Vs]	480	115	1200-1600
Saturation electron velocity [10^7 cm/s]	1	2.2	2.7
Breakdown Field [MV/cm]	0.5	⊥ c: 4.0; ∥ c: 3.0	10
e/h pairs per µm	72	57	36
Typical active thickness [µm]	300	<150µm epi layer possible (50µm studied by us)	<400 (charge collection distance)
Material	Float zone	Epitaxially grown	chemical vapor deposition
e/h pairs MPV	21,600	2,850 (50µm)	14,000
Typical signal (recently measured myself at proton beam with UCSC LGAD-readout board and DRS4-based digitizer)			
Wafer costs	O(<100€)	O(1000€)	O(100,000€)



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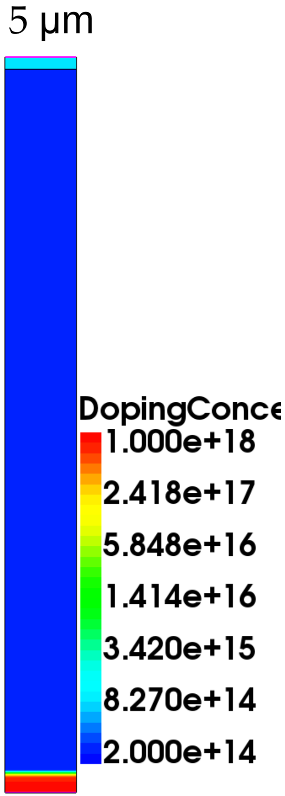
Tackling convergence issues

HEPHY INSTITUTE OF HIGH ENERGY PHYSICS

Lumped resistor approach for breakdown (BD) simulations

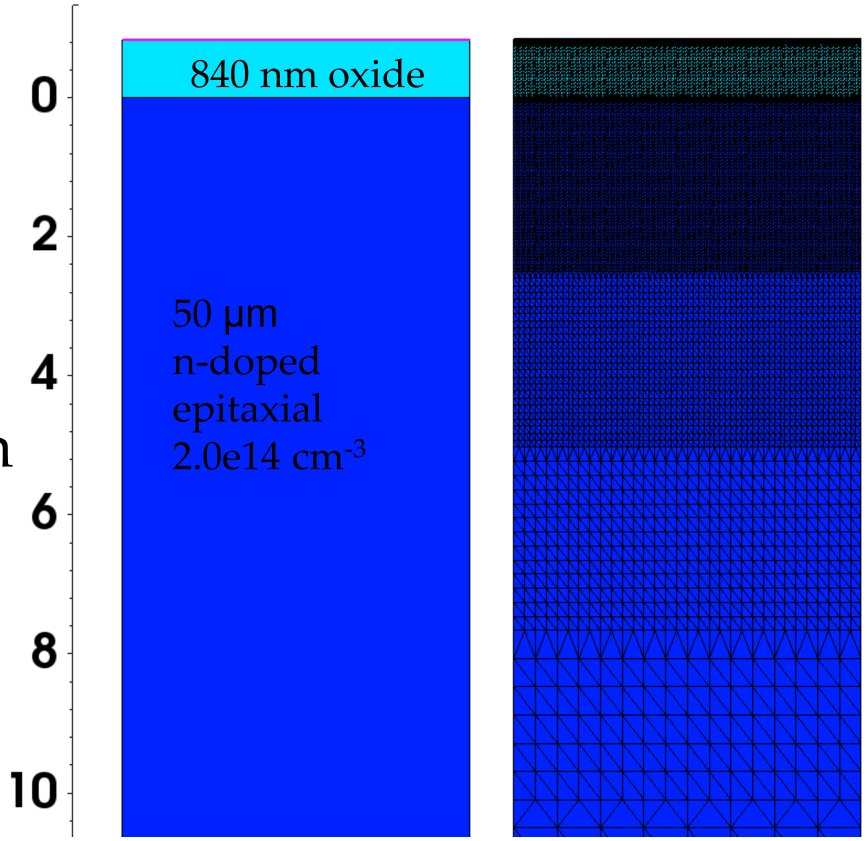
- Improves convergence for reverse bias modeling
- Attaching an external resistor to the ramped electrode (*Resist*=… in *Electrode* section) comparable to the device resistance at the onset of breakdown
- Ramp *outer voltage* to obtain an *inner voltage* corresponding to the bias
- At small bias: Main voltage drop over TCAD-device
  At BD-onset: Series resistance comparable to device resistance → voltage drop is split
  At BD: Device resistance drops, voltage drop mainly over series resistor
- Smoothly increase of outer voltage

Simulations - MOSCAP



Structure:

