A TCAD Simulation Framework for DLTS-based Defect Characterisation in Solid-State Particle Detectors

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Outline

- Motivations
- DLTS-based defect characterisation
- TCAD simulation framework
  - ☐ case studies and simulation setup
  - ☐ challenges and solutions
- Simulation results and their validation
- Summary
- Next Steps

Motivations

TCAD simulation **framework** for **defect characterisation**

- Solid-state **particle detectors** in **future** high-luminosity **collider experiments**

  → increasing radiation levels demand **robust** and **accurate predictive models** for designing and optimising the **detector operation** under **extreme fluences** (above 10^{16} 1 MeV n_{eq}/cm^2).

- A **TCAD** simulation **framework** for **defect characterisation** that enables

  → the **extraction** and **refinement** of **trap parameters** (i.e. *concentration* $\mathbf{N_t}$, thermal *activation energy* $\mathbf{E_A}$, and *capture cross-sections* $\boldsymbol{\sigma_{e,h}}$)

  → systematic **assessment** of the "**effectiveness**" of each **trap** in **reproducing** key device-level **observables** (i.e. leakage current, depletion voltage, and charge collection efficiency)

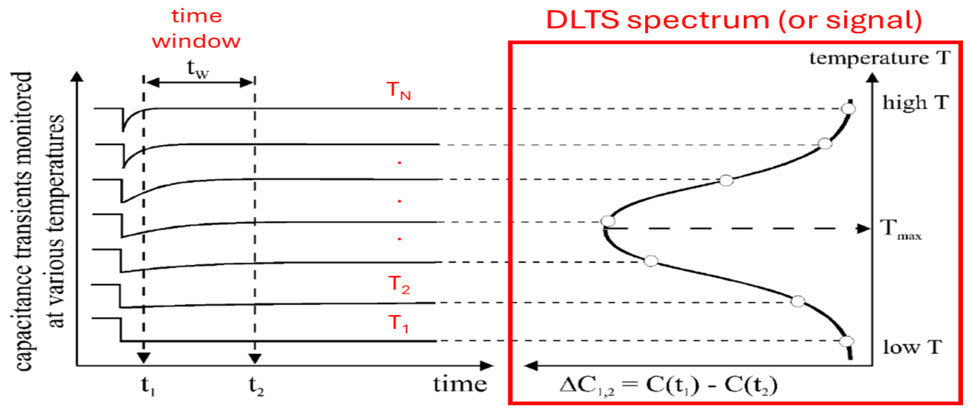
General-purpose TCAD radiation damage model applicable across **different semiconductor materials** (e.g. silicon, silicon carbide, etc.) and **fluence regimes**
→ enhancement of the **predictive power** of **simulation tools**, supporting the **development** of **radiation-hard detectors** for future collider experiments.

DLTS-based defect characterisation

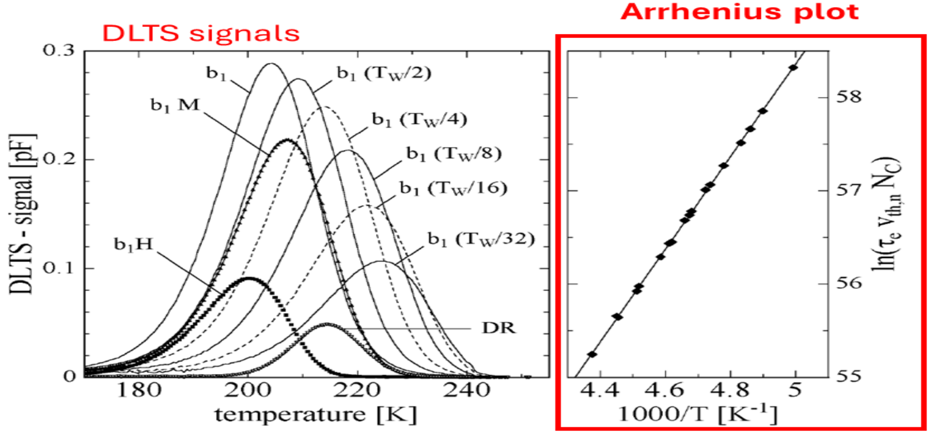
Deep-**L**evel **T**ransient **S**pectroscopy (**DLTS**) – in a nutshell

- **Method**:
  - ☐ ***Current*** (**I-DLTS**) or ***Capacitance*** (**C-DLTS**) based technique
  - ☐ **Measure** change in **current** or **capacitance transients** due to **de-trapping** of **charges from defects** at different temperatures
- **Filling recipes**:
  - ☐ ***Forward* biasing** → *majority* and *minority* carriers
  - ☐ “Zero” biasing → *majority* carriers
  - ☐ ***Light* injection** → *majority* and/or *minority* carriers
- **Results**:
  - ☐ **N_t** (amplitude of current/capacitance transients)
  - ☐ **E_A** (*Arrhenius* relation from transients)
  - ☐ **$\sigma_{e,h}$** (*Arrhenius* relation from transients)

“Double boxcar” method



“Correlator functions” method



Niels Sorgenfrei, *Radiation Damages in Silicon: Acceptor Removal Effect and the X-Defect*, CERN EP R&D Seminar, 01.09.25

M. Moll - PhD thesis 1999

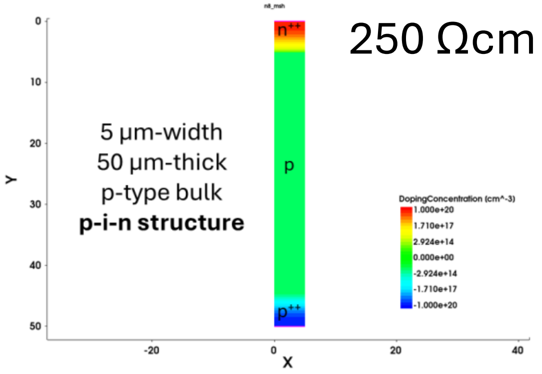
See appendix for more details on DLTS methods

TCAD simulation framework

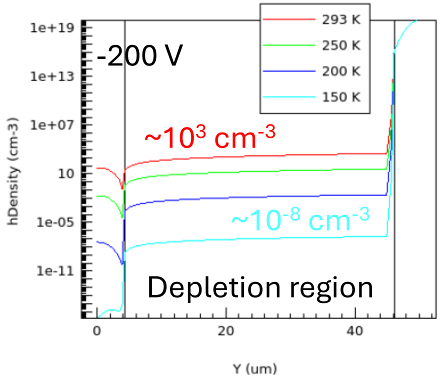
The **developed framework** – in a nutshell

- **Reproduction** of ***I-DLTS* spectra**, i.e. based on ***current* transient measurements** following **laser-induced** charge **carrier injection** in silicon ***p-i-n*** diode – ***C_iO_i*** and ***B_iO_i*** defects.

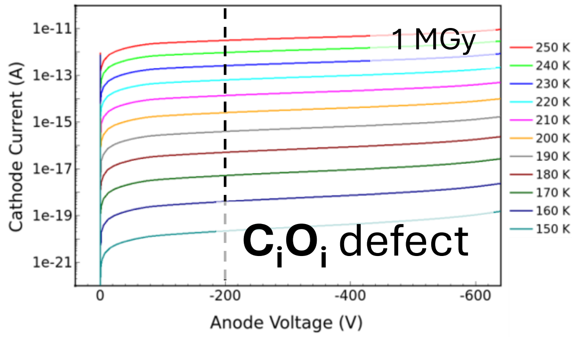
Layout **and *Doping Concentration***



Majority Carrier Density



Current-Voltage (I-V)



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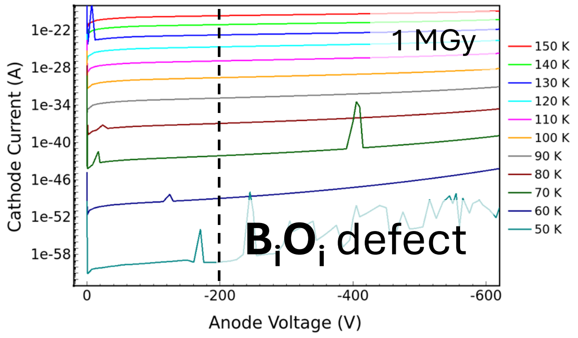
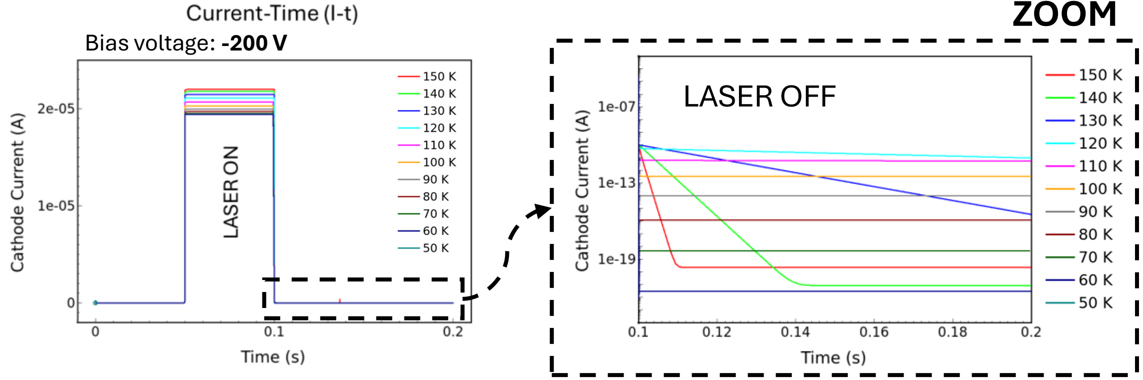


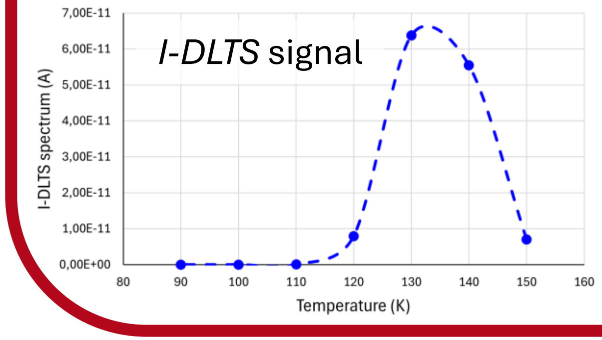
Example: B_iO_i defect @ 1 MGy

Current-Time (I-t)

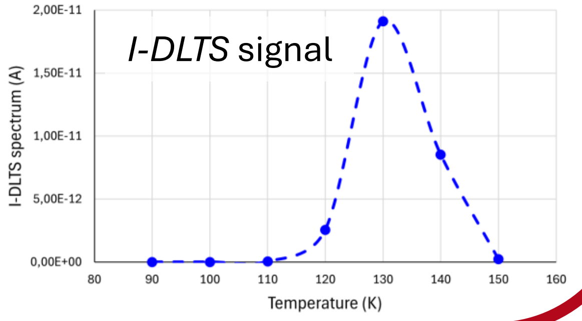
Bias voltage: **-200 V**



"Double Boxcar" Method



"Correlator Function" Method

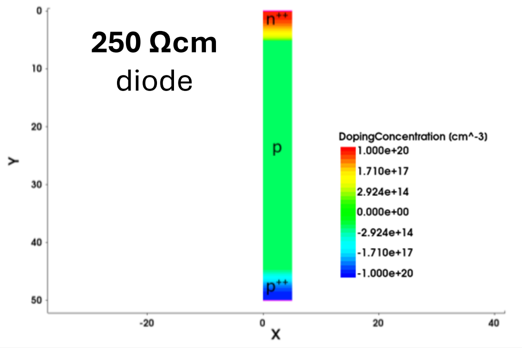


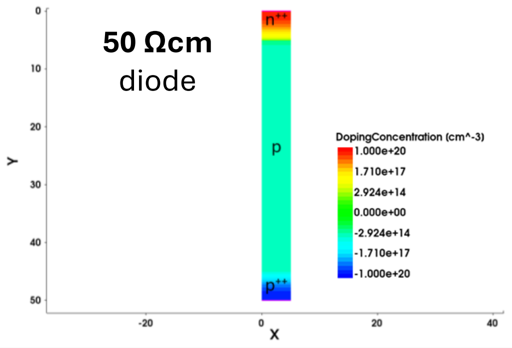
Case studies and simulation setup (1/2)

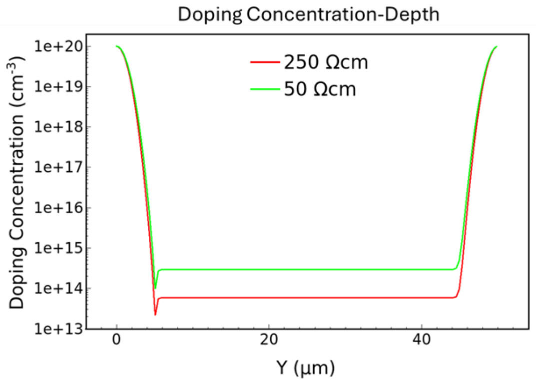
Device Under Test (DUT) – silicon *p-i-n* diode

Layout and **bulk resistivity**

- ☐ **5 µm**-width and **50 µm**-thick structure
- ☐ **250 Ωcm** and **50 Ωcm** *p-type* epitaxial



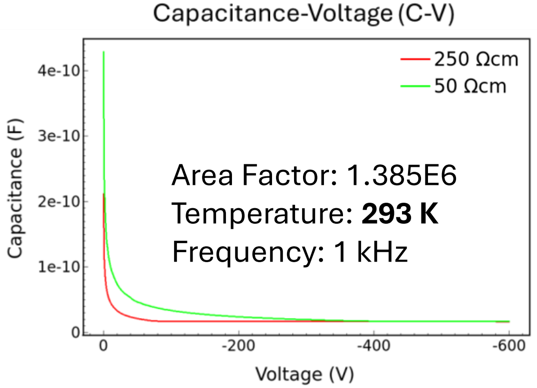




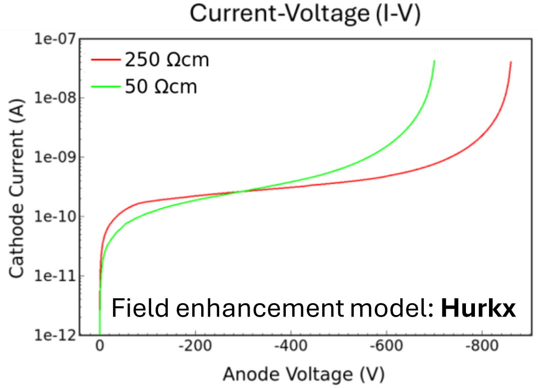
Two different **bulk resistivities** (i.e. bulk **doping concentrations**)

Analyses: before irradiation

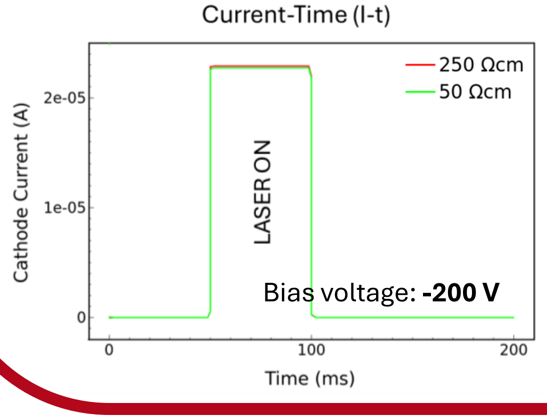
☐ Small-signal (**AC**)



