

A new model for the TCAD simulation of the silicon damage by high fluence proton irradiation

—The Hamburg Penta Trap Model—

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High-Luminosity LHC radiation level for the 1st pixel layer after 3000 fb⁻¹ :

- $\Phi_{eq} \approx 2.3 \cdot 10^{16} \text{ cm}^{-2}$, dose $\approx 12 \text{ MGy}$

TCAD simulations of sensors are valuable in:

- Avoiding designs mistakes
- Understanding and predicting the performance of the sensor
- Optimization for radiation hardness

Requirements:

- Accurate models + parameters describing **bulk** and **surface** radiation damage in TCAD
- Choice of correct boundary conditions

Problems:

- Currently available radiation damage models are not able to describe I-V, C-V and CCE measurements on pad diodes simultaneously for fluences $\geq 1 \cdot 10^{15} \text{ n}_{eq}/\text{cm}^2$
- Is SRH valid (point vs. cluster defects)?
- Accuracy and reproducibility of data



Measurement and simulation program for high fluences with the aim of the development of an accurate model

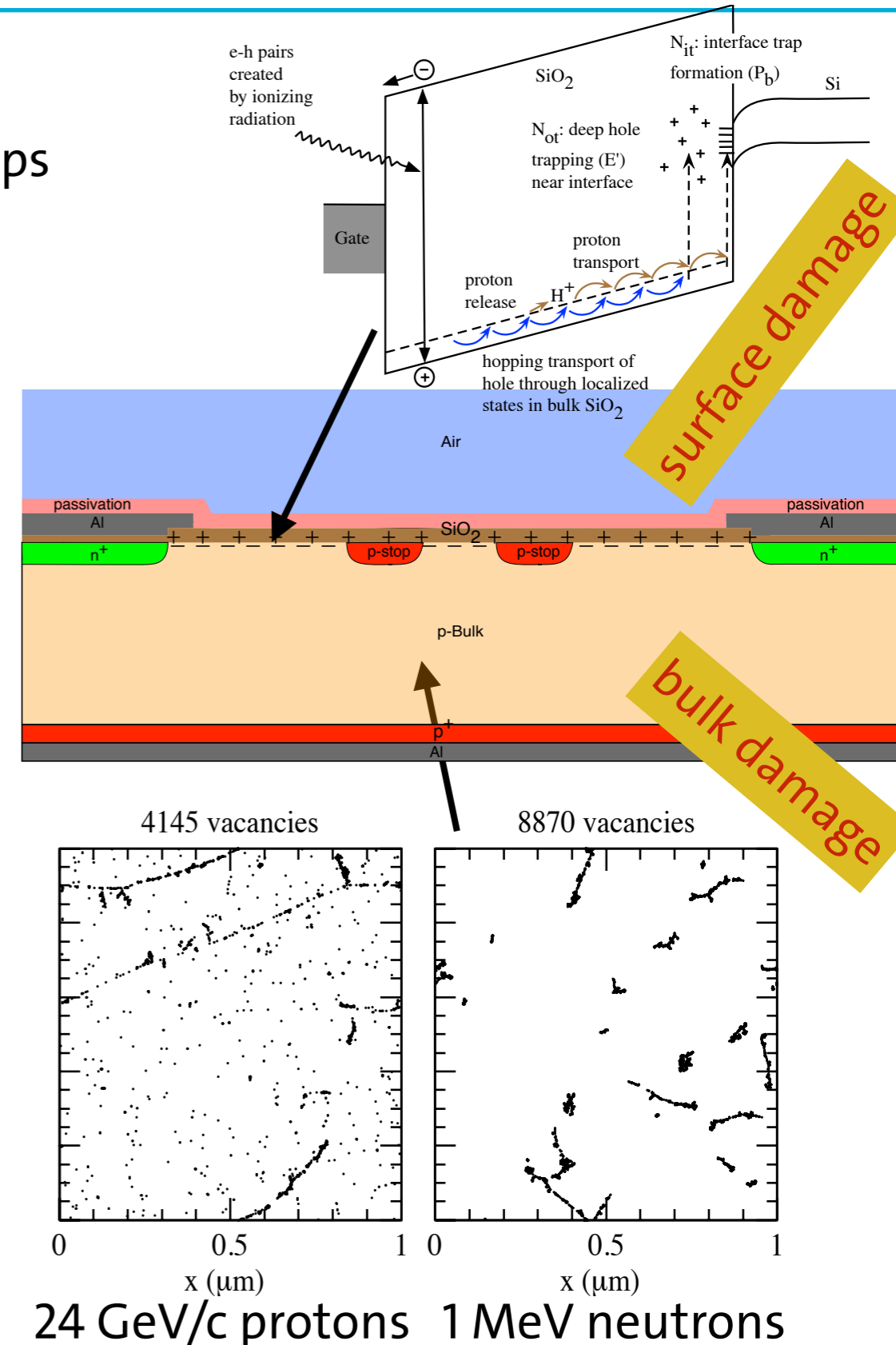
Surface damage (Ionizing Energy Loss):