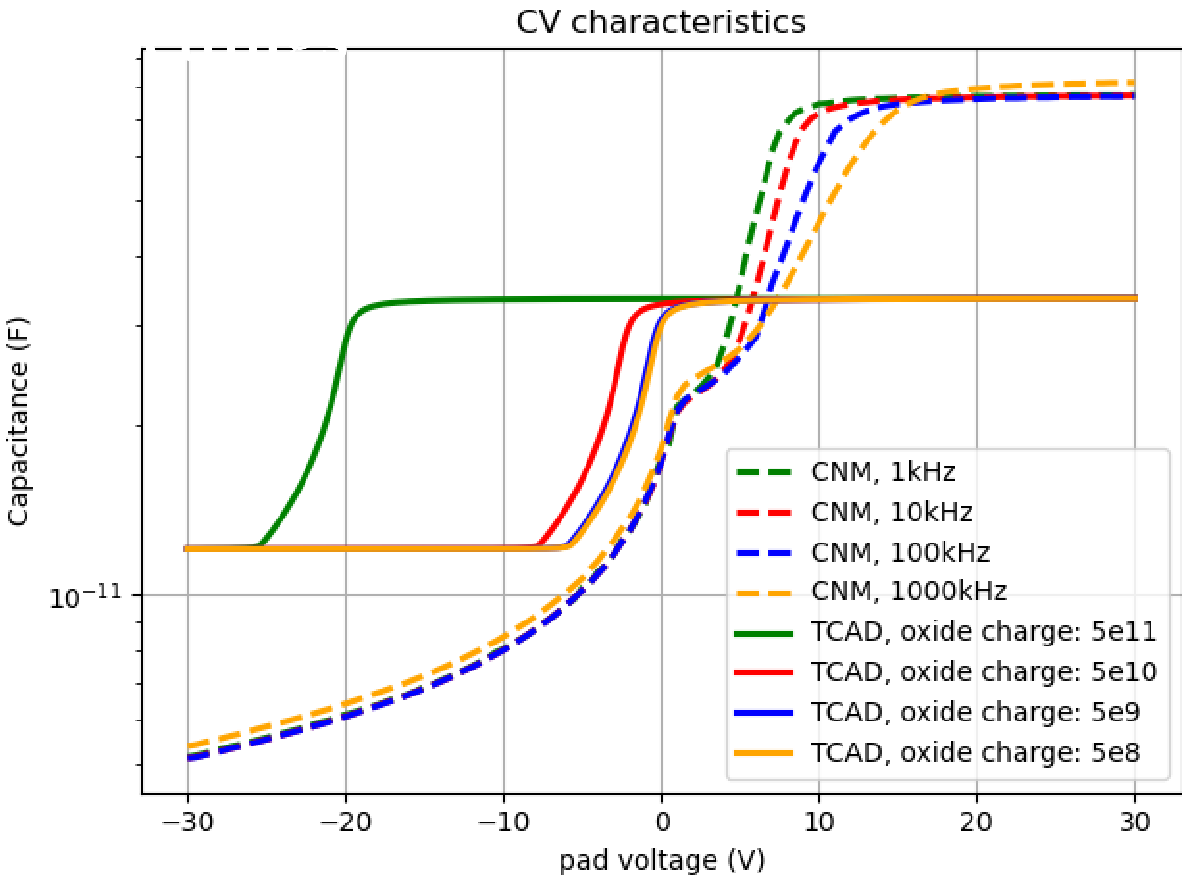
- Used a (very) simple structure
- Only one oxide layer
- Measurements from [-30 V, 30 V]
- Very fine mesh at upper region
- First two layers below oxide needed to be meshed at < 1 Å to reach convergence!!!
- Carried out simulations for different fixed oxide charges