☐ Steady-state (**DC**)



☐ Time-Variant (**TV**)



***Optical* stimulus**

- Monochromatic source (**laser**)
- Wavelength: 800 nm (**near IR**)
- Duration: **50 ms**
- Transition: 50 ns
- Intensity: 6E-4 W/cm^2

Case studies and simulation setup (2/2)

Trap **U**nder **T**est (**TUT**) – *C_iO_i* and *B_iO_i* defects

- **Defects' parameters** obtained from *C-DLTS* measurements of γ-irradiated p-type silicon diodes

Parameter/Defect		**C_iO_i**		**B_iO_i**	
Defect Type		Donor, *hole* trap		Donor, *electron* trap	
Temperature Range (average)		162 – 211 K		108 – 143 K	
Thermal Activation Energy		E_v + 0.36 eV		E_c - 0.25 eV	
***Electron* Capture Cross-Section**		2E-18 cm^2		6E-15 cm^2	
***Hole* Capture Cross-Section**		2E-15 cm^2		6E-18 cm^2	
Bulk resistivity		**250 Ωcm**	**50 Ωcm**	**250 Ωcm**	**50 Ωcm**
Concentration (vs. Dose)	**10 Mrad (0.1 MGy)**	4.40E+11 cm^{-3}	1.02E+11 cm^{-3}	4.38E+11 cm^{-3}	6.16E+11 cm^{-3}
	100 Mrad (1.0 MGy)	5.24E+12 cm^{-3}	1.51E+12 cm^{-3}	4.79E+12 cm^{-3}	5.80E+12 cm^{-3}
	200 Mrad (2.0 MGy)	1.03E+13 cm^{-3}	2.79E+12 cm^{-3}	9.43E+12 cm^{-3}	1.11E+13 cm^{-3}

Anja Himmerlich et al.: *Defects and acceptor removal in ^{60}Co γ-irradiated p-type silicon* (link)

100 rad = 1 Gy

Challenges and solutions (1/3)

Temperature and **charge density** – *DC* analysis

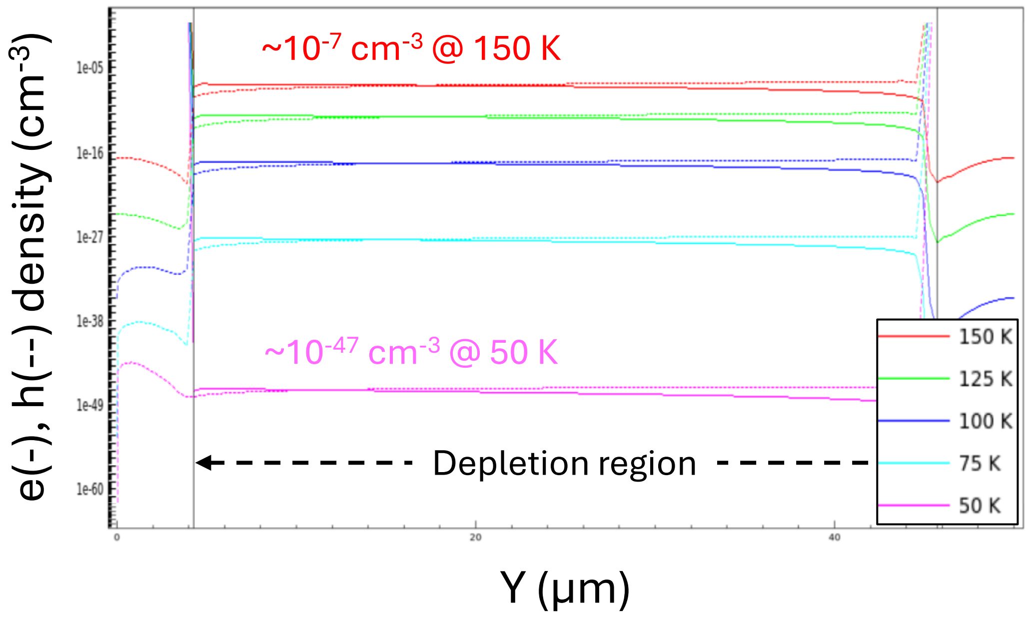
- **Low** values of **temperature** and **charge carrier density** → **convergence *issues*** & **numerical *spikes***

Example: 250 Ωcm diode, **B_iO_i** defect **@ 1 MGy**

☐ **numerical strategies** to ensure convergence

- *ExtendedPrecision* 128-bit, no. *Digits* 25, no. *Iterations* 20, *Blocked* and *ILS* Methods, *ErrRef(e,h)* 1E-50, *RhsMin* 1E-100

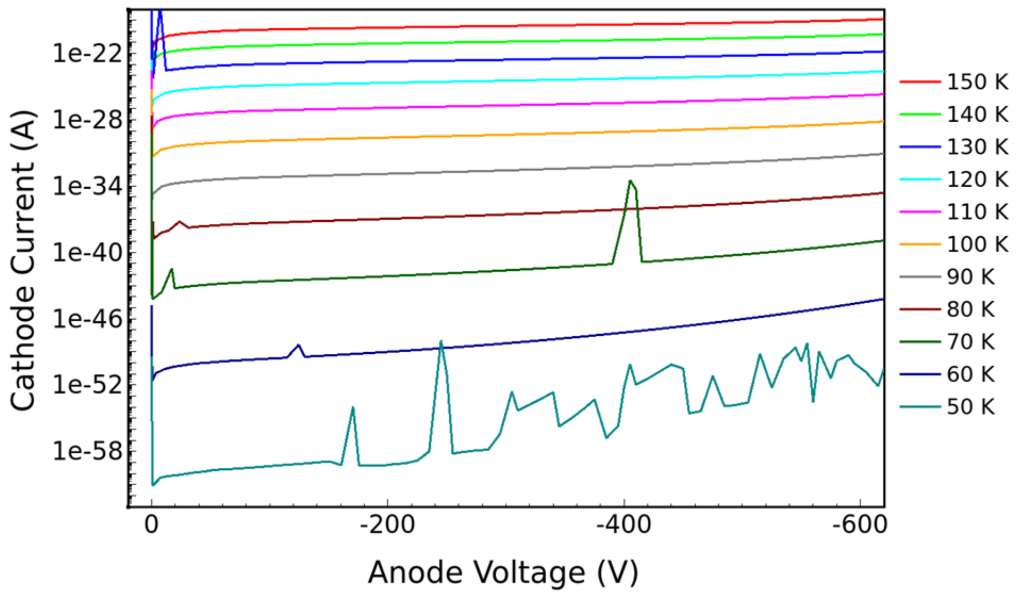
Majority (h) & Minority (e) Density @ -100 V


~10^{-7} cm^{-3} @ 150 K

~10^{-47} cm^{-3} @ 50 K

Depletion region

Current-Voltage (I-V)



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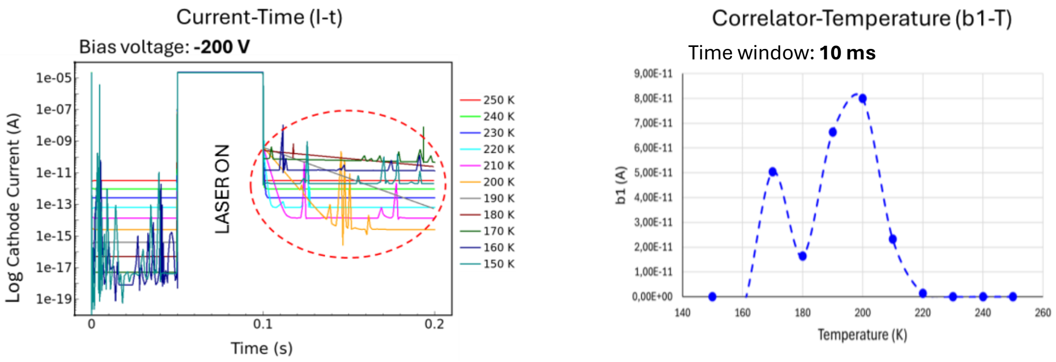
250 Ωcm diode, **C_iO_i** defect **@ 1 MGy**



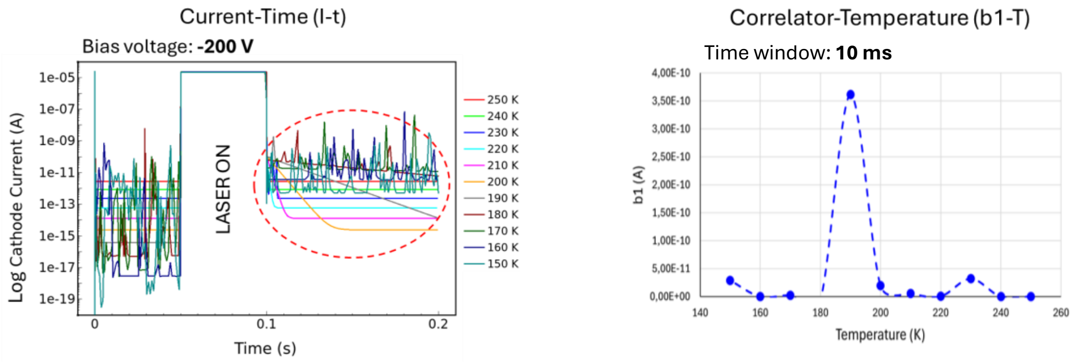
Current-Time (I-t)

Bias voltage: **-200 V**

Correlator-Temperature (b1-T)

Time window: **10 ms**

50 Ωcm diode, **C_iO_i** defect **@ 1 MGy**



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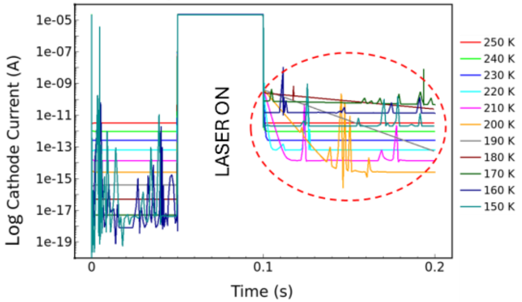

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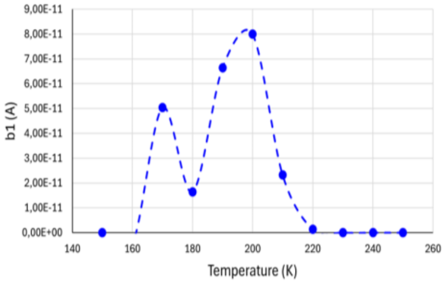

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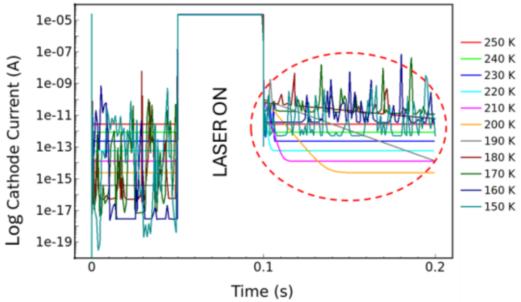

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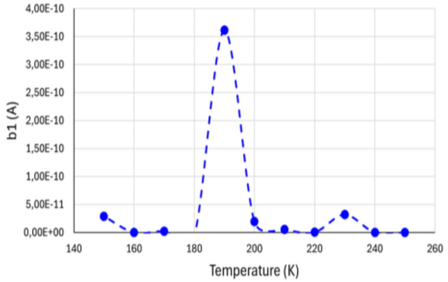
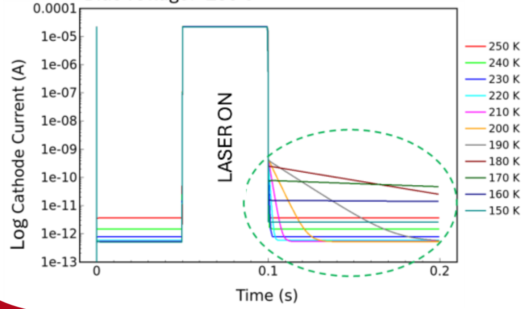


Constant **C**arrier **G**eneration (**CCG**) model → artificially **increasing** of **carrier generation rate** (cm^{-3} s^{-1})

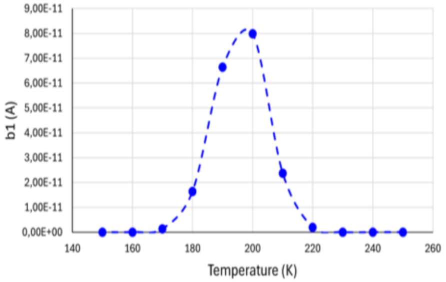
Current-Time (I-t)

Bias voltage: **-200 V**



Correlator-Temperature (b1-T)

Time window: **10 ms**



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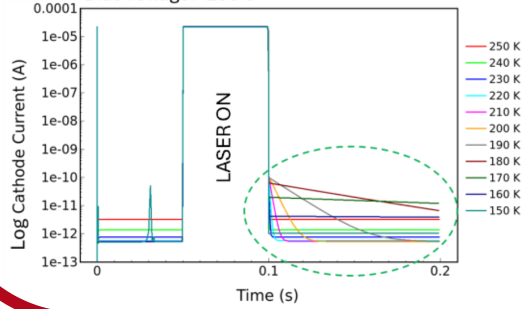

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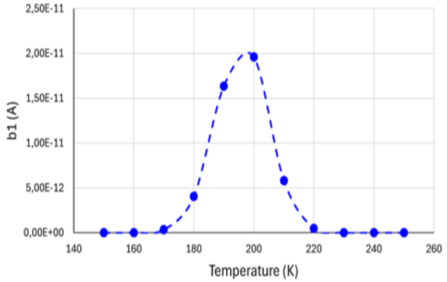

Challenges and solutions (3/3)

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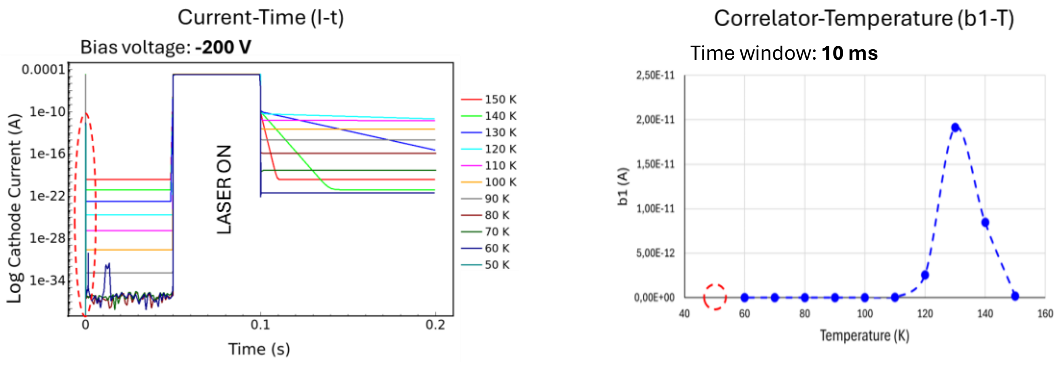
250 Ωcm diode, **B_iO_i** defect **@ 1 MGy**