- Build up of oxide charges, border and interface traps
 - ➔ Increase of surface current
 - ➔ Change of electrical field near to the Si-SiO₂ interface
 - ➔ Trapping near to the Si-SiO₂ interface
- C-V/I-V on MOS capacitors, MOSFET and gate controlled diodes

Bulk damage (NIEL):

- Point and cluster defects in the silicon lattice
 - ➔ Increase of leakage current
 - ➔ Change of the space charge in the depletion region, increase of full depletion voltage
 - ➔ Trapping of drifting charge
- I-V, C-V and CCE on pad diodes

In the following only bulk damage from protons and no surface damage (1 D problem)



Large and small diodes available from the CMS HPK campaign:

1. Material

- **p-type** (p-stop, p-spray)
 - Thinned **float zone FTH200** (200 μm thick)
 - + MCz, Epi, deep diffused FZ

2. Irradiations

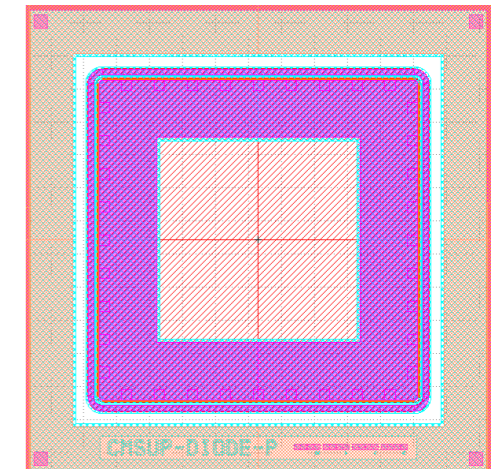
- Protons **24 GeV/c**
 - Fluences: 0.3, 1, 1.5, 2.4, 3, 6, 7.75, $13 \cdot 10^{15} n_{\text{eq}}/\text{cm}^2$

3. Measurements after **80min@60°C** annealing (irrad. 2015) at

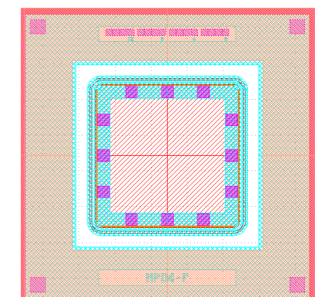
T= -20°C and -30°C with reverse and forward bias applied

- I-V up to 1000 V (reverse) and up to current limit of 0.5 mA (forward)
- C/G-V with 100 Hz - 2 MHz
- TCT with 670 nm (red) and 1063 (IR) nm laser

Diode 5mm x 5mm

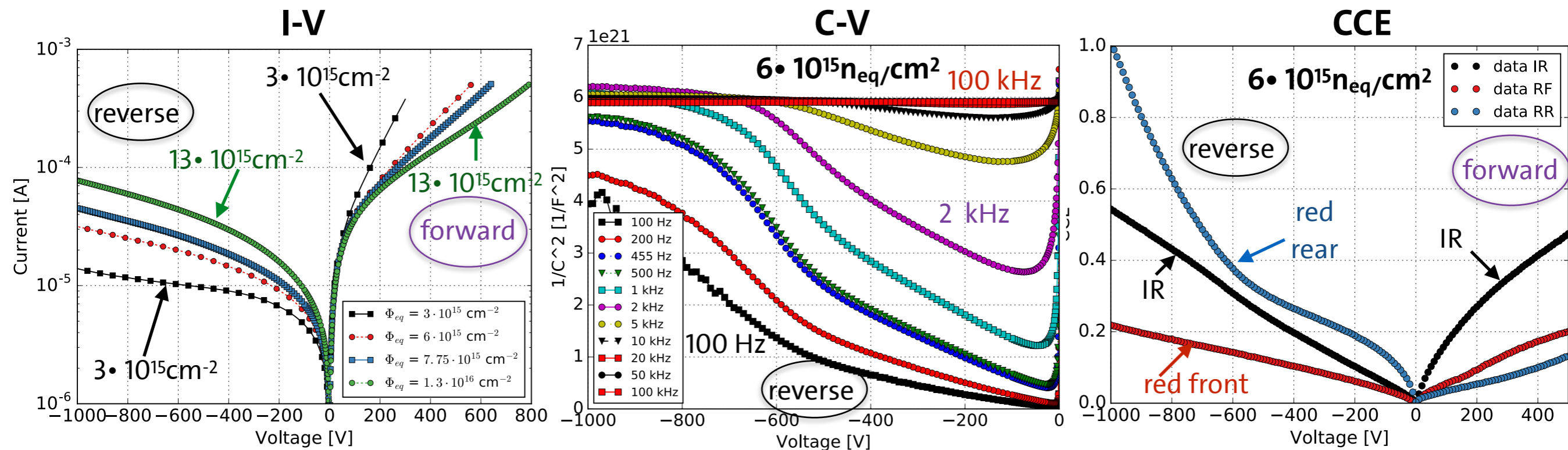


Diode 2mm x 2mm



Large diodes FTH200:

- 24 GeV/c protons with fluences $3, 6, 7.75, 13 \cdot 10^{15} n_{eq}/cm^2$
- 80min@60 °C
- $T = -20$ °C
- CCE from TCT measurements with error below 10 %

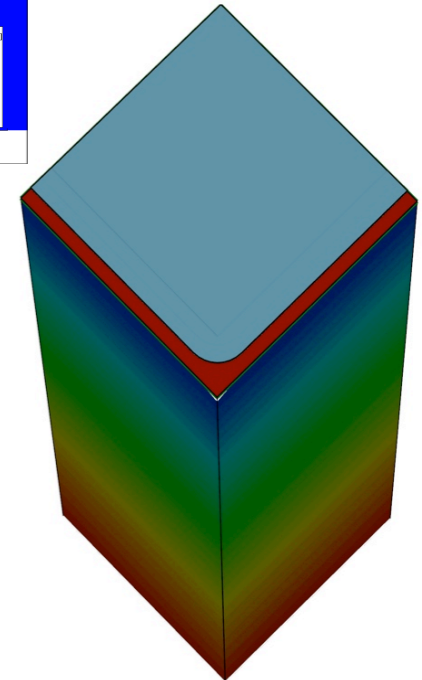
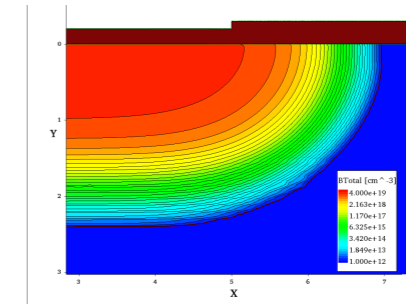


Are we able to reproduce all measurements with simulations?

TCAD (Technology Computer Aided Design):

- Process simulation → doping profile
- Device simulation → electrical behaviour
 - Works by modeling electrostatic potential (Poisson's equation) and carrier continuity equations
 - Takes mesh, applies semiconductor equations + boundary conditions (in discrete form) and solves

2D Boron profile



Poisson $\nabla \cdot \epsilon \nabla \phi = -\rho_{eff}$ with $\rho_{eff} = q[p - n + N_D - N_A] - \rho_{traps}$

Electron continuity $\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_n + R_{net}$ where $\mathbf{J}_n = qn\mu_n \mathbf{E} + qD_n \nabla n$

Hole continuity $\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{J}_p + R_{net}$ where $\mathbf{J}_p = qp\mu_p \mathbf{E} - qD_p \nabla p$

- Different versions of physics models are available (mobility, avalanche, tunnelling etc)
- Radiation damage will change the net recombination rate R_{net} and the charge density due to ρ_{traps}

Radiation damage modelling:

- Usually effective trap levels modelling the measured identified point and cluster defects
- It is assumed that the traps obey **SRH** statistics (still valid at high fluences?)
- Parameters are dependent on the simulator (Synopsys TCAD, Silvaco)