Simulations - MOSCAP

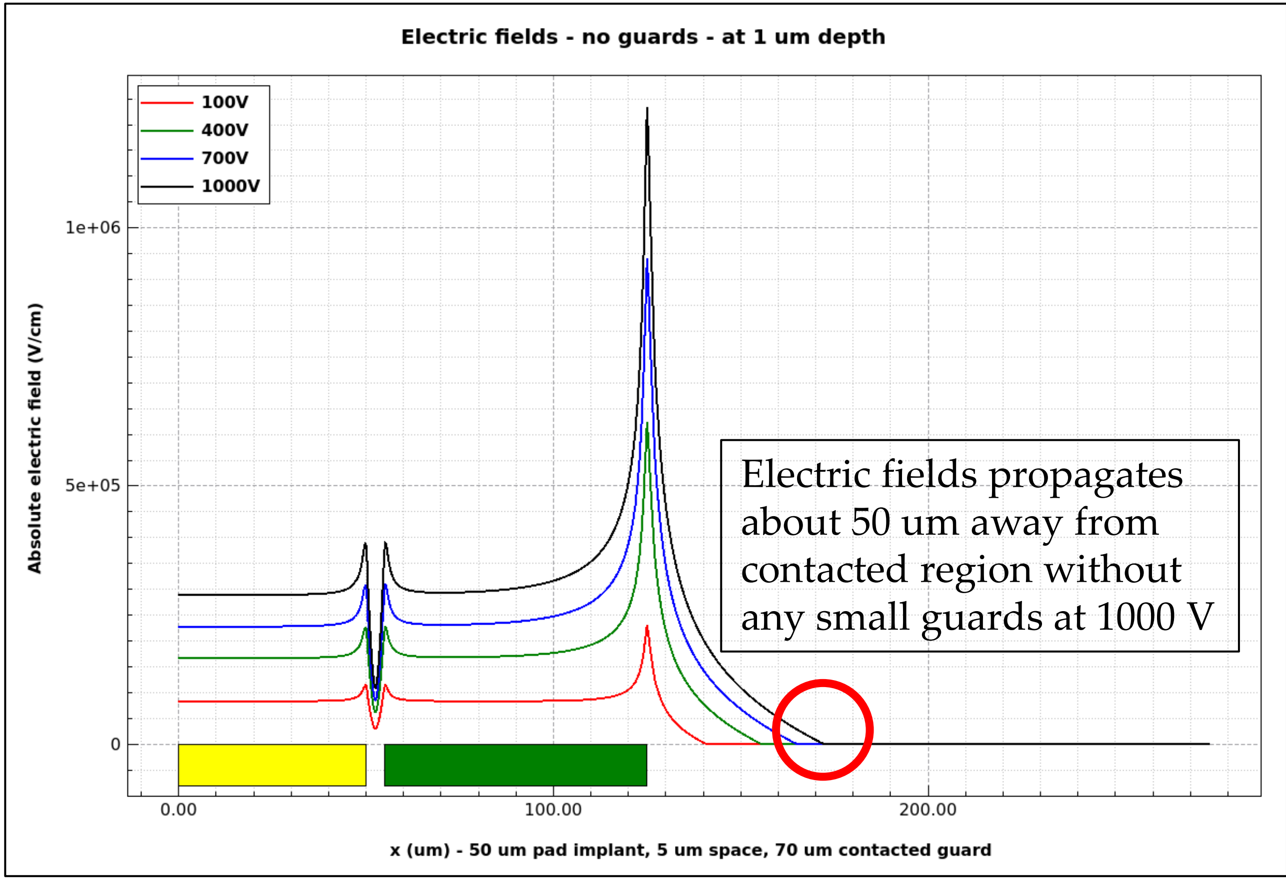
Preliminary results:

- Capacitance is comparable
- Measurements show two “knees” due to the double oxide structure
- Lower oxide charges at interface seem to fit better
- This makes sense due to the thermal oxide at the device
- Further simulation needed



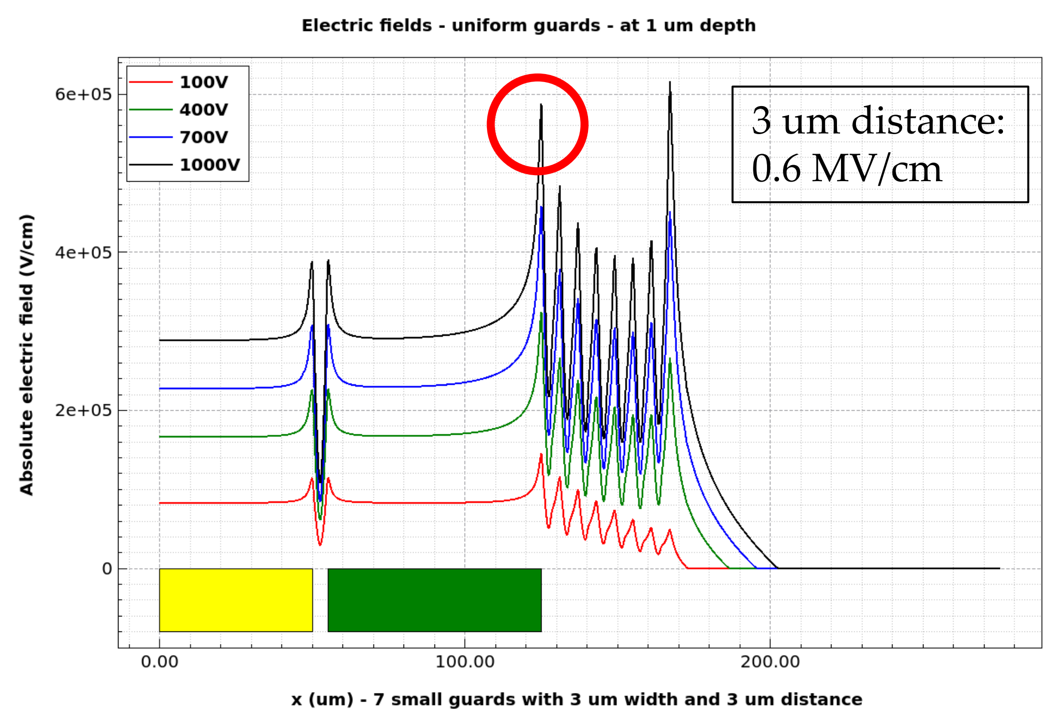
Electric field propagation (1µm depth)