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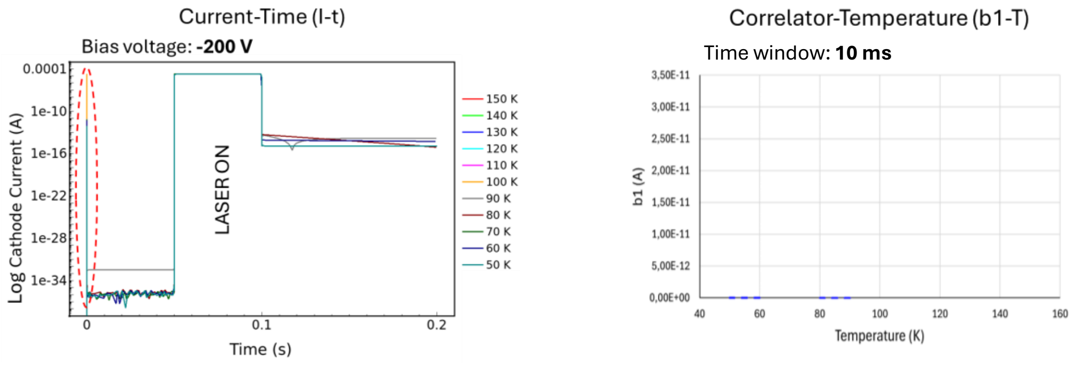

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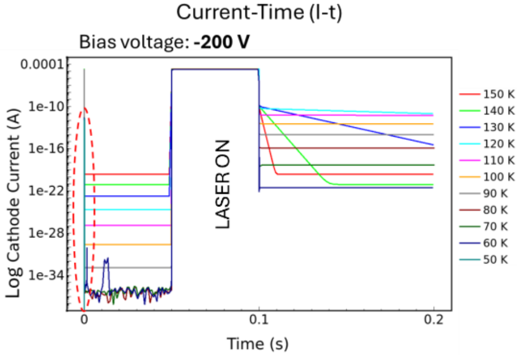
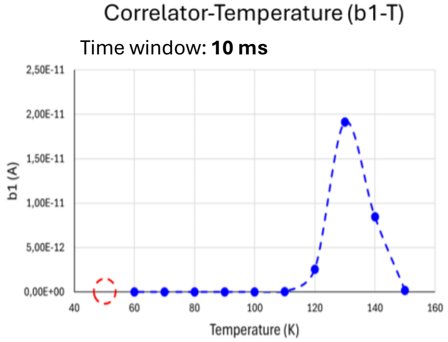

Current-Time (I-t)

Bias voltage: **-200 V**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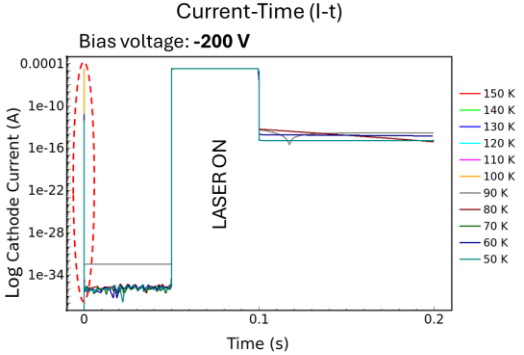
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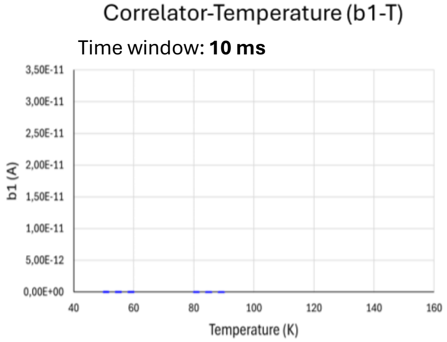
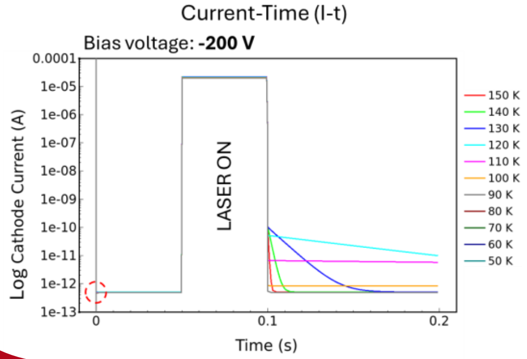

Correlator-Temperature (b1-T)

Time window: **10 ms**

CCG model + **numerical strategies** (e.g. *RhsFactor* 1E100 & *RhsMax* 1E30)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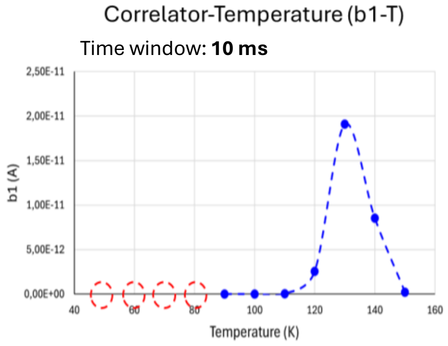
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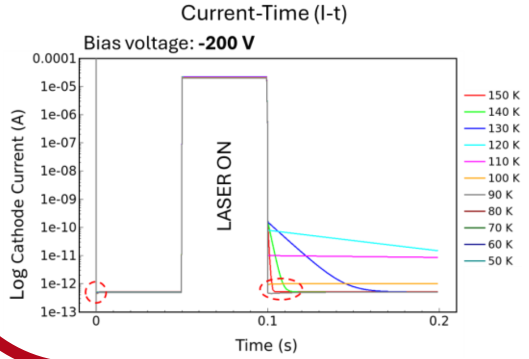
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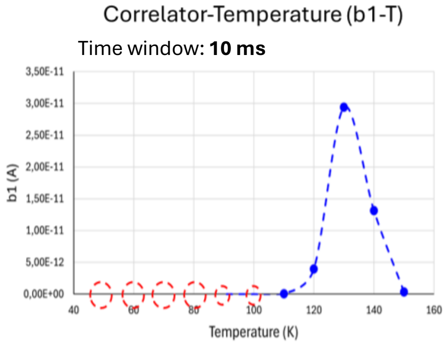

Correlator-Temperature (b1-T)

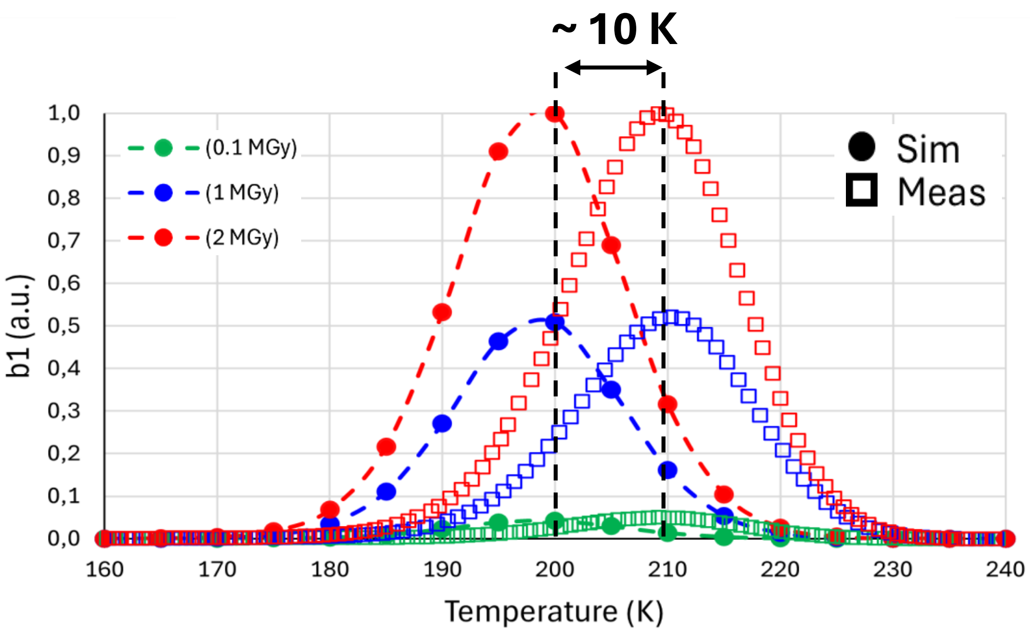
Time window: **10 ms**

Simulation results and their validation (1/2)

I-DLTS spectra, C_iO_i defect – *simulation* vs. *measurement*

- **Evaluation** of the **reliability** of the **TCAD simulation framework** using **I-DLTS measurements**

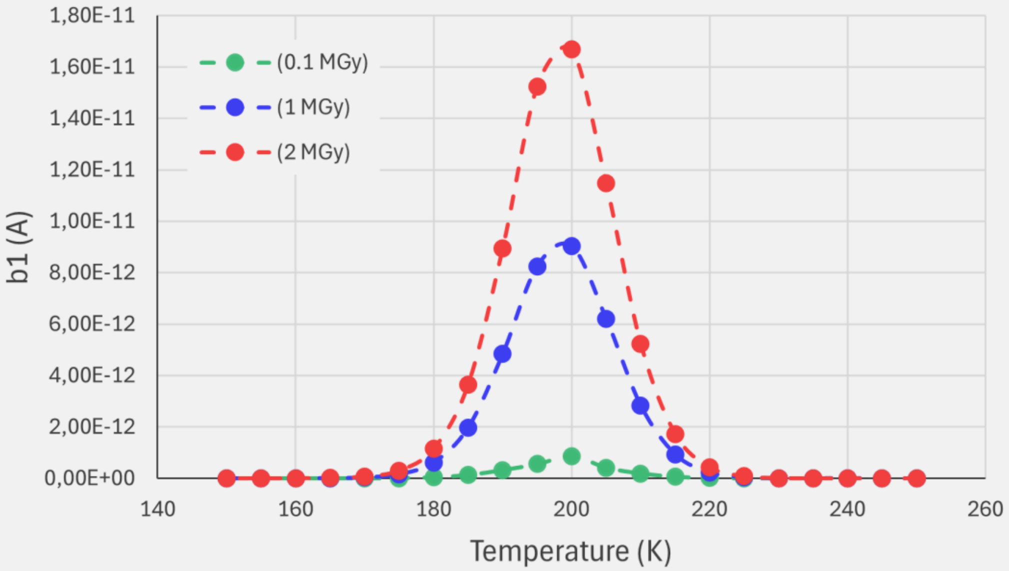
250 Ωcm diode, **C_iO_i** defect **@ 0.1,1 & 2 MGy**



UR = **-100 V**, t_P = **10 ms**, t_0 = **1 ms**, T_W = **10 ms**

50 Ωcm diode , **C_iO_i** defect **@ 0.1,1 & 2 MGy**

ONGOING MEASUREMENTS!



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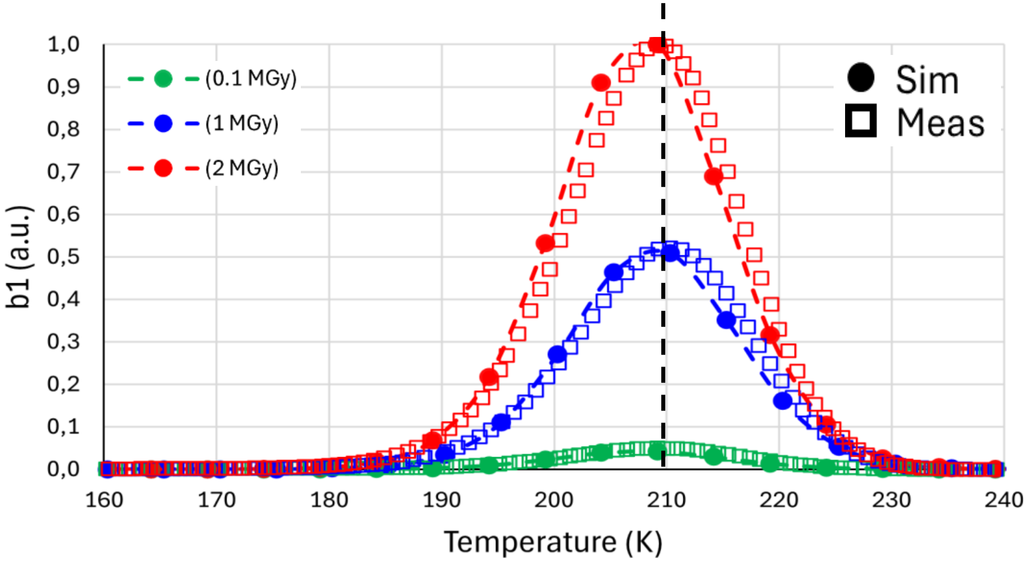
Sim shift **~ 10 K**



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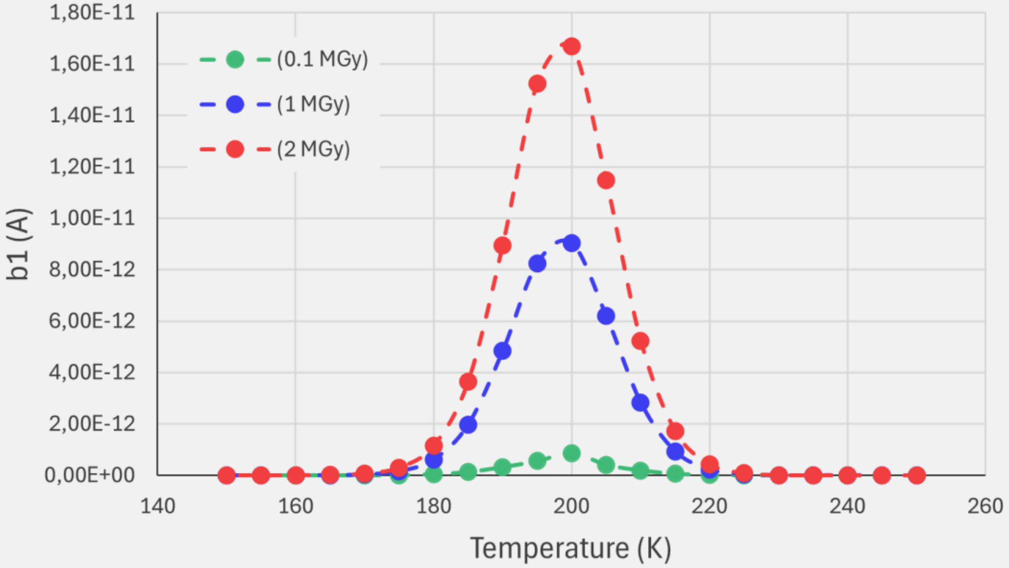