Example: 2 trap model → 6 parameter

1. Concentrations : N_A, N_D
2. Cross sections : $\sigma_e^A, \sigma_h^A, \sigma_e^D, \sigma_h^D$

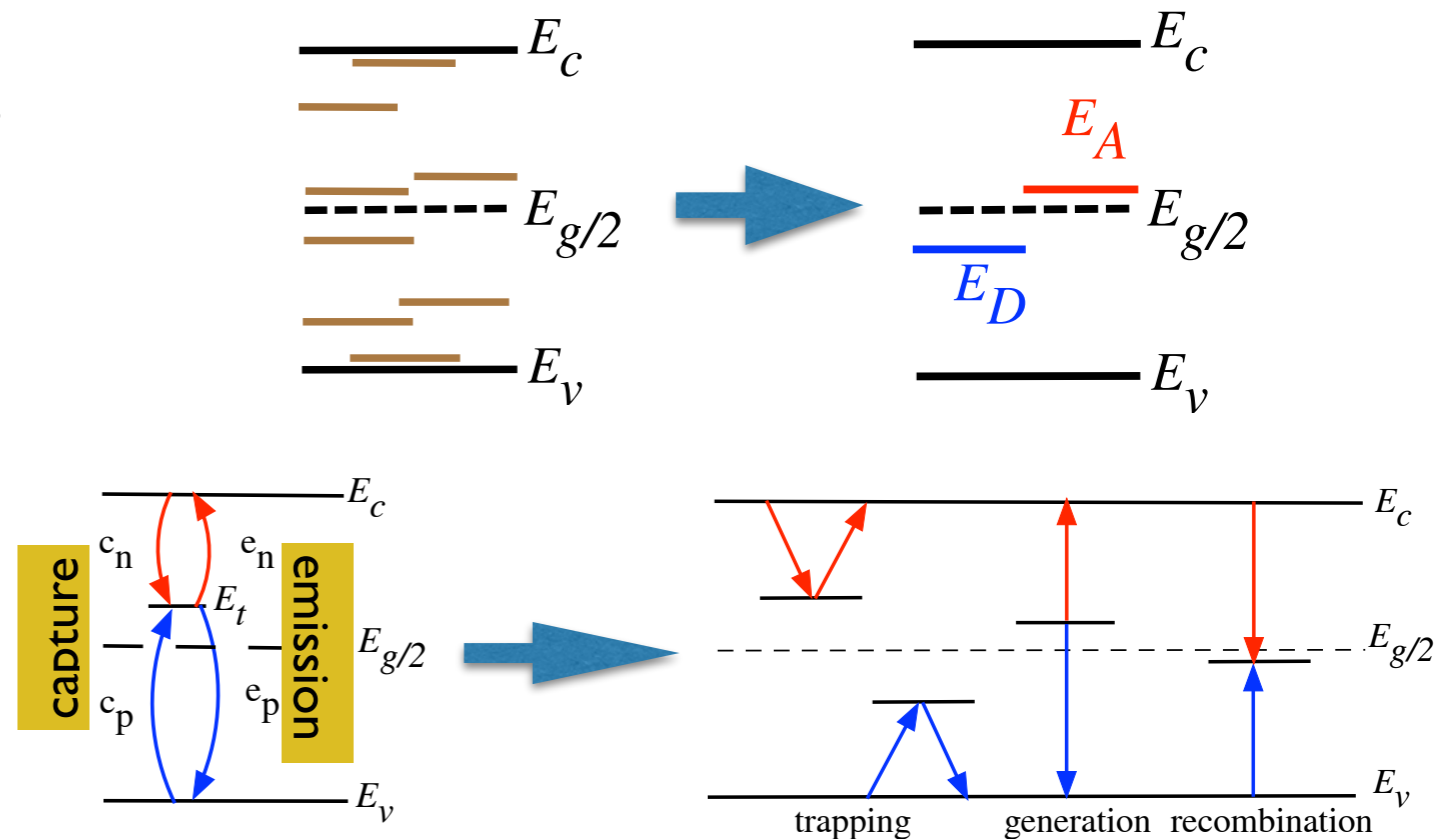
$$\rho_{trap} = q[N_D f_D - N_A f_A]$$

with

$$\left\{ \begin{aligned} f_D &= \frac{v_h \sigma_h^D p + v_e \sigma_e^D n_i e^{E_D/kT}}{v_e \sigma_e^D (n + n_i e^{E_D/kT}) + v_h \sigma_h^D (p + n_i e^{-E_D/kT})} \\ f_A &= \frac{v_e \sigma_e^A n + v_h \sigma_h^A n_i e^{-E_A/kT}}{v_e \sigma_e^A (n + n_i e^{E_A/kT}) + v_h \sigma_h^A (p + n_i e^{-E_A/kT})} \end{aligned} \right.$$

$$R_{net} = \frac{v_h v_e \sigma_h^D \sigma_e^D N_D (np - n_i^2)}{v_e \sigma_e^D (n + n_i e^{E_D/kT}) + v_h \sigma_h^D (p + n_i e^{-E_D/kT})} + \frac{v_h v_e \sigma_h^A \sigma_e^A N_A (np - n_i^2)}{v_e \sigma_e^A (n + n_i e^{E_A/kT}) + v_h \sigma_h^A (p + n_i e^{-E_A/kT})}$$

$$\text{Trapping} \left\{ \begin{aligned} \Gamma_h &= v_h [\sigma_h^D N_D (1 - f_D) + \sigma_h^A N_A f_A] \\ \Gamma_e &= v_e [\sigma_e^A N_A (1 - f_A) + \sigma_e^D N_D f_D] \end{aligned} \right.$$



3-trap Perugia parameters (F. Moscatelli et al IEEE Trans Nucl Sci 2017) for Synopsys TCAD

RADIATION DAMAGE MODEL FOR P-TYPE SUBSTRATES
 (UP TO 7×10^{15} N/CM²)

Type	Energy (eV)	σ_e (cm ⁻²)	σ_h (cm ⁻²)	η (cm ⁻¹)
Acceptor	Ec-0.42	1×10^{-15}	1×10^{-14}	1.613
Acceptor	Ec-0.46	7×10^{-15}	7×10^{-14}	0.9
Donor	Ev+0.36	3.23×10^{-13}	3.23×10^{-14}	0.9

V₂ →
 V₃ →
 C_iO_i →

RADIATION DAMAGE MODEL FOR P-TYPE SUBSTRATES
 (IN THE RANGE $7 \times 10^{15} - 1.5 \times 10^{16}$ N/CM²)