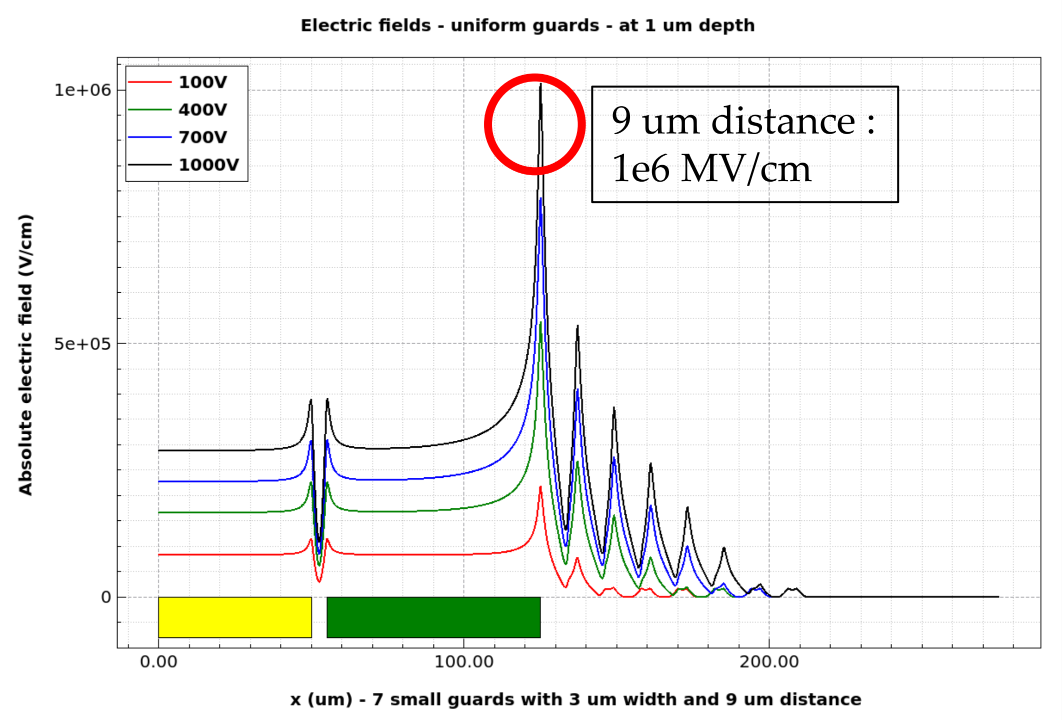
- Without any small guards, we get a peak field right after the biased collector
- This field value is the highest observed value for all structures
- Without any small guards, the electric field propagates to about 50 um after the contacts



Electric field propagation (1µm depth)

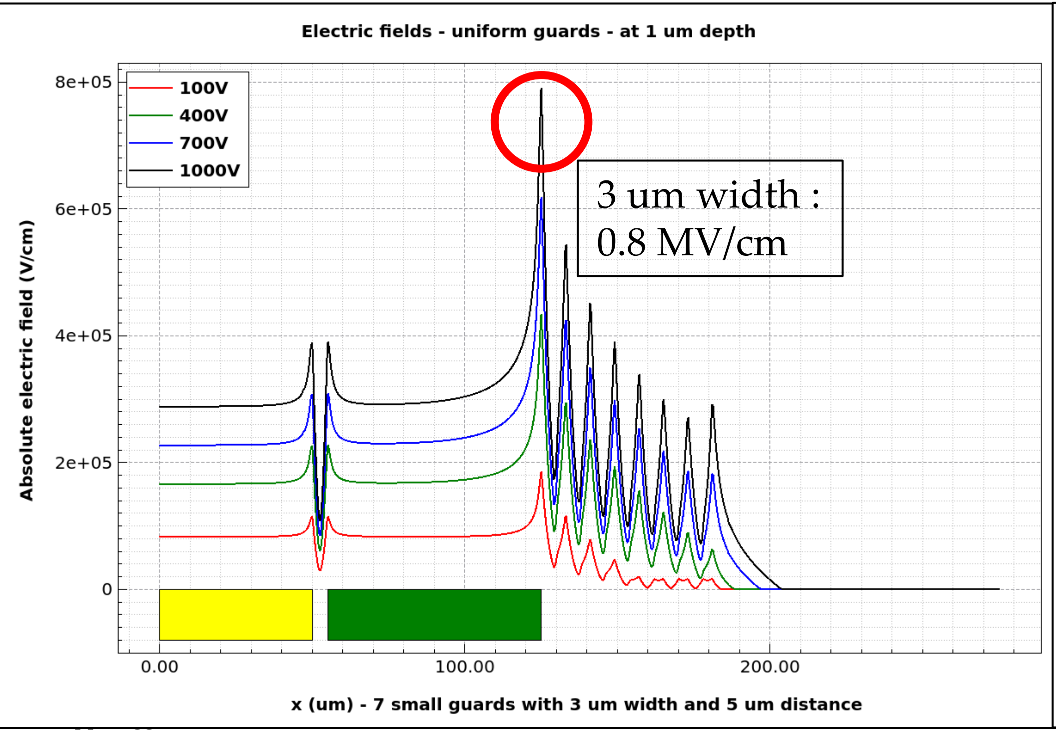
– Small **inter-guard-distances** efficiently weaken the fields directly after the contacted region