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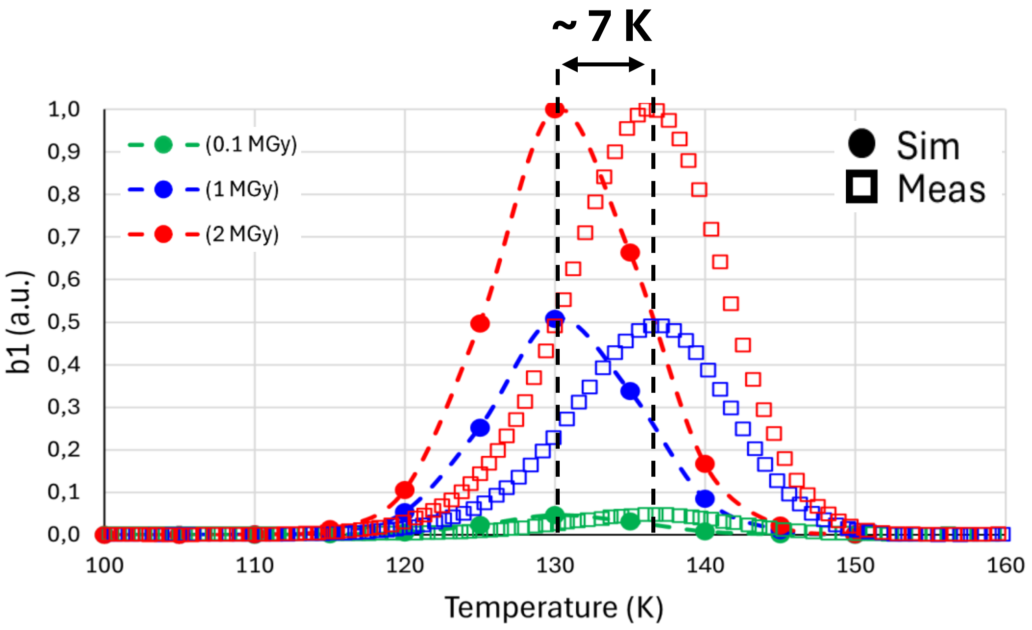

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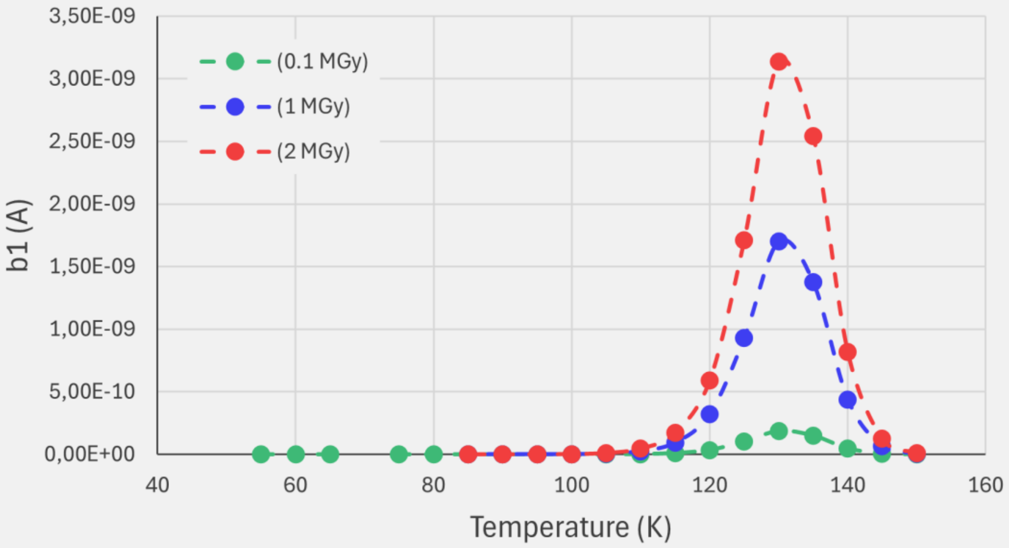
50 Ωcm diode , **B_iO_i** defect **@ 0.1,1 & 2 MGy**

ONGOING MEASUREMENTS!



UR = **-100 V**, t_P = **10 ms**, t_0 = **1 ms**, T_W = **10 ms**

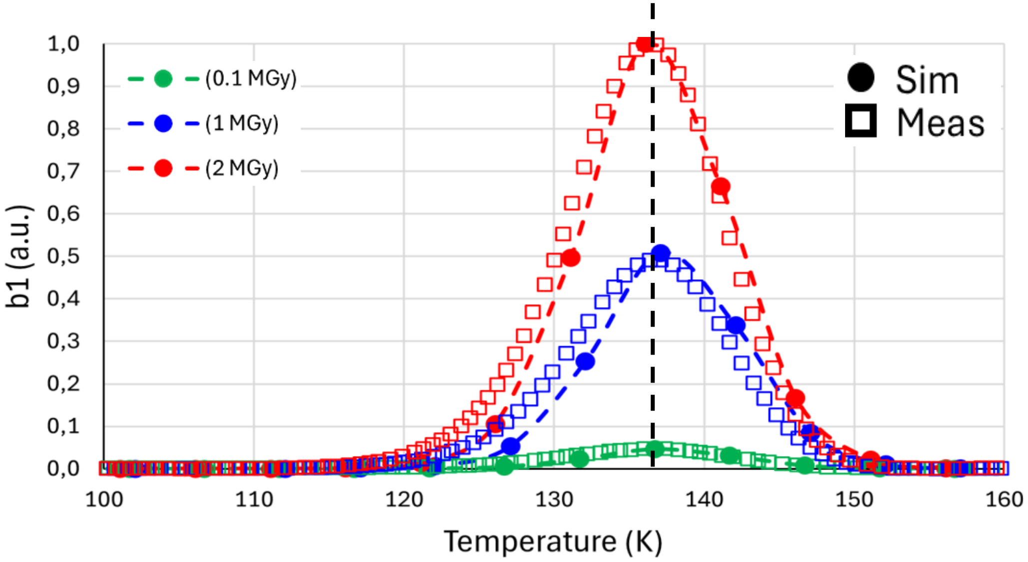
Simulation results and their validation (2/2)

I-DLTS spectra, B_iO_i defect – *simulation* vs. *measurement*

- **Evaluation** of the **reliability** of the **TCAD simulation framework** using **I-DLTS measurements**

250 Ωcm diode, **B_iO_i** defect **@ 0.1,1 & 2 MGy**

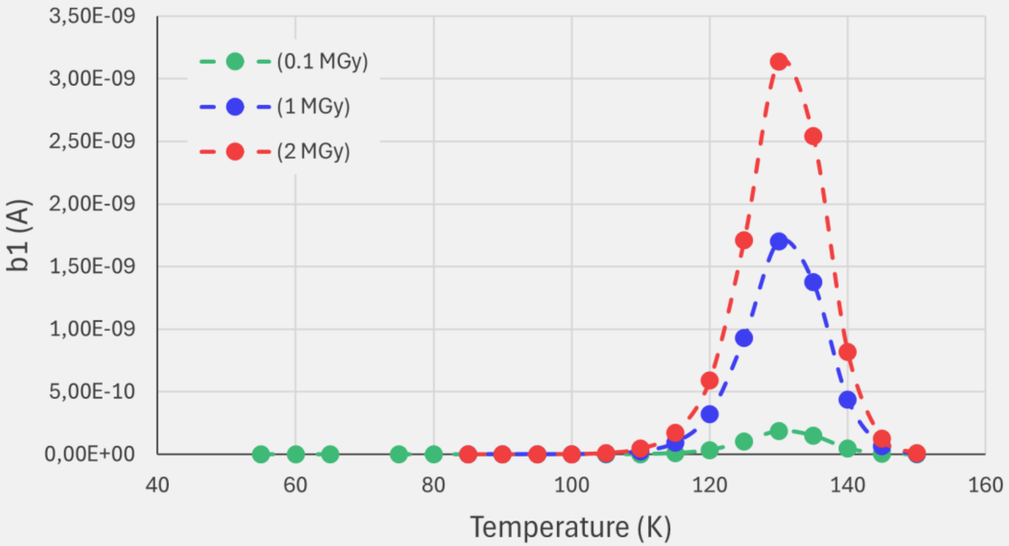
Sim shift **~ 7 K**



UR = **-100 V**, t_P = **10 ms**, t_0 = **1 ms**, T_W = **10 ms**

50 Ωcm diode , **B_iO_i** defect **@ 0.1,1 & 2 MGy**

ONGOING MEASUREMENTS!



UR = **-100 V**, t_P = **10 ms**, t_0 = **1 ms**, T_W = **10 ms**

Summary

- A **TCAD simulation framework** for **DLTS-based defect characterisation** is under development…
- **I-DLTS spectra** of **C_iO_i** and **B_iO_i defects** have been **reproduced** in **p-type silicon** p-i-n diodes with different **bulk resistivities** (250 and 50 Ωcm) at various **irradiation doses** (0.1, 1 and 2 MGy)
- **Numerical strategies** and **specific workarounds** have been **implemented to ensure convergence** at cryogenic temperatures (< 250 K), including
  - ❑ Tuning of **mathematical parameters** (e.g. extended precision floating-point arithmetic, no. Newton Iterations, numerical methods, error criteria)
  - ❑ Artificial **increase** of **carrier generation rate** (i.e. Constant Carrier Generation model)
- **Simulation** results have been **validated** against **experimental data**
  - ❑ A **systematic shift** in **peak positions** (i.e. extracted time constant) has been observed and is under investigation (e.g. **parameters** used by **TCAD models** to extract values)

Next steps

- ***Evaluate* TCAD performance** in simulating **defect behaviour** at **very low temperatures** (e.g. I_2O defect in the 25-75 K range)
- ***Test*** the **developed framework** with **C_iO_i** and **B_iO_i defects** at **higher irradiation doses** (e.g. 5 MGy)
- ***Validate*** the **framework** by **comparing Arrhenius plots** from **simulations** and experimental **measurements**
- ***Reproduce* C-DLTS** spectrum **measurements**
  - ❑ Find a robust procedure for ***capacitance* extraction during *transient*** simulations
  - ❑ Challenge ahead: **small-signal analysis** and **transient** simulations **at cryogenic temperatures**

Thanks for your attention!

A TCAD Simulation Framework for DLTS-based Defect Characterisation in Solid-State Particle Detectors

T. Croci [a,*], F. Rizwan [e], A. Fondacci [b,a], Y. Gurimskaya [g,e], M. Moll [e],
A. Morozzi [a], F. Moscatelli [c,a], D. Passeri [d,a], N. Sorgenfrei [e,f]

(a) Istituto Nazionale di Fisica Nucleare (**INFN**), Perugia Unit, Perugia, Italy
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(c) Consiglio Nazionale delle Ricerche – Istituto Officina dei Materiali (**CNR-IOM**), Perugia Unit, Perugia, Italy
(d) Department of Engineering, University of Perugia (**UNIPG**), Perugia, Italy
(e) European Organization for Nuclear Research (**CERN**), Geneva, Switzerland
(f) Institute of Physics, University of Freiburg (**ALU-FR**), Freiburg, Germany
(g) **Solestial**, Tempe, Arizona, USA

* **Corresponding author** tommaso.croci@pg.infn.it (T. Croci)

Backup

C-DLTS *transient analysis: Double boxcar method*

(from Michael Moll's PhD thesis, Ch. 4, Para. 4.4, pp. 81-88)

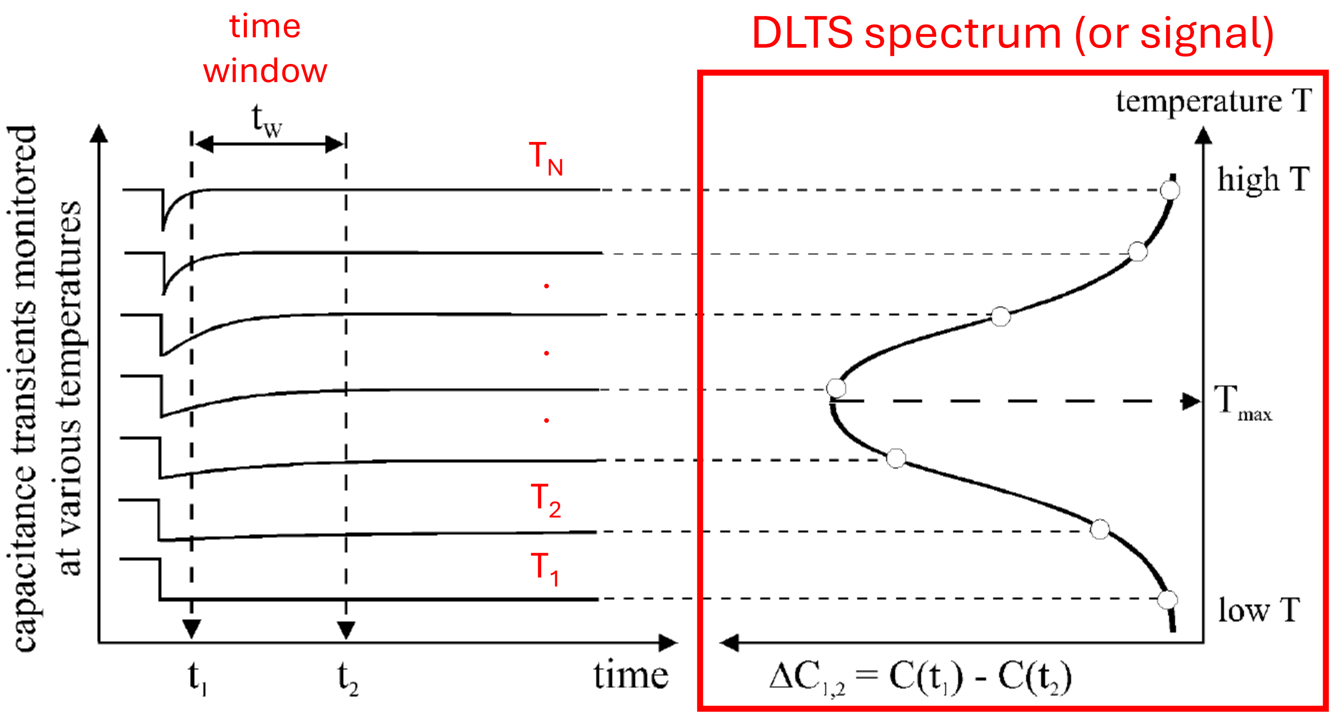


Figure 4.9: The left-hand side shows capacitance transients at various temperatures, while the right-hand side shows the corresponding DLTS signal resulting from using the double boxcar to display the difference between the capacitance at time t_1 and the capacitance at time t_2 as a function of temperature (after [Lan74]). **NB**: after filling pulse, t_p, and delay period t_0

Emission time constant, τ_e, at the **peak maximum temperature**, T_{max}, in the DLTS spectrum **@ time window**

$$\boxed{\tau_e(T_{max}) = \frac{t_1 - t_2}{\ln\left(\frac{t_1}{t_2}\right)}. \qquad (4.16)}$$

Double boxcar integrator method: consists of taking the difference between the measured capacitance, $\Delta C_{1,2} = C(t_1) - C(t_2)$, at two precise moments (t_1 and t_2), **NB**: **after** the filling pulse, t_p, **and** the delay period, t_0 (see previous slide).

DLTS spectrum: difference $\Delta C_{1,2} = C(t_1) - C(t_2)$ plotted **versus** the temperature, **T**.