Type	Energy (eV)	σ_e (cm ⁻²)	σ_h (cm ⁻²)	η (cm ⁻¹)
Acceptor	Ec-0.42	1×10^{-15}	1×10^{-14}	1.613
Acceptor	Ec-0.46	3×10^{-15}	3×10^{-14}	0.9
Donor	Ev+0.36	3.23×10^{-13}	3.23×10^{-14}	0.9

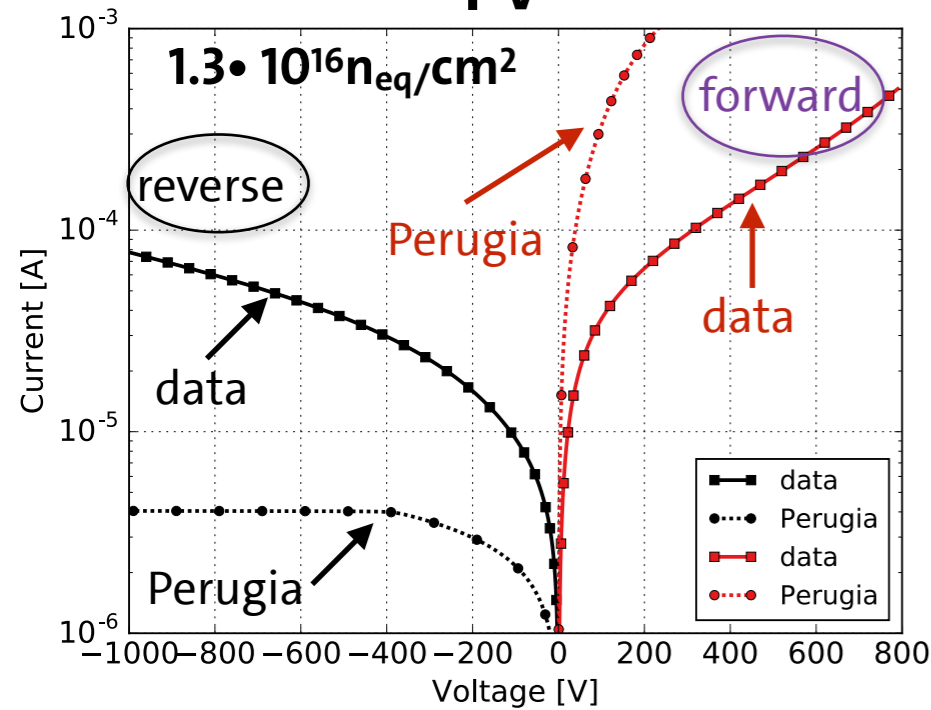
RADIATION DAMAGE MODEL FOR P-TYPE SUBSTRATES
 (IN THE RANGE $1.6 \times 10^{16} - 2.2 \times 10^{16}$ N/CM²)

Type	Energy (eV)	σ_e (cm ⁻²)	σ_h (cm ⁻²)	η (cm ⁻¹)
Acceptor	Ec-0.42	1×10^{-15}	1×10^{-14}	1.613
Acceptor	Ec-0.46	1.5×10^{-15}	1.5×10^{-14}	0.9
Donor	Ev+0.36	3.23×10^{-13}	3.23×10^{-14}	0.9

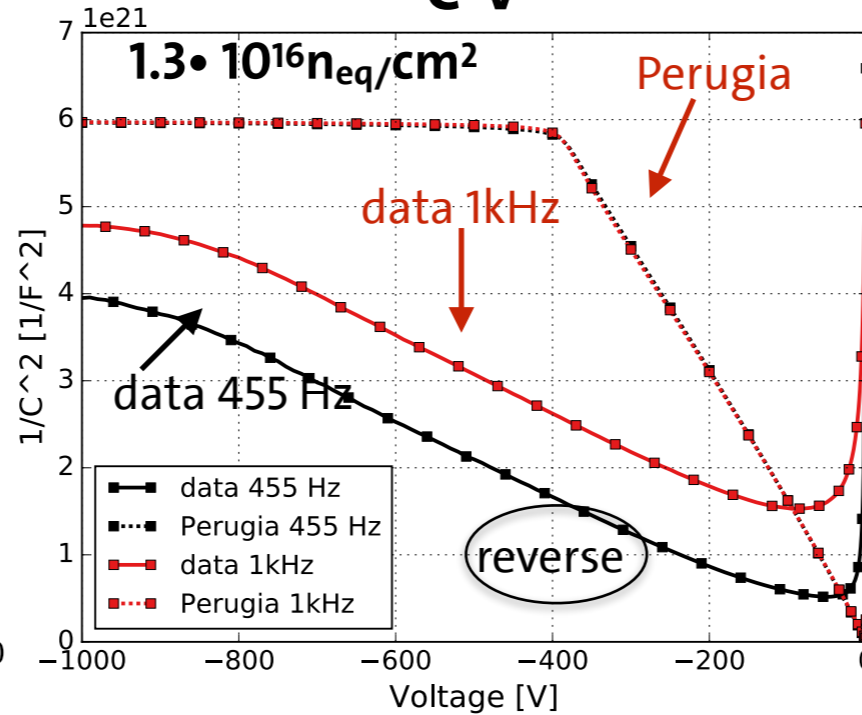
Fluence depending!!