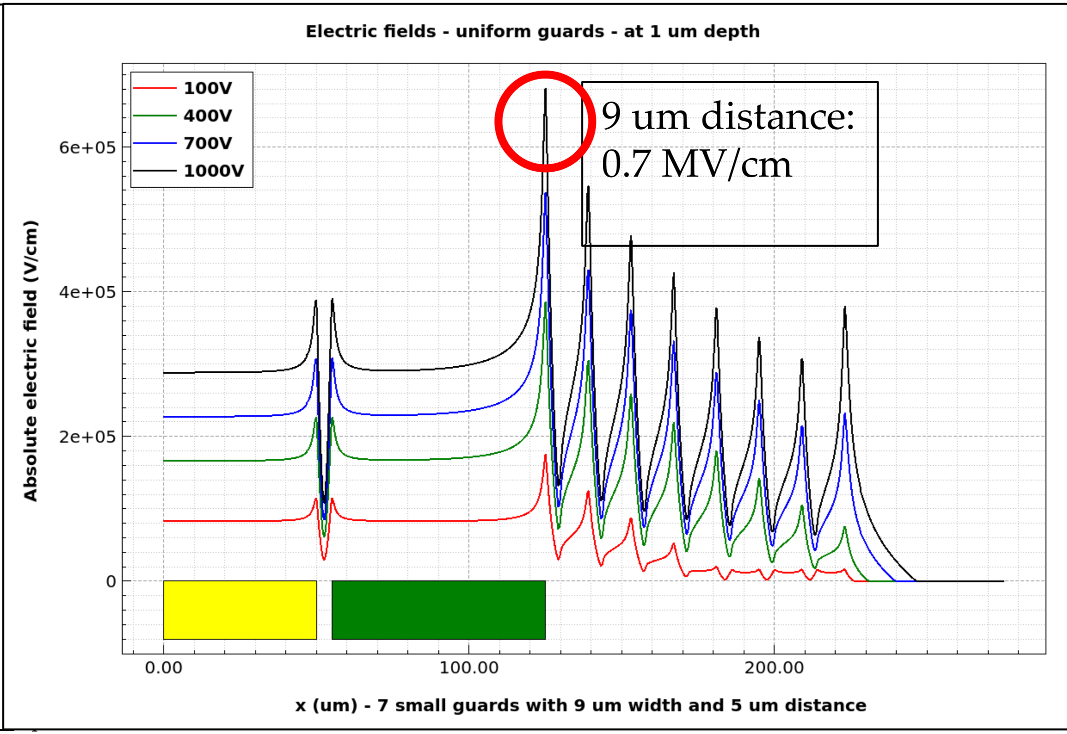




Electric field propagation (1μm depth)