- **Zero** @ T_{low} & T_{high} where the emission process is too slow and too fast, respectively.
- **Max** @ T_{max} where the emission time constant, $\tau_e(T_{max})$, fits the chosen time window, t_W, depending on t_1 and t_2 (Eq. 4.16).

Arrhenius plot: can be constructed from a set of data ($T_{max,i}$, $\tau_e(T_{max,i})$) obtained performing several temperature scans with different time windows.

Drawback: the outcoming DLTS signal is fully influenced by the behaviour of the transient signal at the two sampling points.

C-DLTS *transient analysis: Correlator functions* (1/2)

(from Michael Moll's PhD thesis, Ch. 4, Para. 4.4, pp. 81-88)

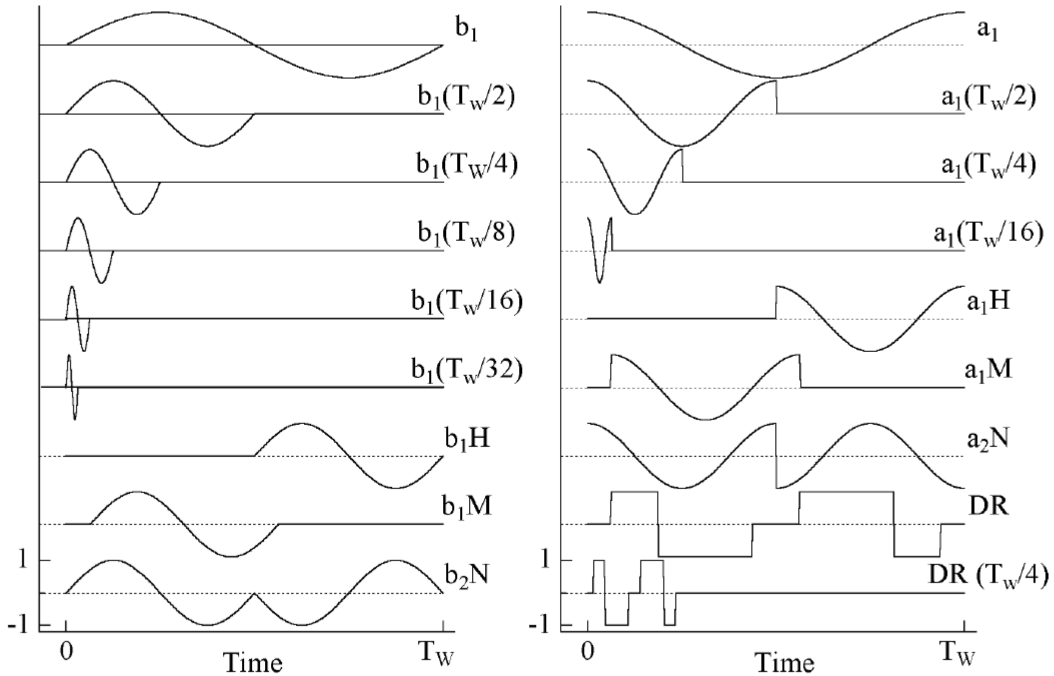


Figure 4.10: The 18 correlator functions used for the *maximum evaluation*.

$$b_1 = \frac{2\,\Delta C_0}{T_W}\int_0^{T_W} \exp\left(-\frac{t+t_0}{\tau_e}\right)\sin\left(\frac{2\pi}{T_W}t\right)dt \qquad (4.17)$$

$$\tau_e(T_{max}) = 0.43 \times T_W. \qquad (4.18)$$

Correlator function: the **complete capacitance transient** is used by **folding** it with a **correlator function**, e.g. a sine, namely by doing the **convolution** between the **measured signal** and a **known function**, called **correlator**. The result is a correlator function, e.g. b_1 (Eq. 4.17), where T_W is the time window.

DLTS spectrum: correlator, e.g. $\mathbf{b_1}$, plotted **versus** the temperature, **T**. NB: in this case, the **emission time constant**, $\tau_e(T_{max})$, can only be **calculated numerically** (Eq. 4.18), where 0.43 corresponds to 512 time bins.

Arrhenius plot: can be constructed from **18 pairs** $(T_{max,i}, \tau_e(T_{max,i}))$ **for each time window** (usually 20, 200 and 2000 ms), by using in total **18 different correlator** functions (Fig. 4.10). See **example** in the next slide.

C-DLTS *transient analysis: Correlator functions* (2/2)

(from Michael Moll's PhD thesis, Ch. 4, Para. 4.4, pp. 81-88)

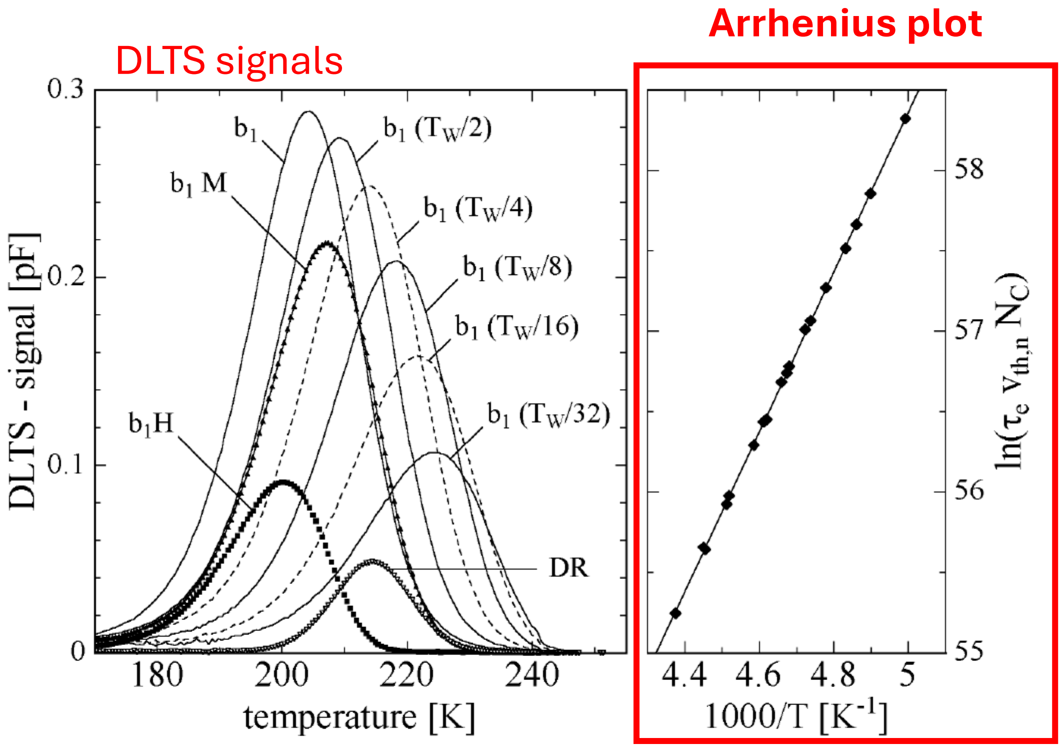


Figure 4.11: DLTS spectra obtained with various different correlators (see Fig. 4.10). For better visibility not all of the 18 used correlators are shown. However, the Arrhenius plot on the right-hand contains the data obtained with all 18 correlators. (transition: $VV^{(-/0)}$, sample M21009, $V_R = -10\,\mathrm{V}$, $V_P = 0\,\mathrm{V}$, $T_W = 200\,\mathrm{ms}$, $t_0 = 6\,\mathrm{ms}$, ^{60}Co-γ-irradiated: 107 kGy)

Example:

DLTS signals corresponding to 9 different correlators (on the left) and an **Arrhenius plot** (on the right).

This **method** is called ***maxima evaluation***.

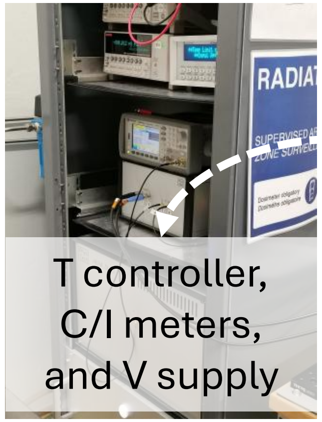
Usually, **three different time windows** T_w of 20, 200 and 2000 ms used **during one temperature scan**.

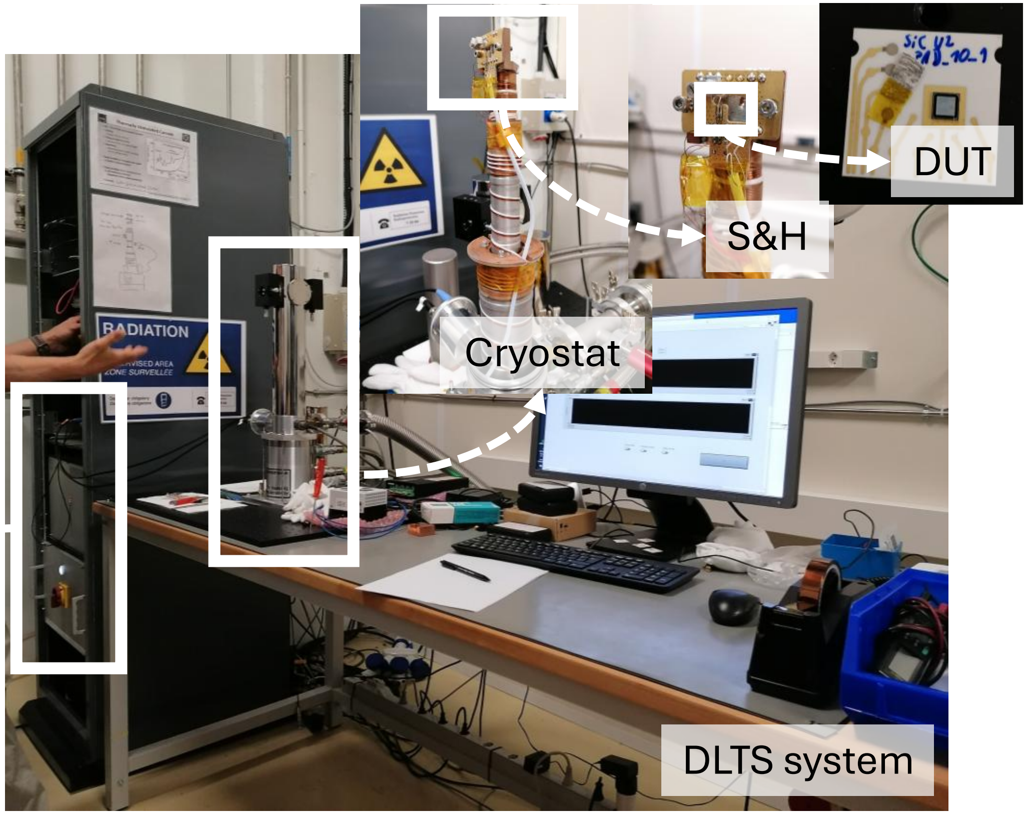
NB: the **measured temperature dependence** of the **characteristic emission time constant** of the capacitance transient, **τ_e**, can be used to establish an **Arrhenius plot** to determine the **capture cross-section**, $\sigma_{n,p}$, and the **activation energy**, $\Delta H'_{n,p}$, of the defect from the **intercept with the ordinate** and from the **slope**, respectively.

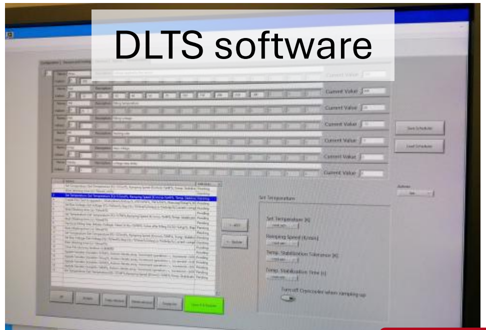
Research activities and achievements

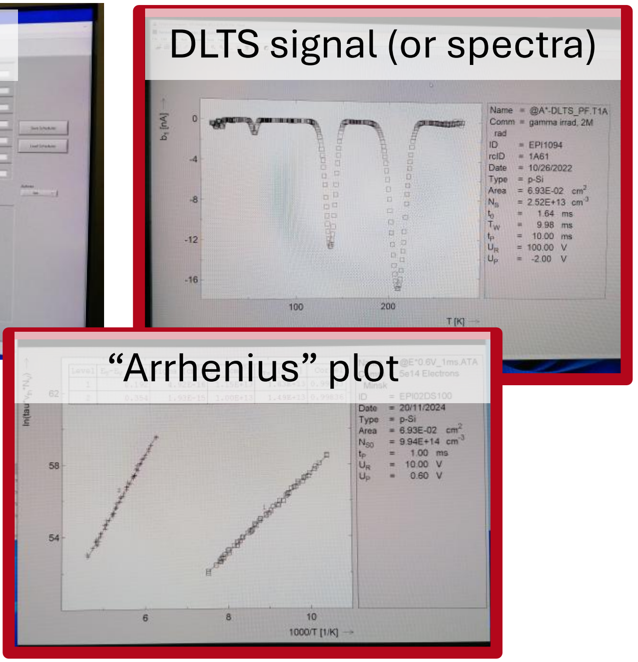
Experimental measurements – 2nd academic year

- **Defect spectroscopy**: *supervised training* and *measurements* at Deep Level Transient Spectroscopy (**DLTS**) system – SSD Lab, CERN EP-DT group (Apr-Sep ’25).