Does it describe our data?

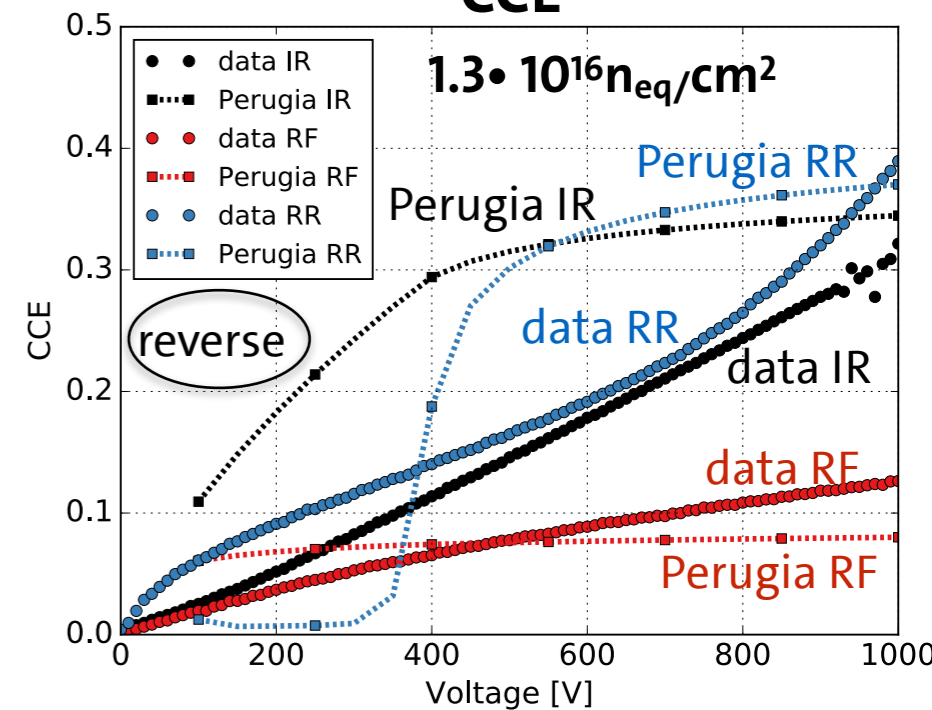
I-V



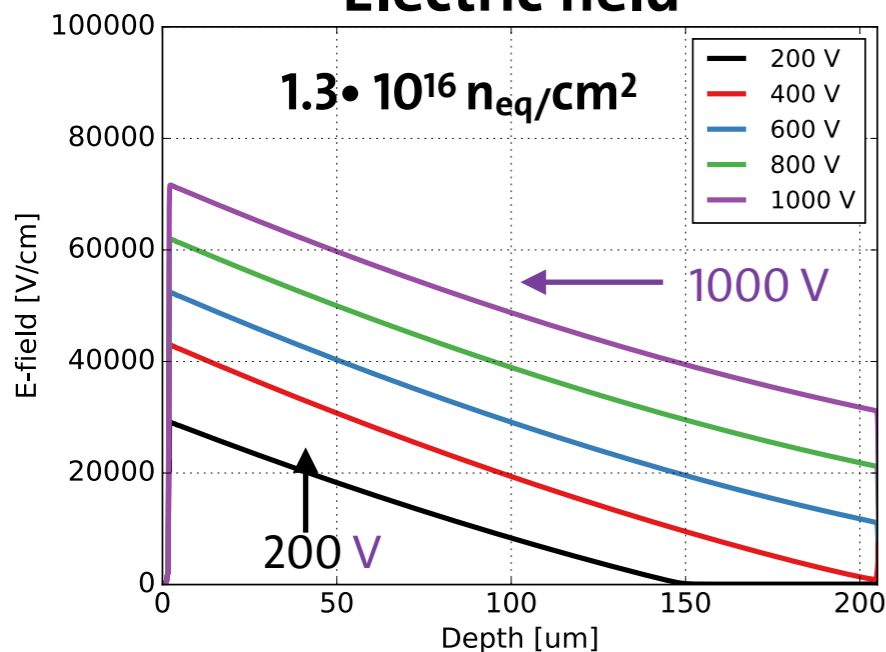
C-V



CCE

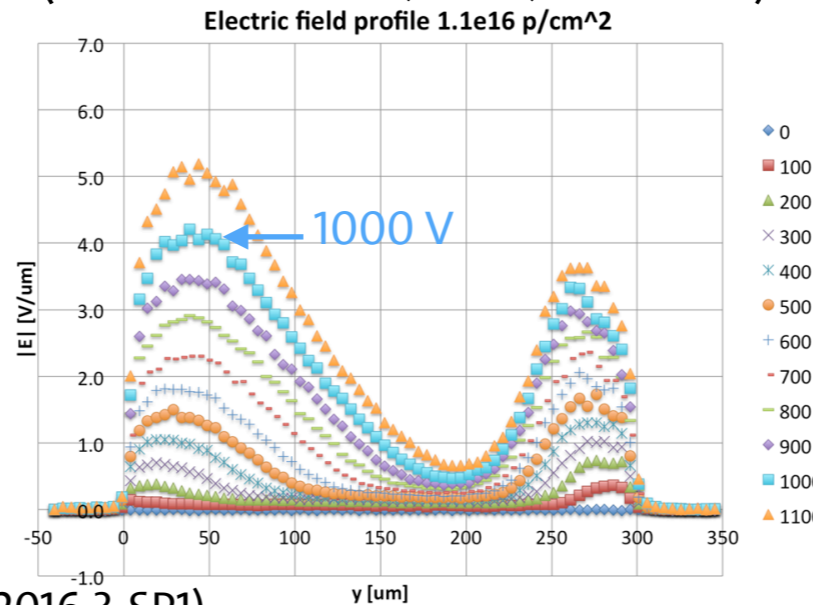


Electric field



Edge-TCT measurements

(M. Mikuž: Tredi, Paris, FEB 2016)



- Reverse current too low
- CV shows no frequency dependence
- CCE has not the correct voltage dependence
- No double peak

*) All simulations done with Synopsys TCAD (L-2016.3-SP1)

Attempts for the determination of new damage parameters:

- Simulation of the I-V, C-V and CCE with **infrared** of diodes for the fluences **3, 6, 13** • $10^{15} n_{eq}/cm^2$ and using the **optimizer** of TCAD for the determination of the free parameters i.e. minimize the relative deviation between the simulations and measurements over a large voltage range or more precise: Minimize simultaneously for every fluence