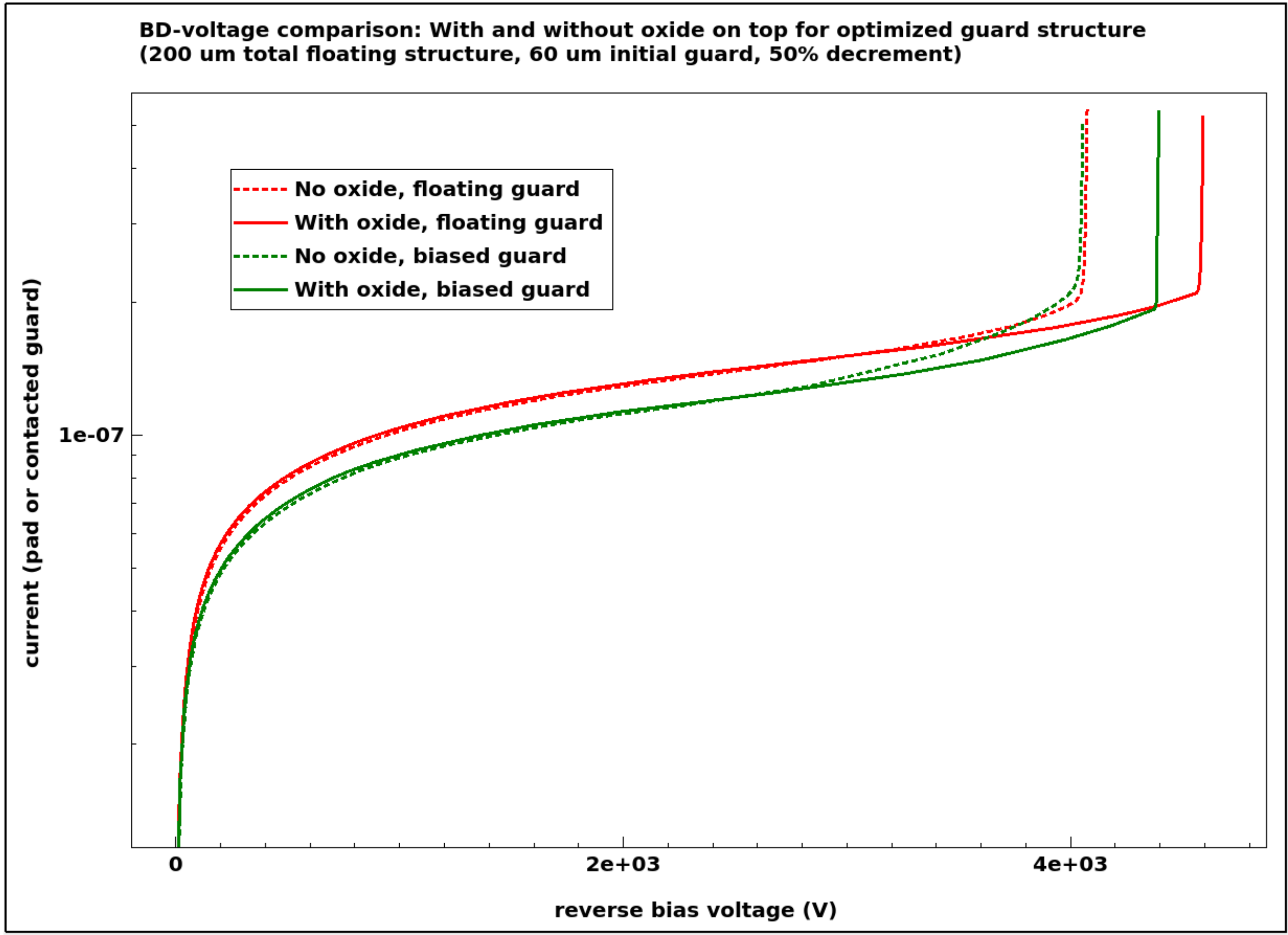
– Regarding the **guard-widths**: Broader guards lower the peak field after the contact better