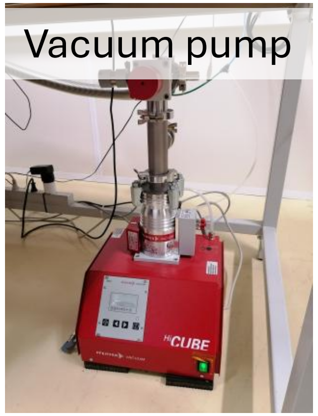






Name = @A*-DLTS_PF.T1A
Comm = gamma irrad, 2M rad
ID = EPI1094
rcID = 1A61
Date = 10/26/2022
Type = p-Si
Area = 6.93E-02 cm^2
N_S = 2.52E+13 cm^{-3}
t_0 = 1.64 ms
T_W = 9.98 ms
t_P = 10.00 ms
U_R = 100.00 V
U_P = -2.00 V

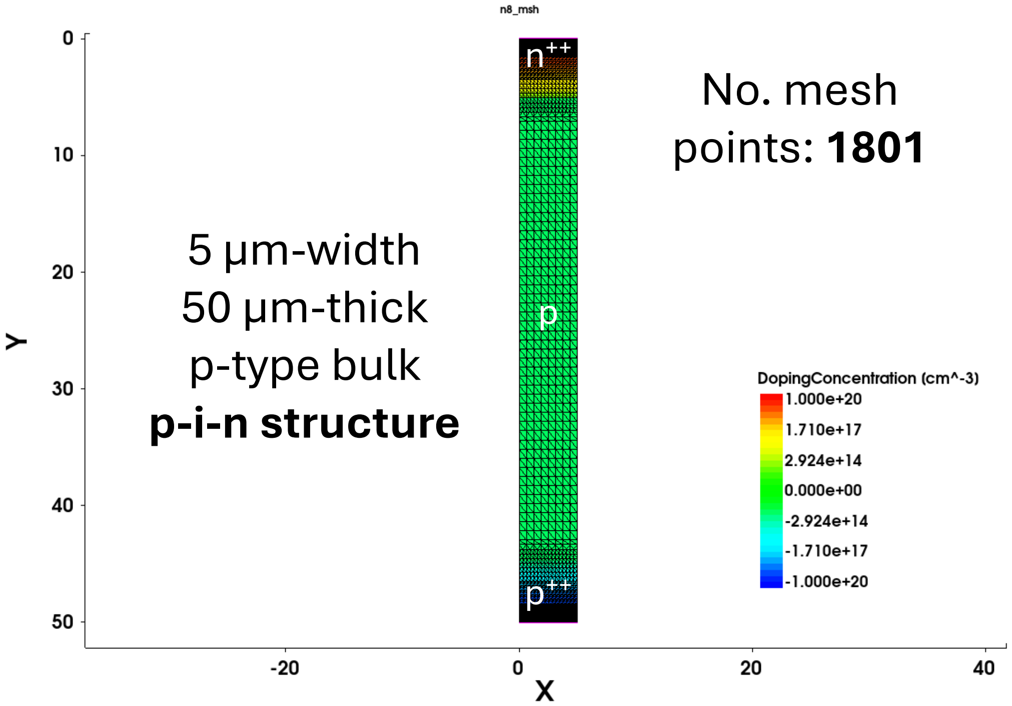
Name = @E*0.6V_1ms.ATA
Comm = 5e14 Electrons Minsk
ID = EPI02DS100
Date = 20/11/2024
Type = p-Si
Area = 6.93E-02 cm^2
N_{S0} = 9.94E+14 cm^{-3}
t_P = 1.00 ms
U_R = 10.00 V
U_P = 0.60 V



Defect parameters:
N_t, E_a and $\sigma_{e,h}$

Layout, Doping Concentration & **Mesh (v4.A2)**

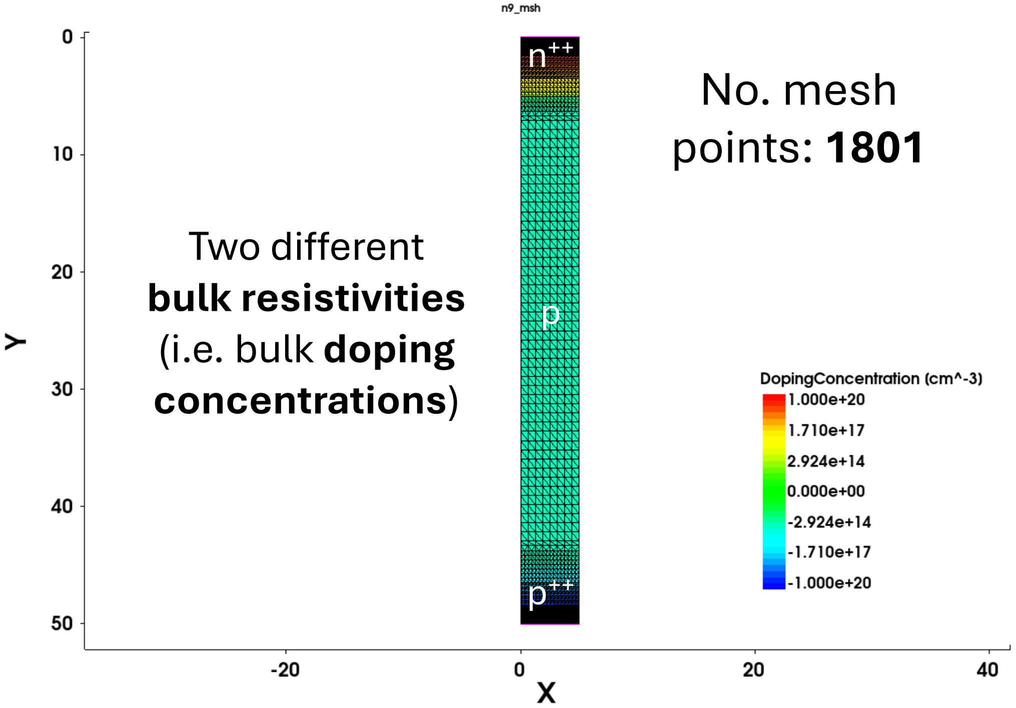
250 Ωcm



No. mesh points: **1801**

5 µm-width
50 µm-thick
p-type bulk
p-i-n structure

50 Ωcm

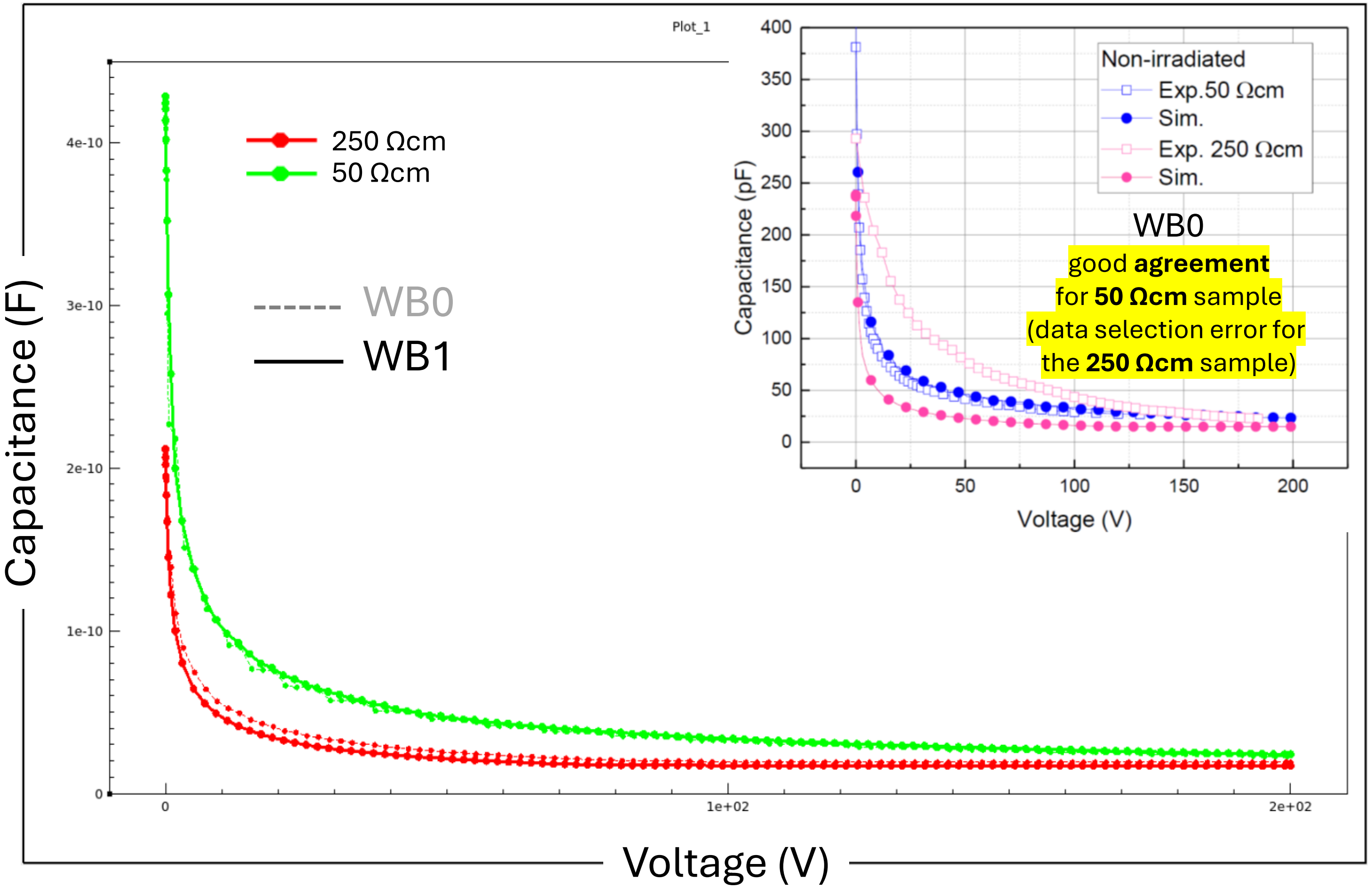


No. mesh points: **1801**

Two different **bulk resistivities** (i.e. bulk **doping concentrations**)

Small-Signal (AC) Analysis – **Sim vs. Meas**

before irradiation



WB0
good **agreement**
for **50 Ωcm** sample
(data selection error for
the **250 Ωcm** sample)

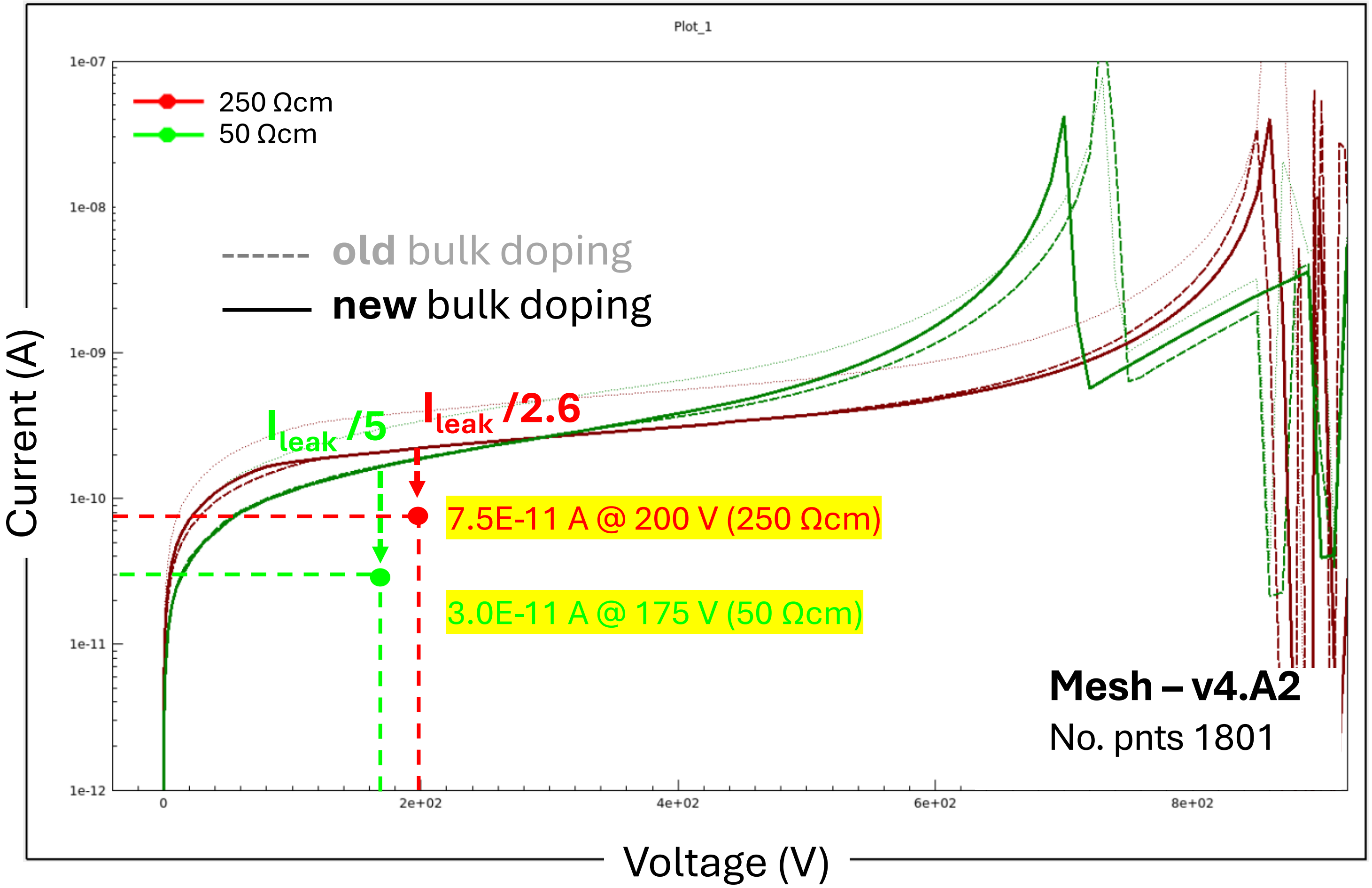
WB0	**WB1**
e/hRecVelocity	-
T = 300 K	T = 293 K
$N_{50\Omega}$ = 2.67E14 $N_{250\Omega}$ = 8.33E13	$N_{50\Omega}$ = 2.95E14 $N_{250\Omega}$ = 5.88E13
$\tau_{n,p}$ = default (max)	$\tau_{n,p}$ = 1 ms (max)
.par file	.par file (PG)
Mesh v0	Mesh v4.A2

Area Factor, **1.385E6**
Frequency, **1 kHz**

Steady-State (DC) Analysis – **Sim vs. Meas**

before irradiation

Perugia Parameter file

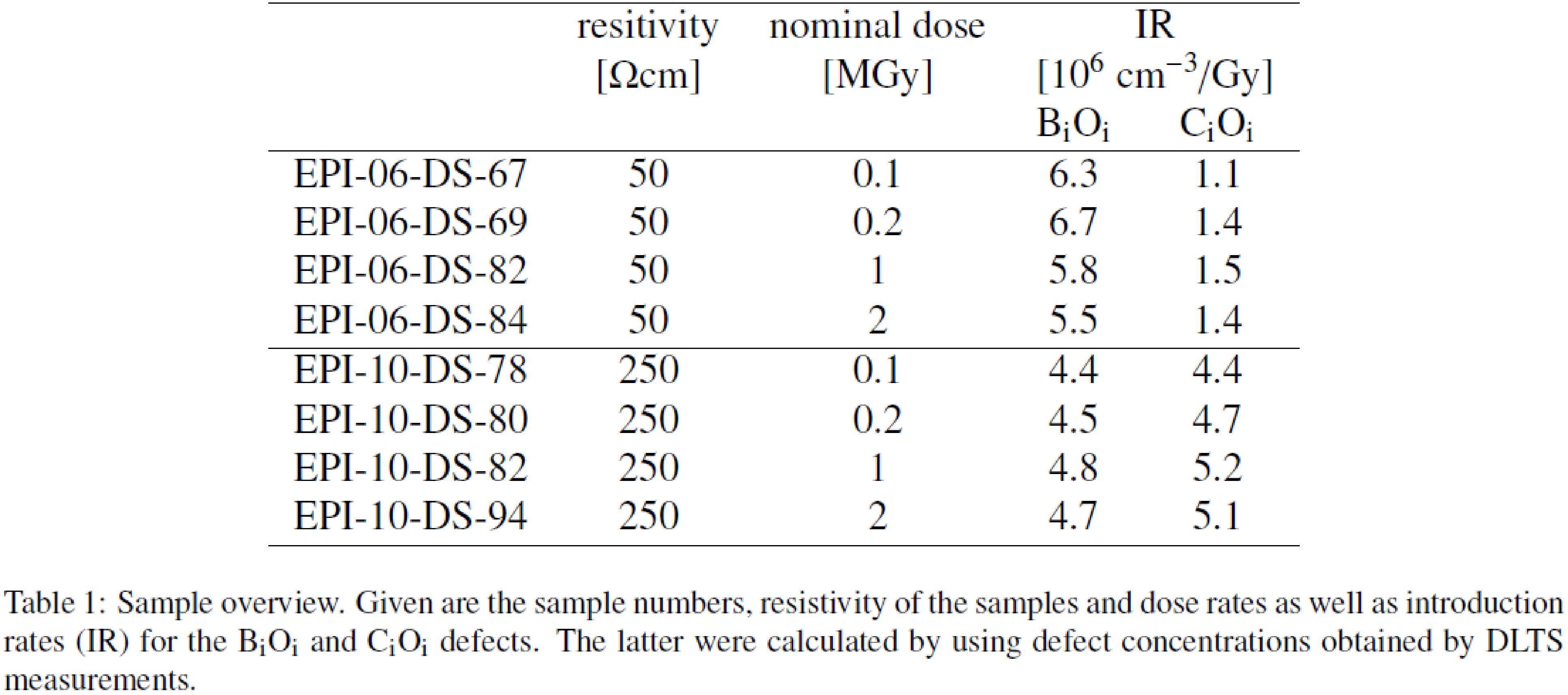


- - - - **MEAS**

Temperature, **293 K**
Area Factor, **1.385E6**

C_iO_i and B_iO_i defects

Sample overview, from *A. Himmerlich* NIMA Article (link)