$$\begin{aligned}
 F = & \int_{-5V}^{-900V} \left(1 - \frac{I_{sim}}{I_{mes}}\right)^2 dV + \int_{-5V}^{-600V} \left(1 - \frac{C_{sim}^{455Hz}}{C_{mes}^{455Hz}}\right)^2 dV + \int_{-5V}^{-600V} \left(1 - \frac{C_{sim}^{1kHz}}{C_{mes}^{1kHz}}\right)^2 dV \\
 & + \int_{-200V}^{-1000V} \left(1 - \frac{CCEir_{sim}}{CCEir_{mes}}\right)^2 dV
 \end{aligned}$$

with I_{sim} simulated current, I_{mes} measured current

C_{sim} simulated capacitance, C_{mes} measured capacitance

$CCEir_{sim}$ simulated CCE, $CCEir_{mes}$ measured simulated

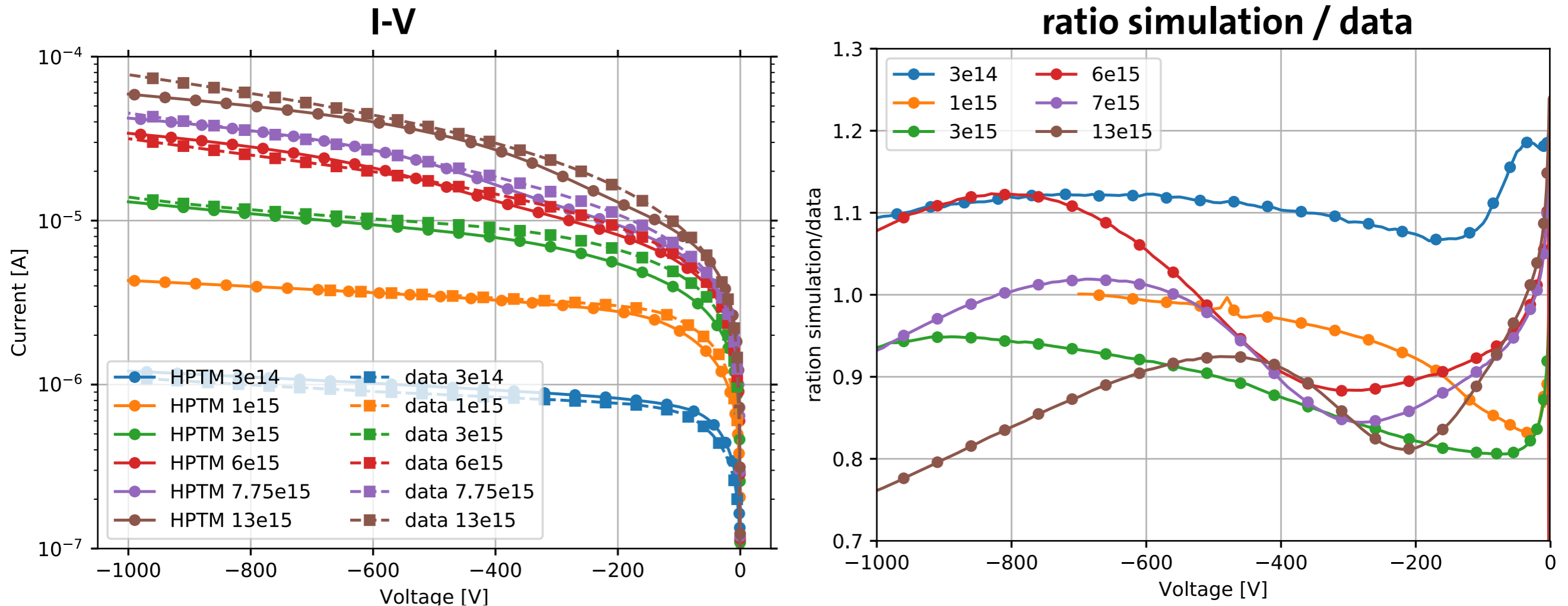
- I-V and C-V are simulated in 1D (CPU time: ≈ 3 min)
- CCE is simulated in 2D (r, ϕ) at 5 voltages (CPU time: ≈ 50 min)