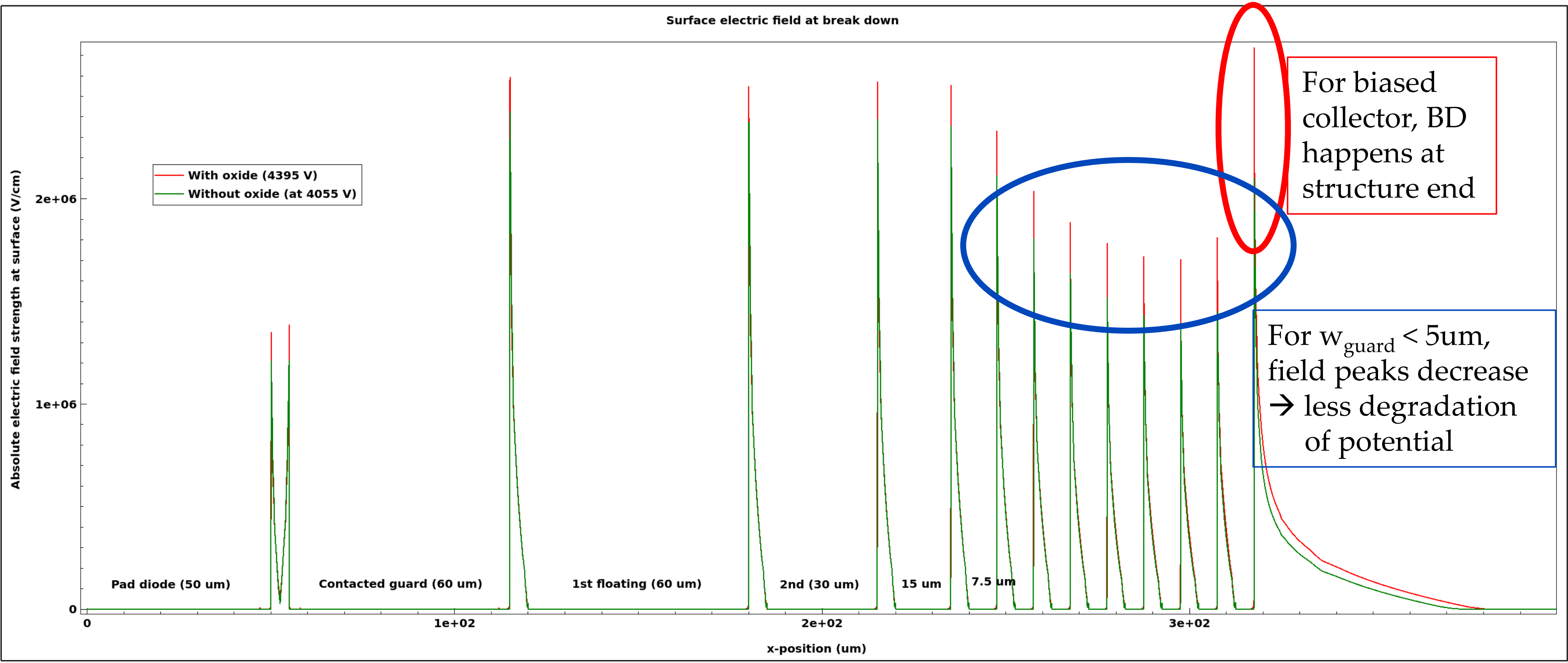


Increment for guard distances

- A higher BD-voltage could be reached after including the oxide
- **No-oxide: 4083 V**
  oxide-floating: 4593 V
  oxide-biased: 4394 V
  50 um: +120 V
- Different BD for biased and floating guard (collector) indicate we can improve further