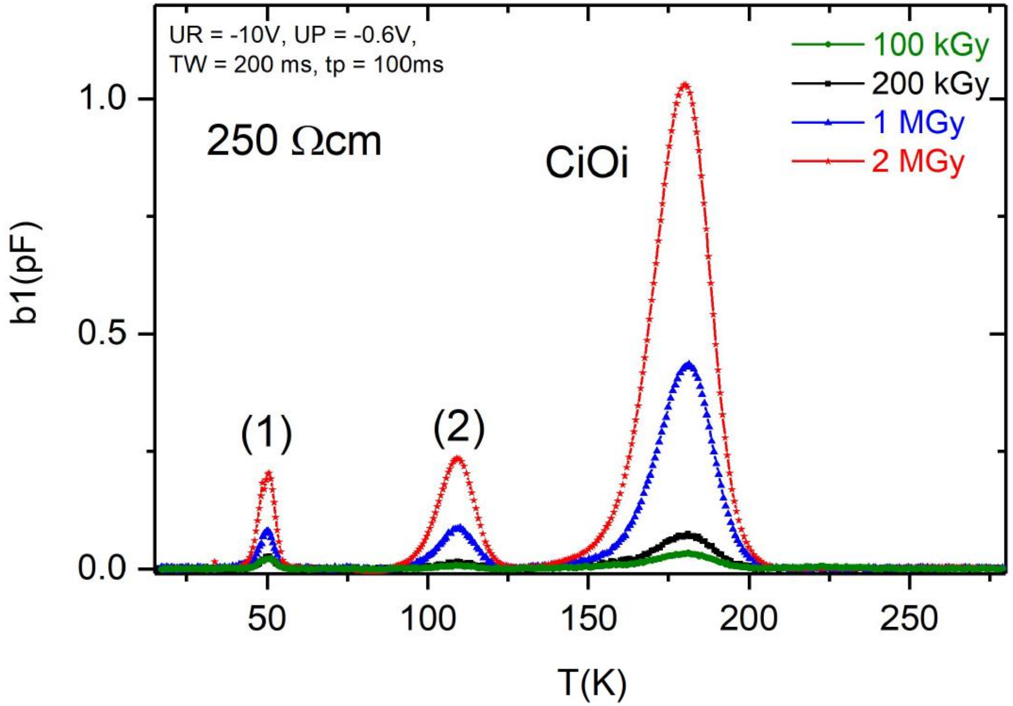
	resitivity [Ωcm]	nominal dose [MGy]	IR [10^6 cm^{-3}/Gy]	
			B_iO_i	C_iO_i
EPI-06-DS-67	50	0.1	6.3	1.1
EPI-06-DS-69	50	0.2	6.7	1.4
EPI-06-DS-82	50	1	5.8	1.5
EPI-06-DS-84	50	2	5.5	1.4
EPI-10-DS-78	250	0.1	4.4	4.4
EPI-10-DS-80	250	0.2	4.5	4.7
EPI-10-DS-82	250	1	4.8	5.2
EPI-10-DS-94	250	2	4.7	5.1

Table 1: Sample overview. Given are the sample numbers, resistivity of the samples and dose rates as well as introduction rates (IR) for the B_iO_i and C_iO_i defects. The latter were calculated by using defect concentrations obtained by DLTS measurements.

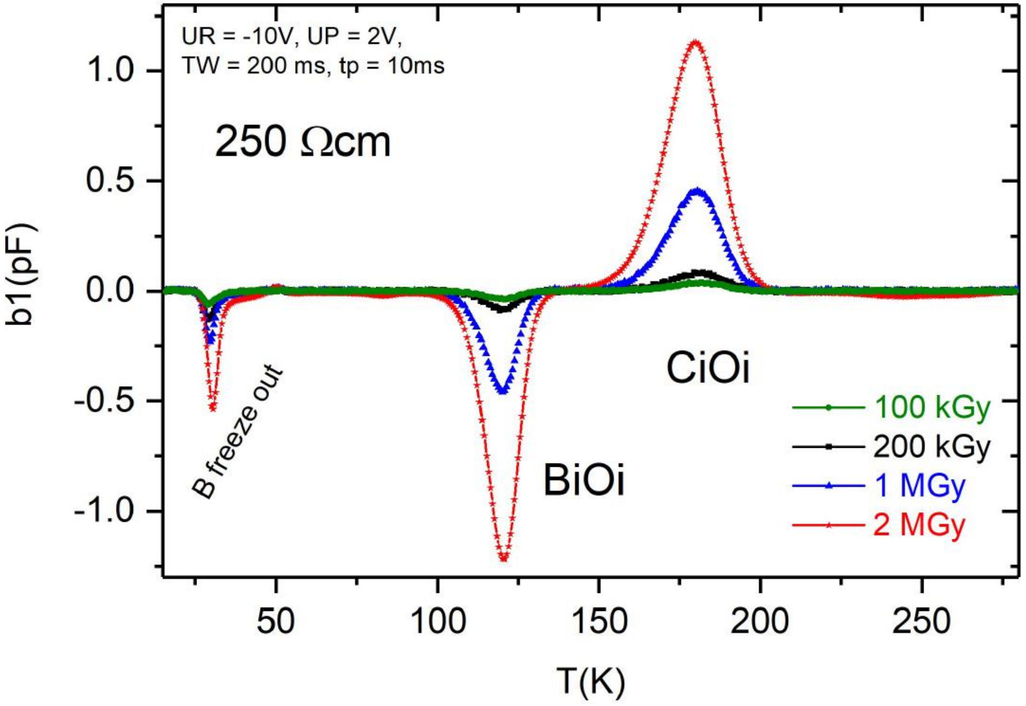
C_iO_i and B_iO_i defects – 250 Ωcm sample

C-DLTS spectra, from *A. Himmerlich* NIMA Article (link)

Majority **carrier injection**



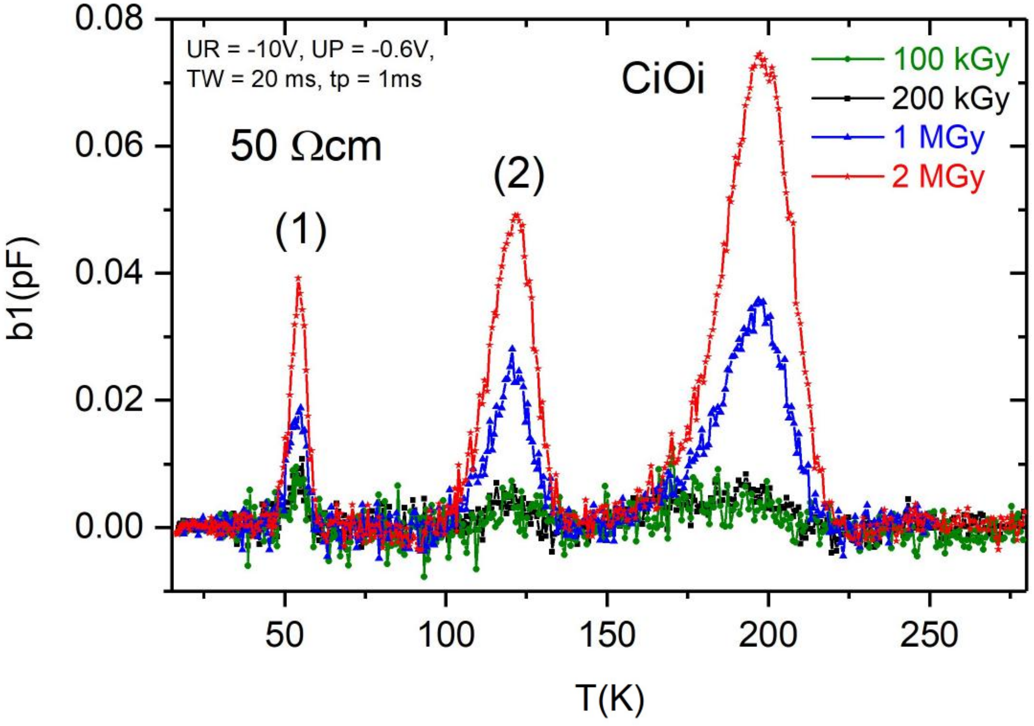
Majority **and** ***Minority*** **carrier injection**



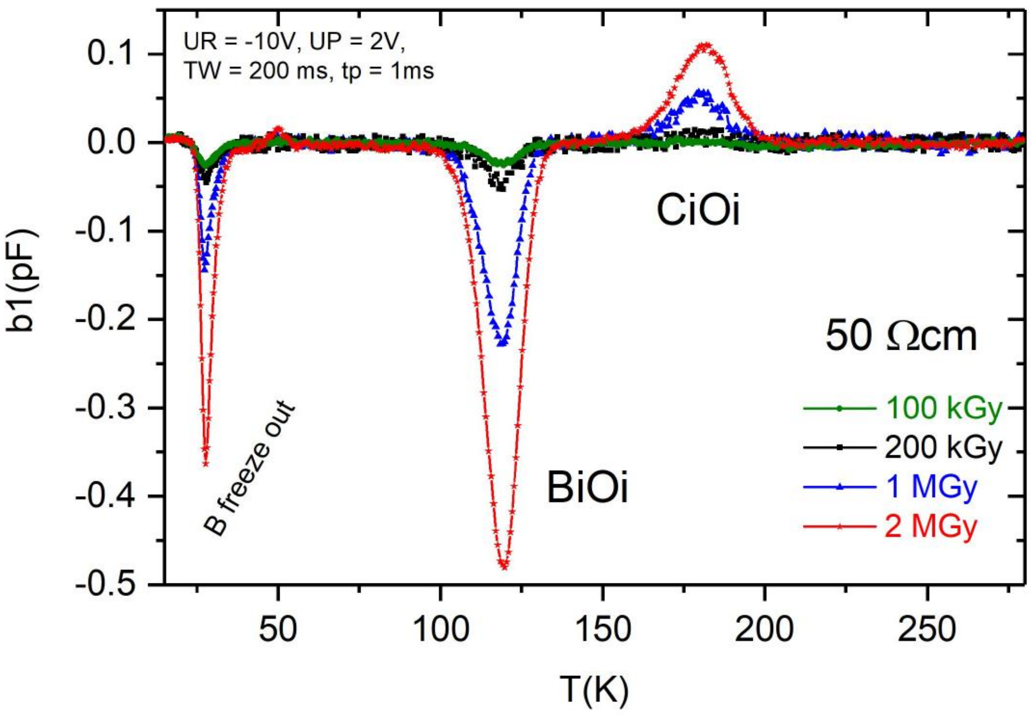
C_iO_i and B_iO_i defects – 50 Ωcm sample

C-DLTS spectra, from *A. Himmerlich* NIMA Article (link)

Majority **carrier injection**



Majority **and** ***Minority*** **carrier injection**



C_iO_i and B_iO_i defects

Concentration, from *A. Himmerlich* NIMA Article (link)

250 Ωcm

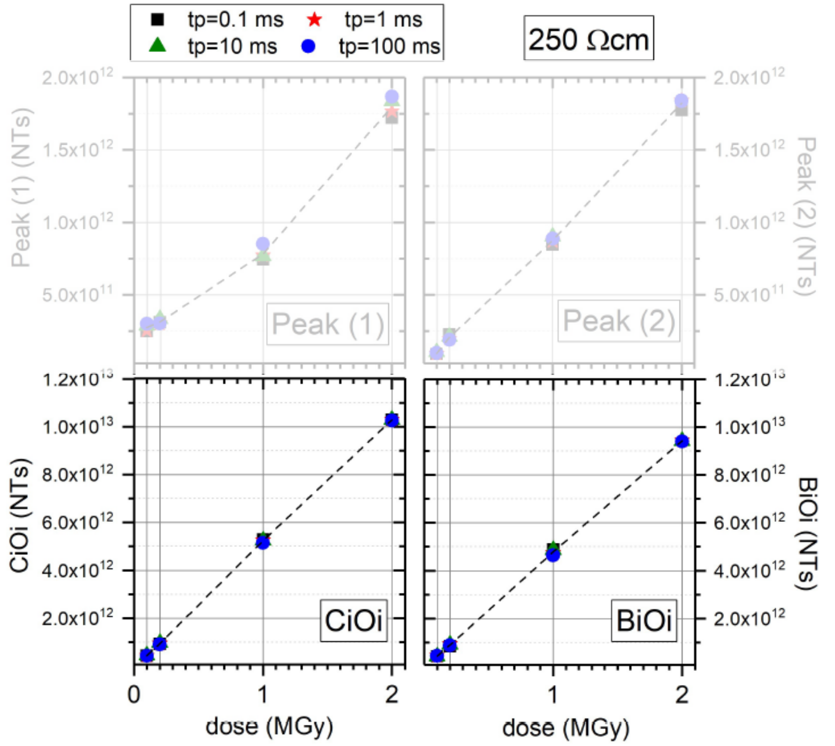


Figure 5: Concentrations of the four dominant defects measured by DLTS on 250 Ωcm ^{60}Co gamma irradiated EPI diodes. Each diode was measured by varying the pulse duration t_p between 0.1 ms and 100 ms. The dotted lines indicate the mean concentration values of all t_p at each radiation dose and guides the eye between measured doses.

50 Ωcm

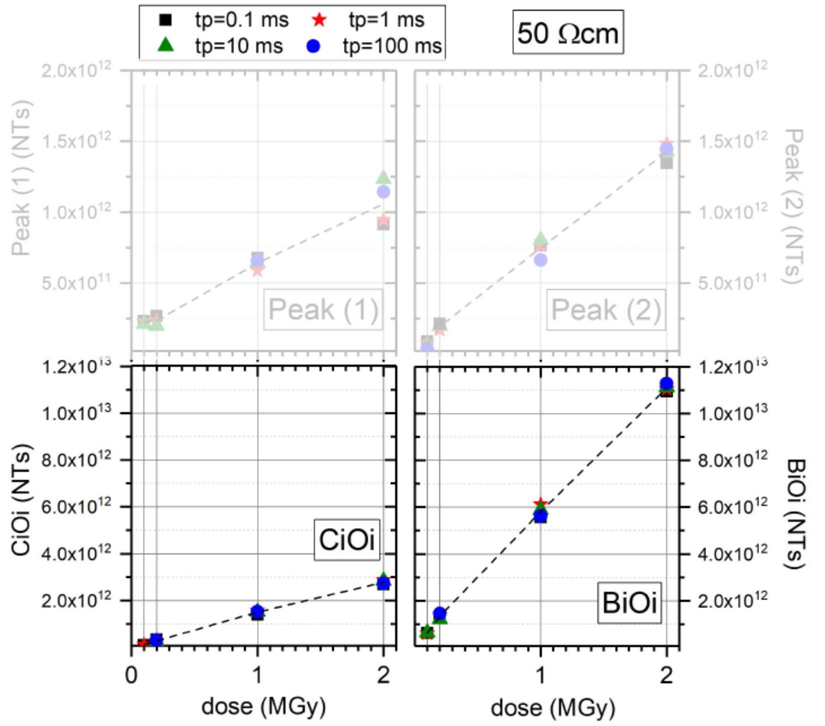
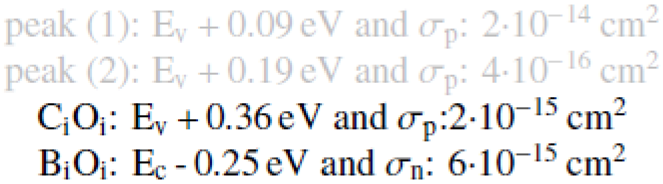


Figure 4: Concentrations of the four dominant defects measured by DLTS on 50 Ωcm ^{60}Co gamma irradiated EPI diodes. Each diode was measured by varying the pulse duration t_p between 0.1 ms and 100 ms. The dotted lines indicate the mean concentration values of all t_p at each radiation dose and guides the eye between measured doses.

C_iO_i and B_iO_i defects

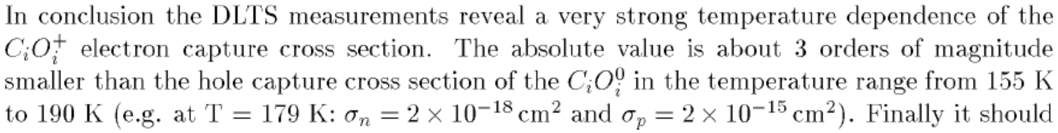
Activation Energy & Capture Cross-Sections

From *A. Himmerlich* NIMA Article (link)



peak (1): $E_V + 0.09\,\text{eV}$ and σ_p: $2{\cdot}10^{-14}\,\text{cm}^2$
peak (2): $E_V + 0.19\,\text{eV}$ and σ_p: $4{\cdot}10^{-16}\,\text{cm}^2$
C_iO_i: $E_V + 0.36\,\text{eV}$ and σ_p:$2{\cdot}10^{-15}\,\text{cm}^2$
B_iO_i: $E_c - 0.25\,\text{eV}$ and σ_n: $6{\cdot}10^{-15}\,\text{cm}^2$

From *M. Moll* PhD Thesis (link)
(chap. 6, par. 6.4, p. 149)



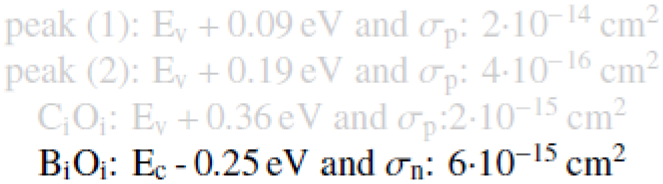
In conclusion the DLTS measurements reveal a very strong temperature dependence of the $C_iO_i^+$ electron capture cross section. The absolute value is about 3 orders of magnitude smaller than the hole capture cross section of the $C_iO_i^0$ in the temperature range from 155 K to 190 K (e.g. at T = 179 K: $\sigma_n = 2 \times 10^{-18}\,\text{cm}^2$ and $\sigma_p = 2 \times 10^{-15}\,\text{cm}^2$). Finally it should

B_iO_i defect

Activation Energy & Capture Cross-Sections

From *A. Himmerlich* NIMA Article (link)

EPI-250 & EPI-50



peak (1): $E_V + 0.09\,\mathrm{eV}$ and σ_p: $2\cdot10^{-14}\,\mathrm{cm}^2$
peak (2): $E_V + 0.19\,\mathrm{eV}$ and σ_p: $4\cdot10^{-16}\,\mathrm{cm}^2$
C_iO_i: $E_V + 0.36\,\mathrm{eV}$ and σ_p:$2\cdot10^{-15}\,\mathrm{cm}^2$
B_iO_i: $E_C - 0.25\,\mathrm{eV}$ and σ_n: $6\cdot10^{-15}\,\mathrm{cm}^2$

From *I. Pintilie* DRAFT Article (link)

EPI-250 (& EPI-50?)

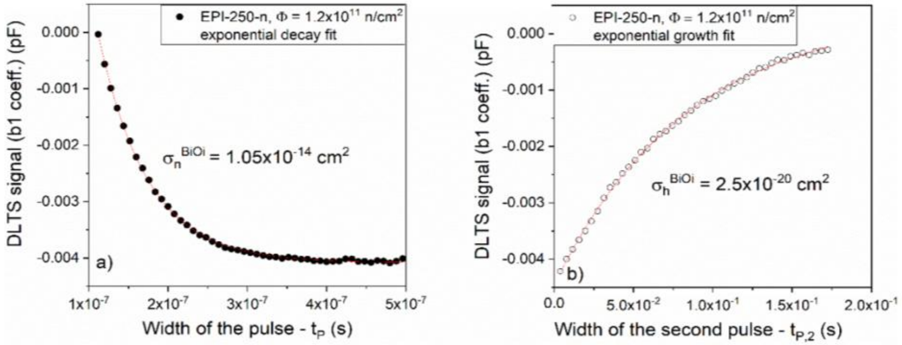


Figure 3. Direct measurement of the capture cross sections ($\sigma_{n,p}$) of the $B_iO_i^{0/+}$ defect energy level at 120K: a) σ_n, after injection pulses of $U_P = 1$ V and different pulse widths; b) σ_p, after double injection pulses, first with $U_{P,1} = 1$ V, t_P= 100 ms followed by the second one with $U_{P,2} = -0.2$ V.

Convergence & Error Control (1/2)

Chap. 6, SDevice User Guide

- **Convergence** of a **solution** is **determined** by calculating and examining at each Newton iteration (AND):
  - *RHS norm* (residual of the equations)
  - *Update error* (updates to the equation variables)
- **Convergence** condition (OR):
  - *RHS norm < RhsMin*
  - *Update error < 1*
- **Divergence** condition (OR):
  - *RHS norm* increase by more than a factor of *RhsFactor*
  - *RHS norm > RhsMax* (for transient simulations) *RhsMaxQ* (for non transient simulations)

Note: use of *CheckRhsAfterUpdate* can sometimes improve the quality of a solution, and might result in better overall convergence – performs an additional check on the *RSH norm* making it smaller after the *Update error* criteria is satisfied

Convergence & Error Control (2/2)

Chap. 6, SDevice User Guide

- *Math* parameters that determine **when** a **coupled solution diverges** or **converges**:
  - *Iterations* → limits the no. of Newton iterations
  - *RhsFactor*, *RhsMin*, *RhsMinFactor*, *RhsMax*, *RhsMaxQ*
  - *CheckRhsAfterUpdate* → when using extended-precision accuracy, large value for *Iterations* might be needed
  - *RelErrControl* → error criterion (*relative* for large values of an equation variable x, *absolute* for small values of x) for calculation of the *Update error*
  - *Digits* → $10^{-\text{Digits}}$ is the relative error ε_R
  - *ErrRef* → reference error parameter x_{ref}
  - *Error* → *absolute error* ε_A
  - *UpdateIncrease*, *UpdateMax* → detect divergence of Newton algorithm if (OR)
    - *Update error* > UpdateMax
    - *Update error* increase exceeds *UpdateIncrease*

Constant Carrier Generation (CCG) Model

SDevice User Guide, Chap. 16, pp. 513-514

- The simplest **generation model** computes a **constant carrier generation** G_{const} and is activated in the Physics section as follows:

```
Physics {
    Recombination (
        ConstantCarrierGeneration (value = 1e10) # [cm^-3 s^-1]
    )
}
```

- To visualize G_{const}, plot the value of *PMIRecombination*:

```
Plot {
    PMIRecombination
}
```

- Note: the constant carrier generation **model** is **functionally equivalent** to the **constant optical generation model** (see Constant Optical Generation on page 680).

Trap modelling in TCAD Sentaurus

from SDevice Tutorial, Chap. 13 “Special Focus: Traps”

- *Acceptor* trap
  - **uncharged** (**0**) when unoccupied
  - **negatively charged** (**-**) when capturing an electron
- *Donor* trap
  - **uncharged** (**0**) when unoccupied (i.e. when capturing an electron)
  - **positively charged** (**+**) when capturing a hole

- **Note**: the TCAD manual refer to **occupation** as occupied **with electrons**, a state when a ***donor*** is **neutral** (0) and an ***acceptor*** **negatively charged** (-).

Silicon material – **Parameter File**

Perugia parameter file

```
MaterialInterface = "Silicon/Oxide" {
 SurfaceRecombination {
  S0 = @s0@, @s0@ * [cm/s]
  Sref = 0 * [1]
 }
}


Material="Silicon"{
  …
}
```

```
Material="Silicon"{
 …
 Scharfetter * relation and trap level for SRH recombination:
 { * tau = taumin + ( taumax - taumin ) / ( 1 + ( N/Nref )^gamma)
  * tau(T) = tau * ( (T/300)^Talpha )        (TempDep)
  * tau(T) = tau * exp( Tcoeff * ((T/300)-1) ) (ExpTempDep)
         taumin          = 0.0000e+00 ,          0.0000e+00  # [s]
         taumax          = @tau_n@ , @tau_p@     # [s]
         Nref      = 1.0000e+16 ,        1.0000e+16  # [cm^(-3)]
         gamma           = 1 ,           1             # [1]
         Talpha          = -1.5000e+00 ,         -1.5000e+00 # [1]
         Tcoeff          = 2.55 ,        2.55          # [1]
         Etrap           = 0.0000e+00                # [eV]
 }
 …
}
```

tau_n = 1E-5 s, tau_p = 3E-6 s (default)

@tau_n@ = @tau_p@ = 1 ms (Perugia)

Transient Analysis – Command File (1/4)

Physics section

```
Physics {
        AreaFactor = 1.3854e6 ; xmax = 5
        Temperature = @T@
        Mobility (
         ; Constant Mobility Model due to phonon scattering in undoped materials – active by default.
         DopingDependence ; mobility degradation due to impurity scattering in doped materials.
         eHighFieldSaturation hHighFieldSaturation Enormal
         ; mobility degradation in high electric field.
         CarrierCarrierScattering  ; Philips Unified Mobility Model accounts for both impurity and carrier-carrier scattering .
        )
Recombination (
        SRH (
         DopingDependence ; Scharfetter Relation models the doping dependence of carriers' lifetime.
         Tunneling(Hurkx) ; models the carriers' lifetime decrease in regions of strong electric fields (Lifetime = Hurkx)
        )
        Auger (withGeneration) ; band-to-band temperature-dependent recombination that decreases at high carrier densities (WithGeneration option allows for generation of electron–hole pairs)
        Avalanche (UniBo Eparallel) ; when UniBo model is active, also Auger generation is activated. Eparallel is the driving force that computes the accelerating field.
        Band2Band (Hurkx) ; selects the band-to-band recombination Hurkx model without density correction.
)

EffectiveIntrinsicDensity (BandGapNarrowing (OldSlotboom)) ; doping-dependent bandgap narrowing in p- and n-type doped materials – BennettWilson bandgap model active by default.
}
```

Transient Analysis – Command File (2/4)

Physics section

```
Physics {
…
Optics (
        OpticalGeneration (
          ComputeFromMonochromaticSource (
                TimeDependence (
                        WaveTime = (50e-3 100e-3)
                        WaveTSigma = 50e-9
                )
                Scaling = 0
          )
        )
        …
```

- *ComputeFromMonochromaticSource* is the **method** used **to compute** the **optical generation rate, G_{opt}**, when an optical wave with a single wavelength, λ, is absorbed by a medium and produces e-h pairs.
- G_{opt} is computed as the **product of** the **absorbed photon density, $\rho_{abs\ ph}$**, and the **quantum yield**, **Q_γ**, for every semiconductor region
$$G_{opt} = \rho_{abs\ ph} * Q_\gamma$$
- *Scaling* applies only **for Quasistationary** (**QS**) **simulations**.
- In the case of **transient simulations** (transient) a **time-dependent scaling factor** can be used **to model the response to a light pulse**, or any other time-dependent light signal.
- To model the electrical response of a light pulse, i.e. to scale the G_{opt} in a transient simulations:
  - *TimeDependence* directly in the *OpticalGeneration* section to describe the light signal over time globally.
  - **The given time dependency scales** the G_{opt} resulting from a stationary solution of the optical problem **as a function of time**. It **works only if a *Transient* statement in the *Solve* section is set.** The corresponding scaling factor is automatically written to the Current file under the name *TimeDependence(Ft)*.
  - The scaling factor can be set directly within the *TimeDependence* section. **If no time dependency has been specified, a scaling factor of 1 is used.**

Transient Analysis – Command File (3/4)

Physics section

```
Physics {
…
Optics (
        …
        Excitation (
                Wavelength = 0.8 *um ; upper/lower limit red/IR
                Intensity = 0.0006 *W/cm2 ; 6E-4 W/cm2
                Window("L1") (
                   Origin = (2.5,-10) ; global location of the of the LCS
                   OriginAnchor = Cente; (default)
                   Line ( Dx = 10 ) ; xmin = 0 xmax = 10, bounding box limits
                   )
                Theta = 0 ; angle between local Y'-axis to the local X'-axis
        )
        …
```

- *Excitation* section specifies the **details of the light source**, such as the **angle of incidence** *Theta* (deg), the **wavelength** (µm), the **intensity** (W/cm^2).
- In combination with the *OptBeam* optical solver (see next slide), a *Window* section is required to specify the parameters of the **illumination window**.
- *Origin* specifies the global location of the origin of the **local coordinate system**, whose default is (0, 0, 0).

Transient Analysis – Command File (4/4)

Physics section

```
Physics {
...
Optics (
          ...
          OpticalSolver (
                    OptBeam (
                              LayerStackExtraction (
                               WindowName ="L1"
                               WindowPosition = Center
                               Mode = ElementWise
                               )
                              )
                    )
          ...
```

- *OptBeam is the optical solver that* computes the **absorbed photon density, $\rho_{\text{abs ph}}$**.
- The **illumination window** is described using a **local coordinate system** specified by the global location of its origin and the x- and y-directions.