Increment for guard distances

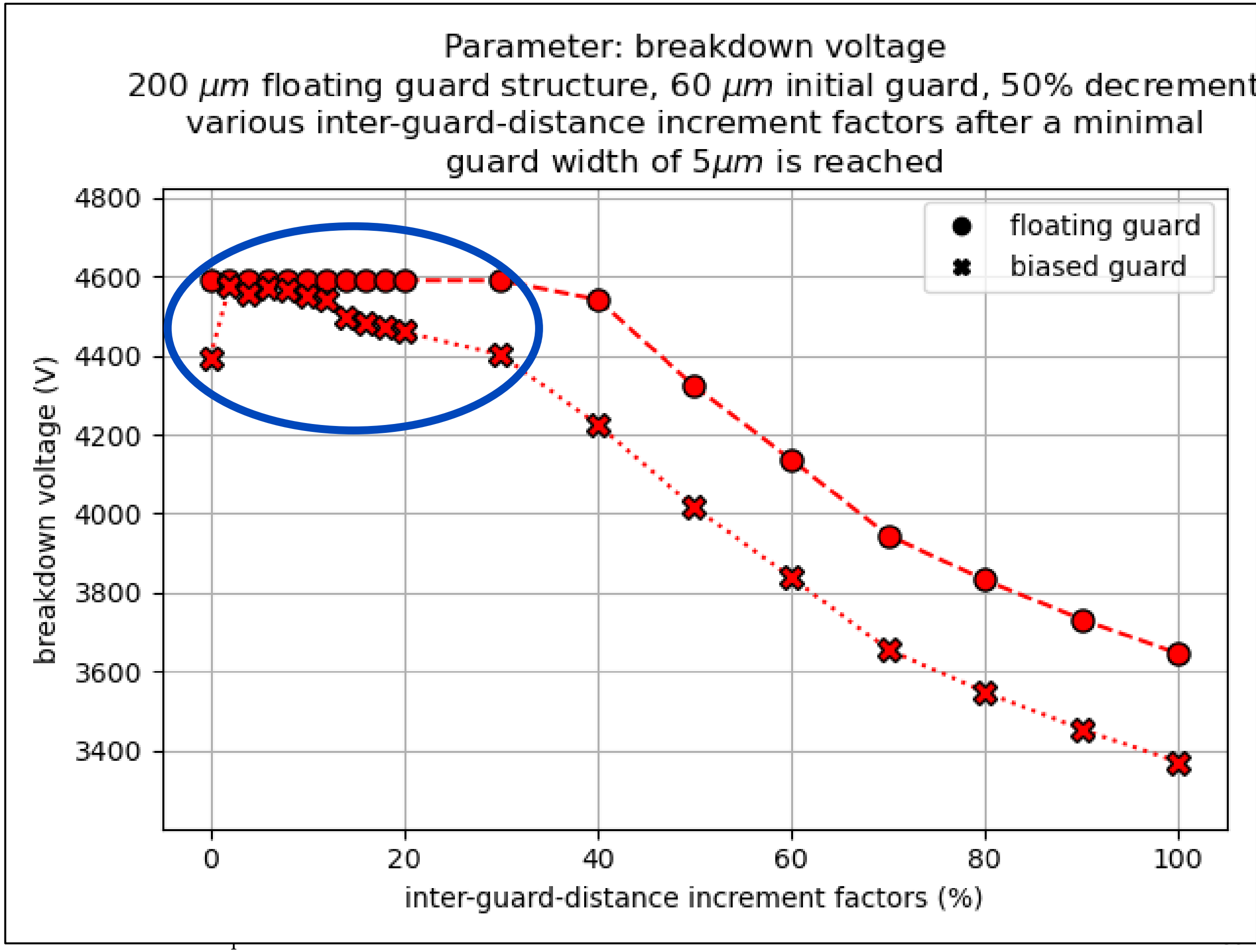


For biased collector, BD happens at structure end

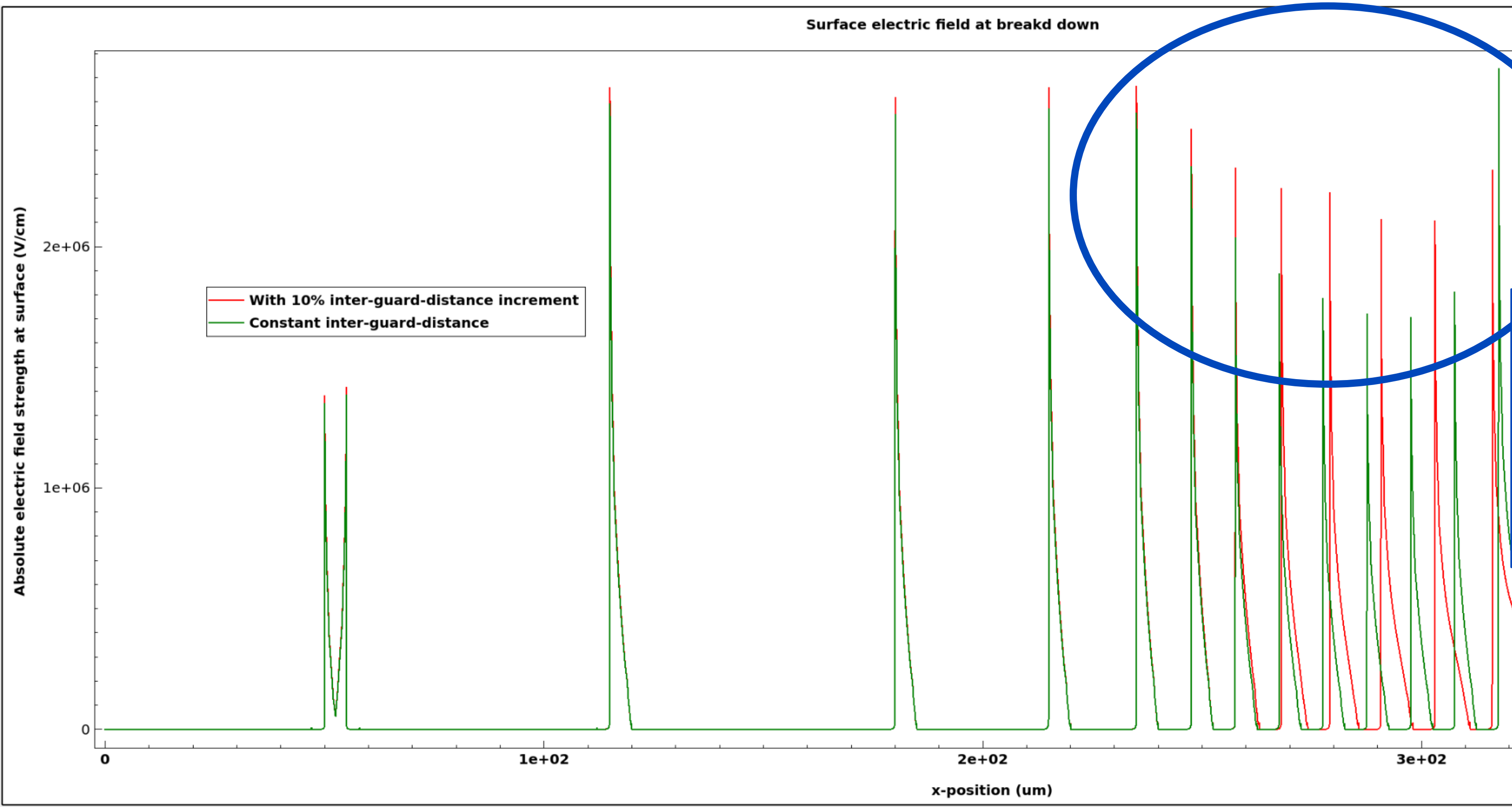
For $w_{guard} < 5$um, field peaks decrease → less degradation of potential

Increment for guard distances

- Simulation run: increment = [0%-100%]
- Obtain a nice optimum between 2.5%-12.5%
- For this structure, BD-behavior for biased and floating collector are (almost) equal again



Increment for guard distances



After introduction of a distance increment, field peaks become more balanced and Potential deterioration is improved

4H-SiC Samples

- Planar 4H-SiC p-in-n diodes from run 13575 of CNM Barcelona [2]
- 3 x 3 mm² active area, 50 µm epi
- Full depletion voltage : 300-400 V, C_{det} = 18 pF
- Neutron irradiated ($5 \cdot 10^{14} – 1 \cdot 10^{16}$ n_{eq}) at ATI Vienna
- Characterization after neutron irradiation [13, 14]