Result of tuning: Hamburg Penta Trap Model (HPTM)

Defect	Type	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
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

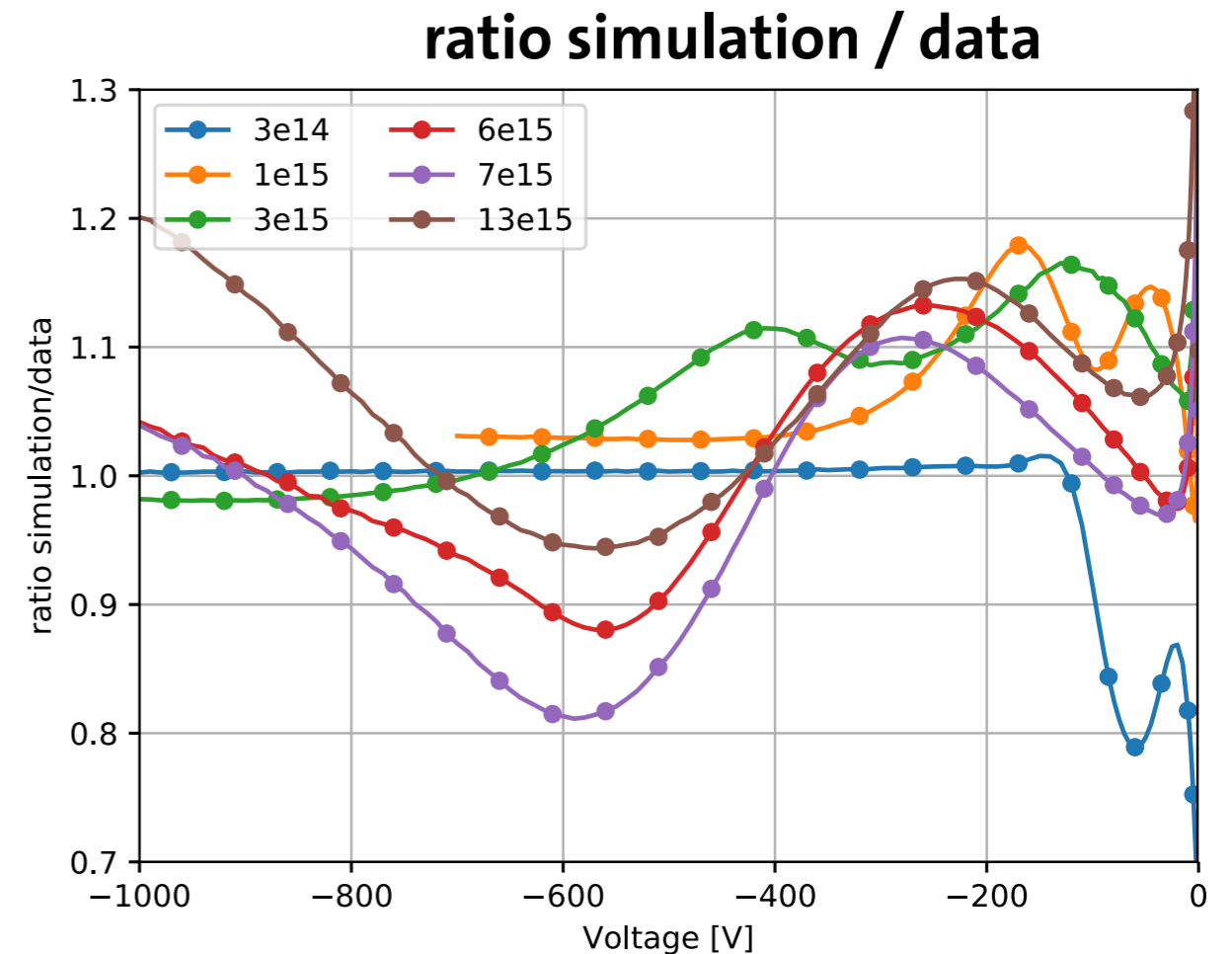
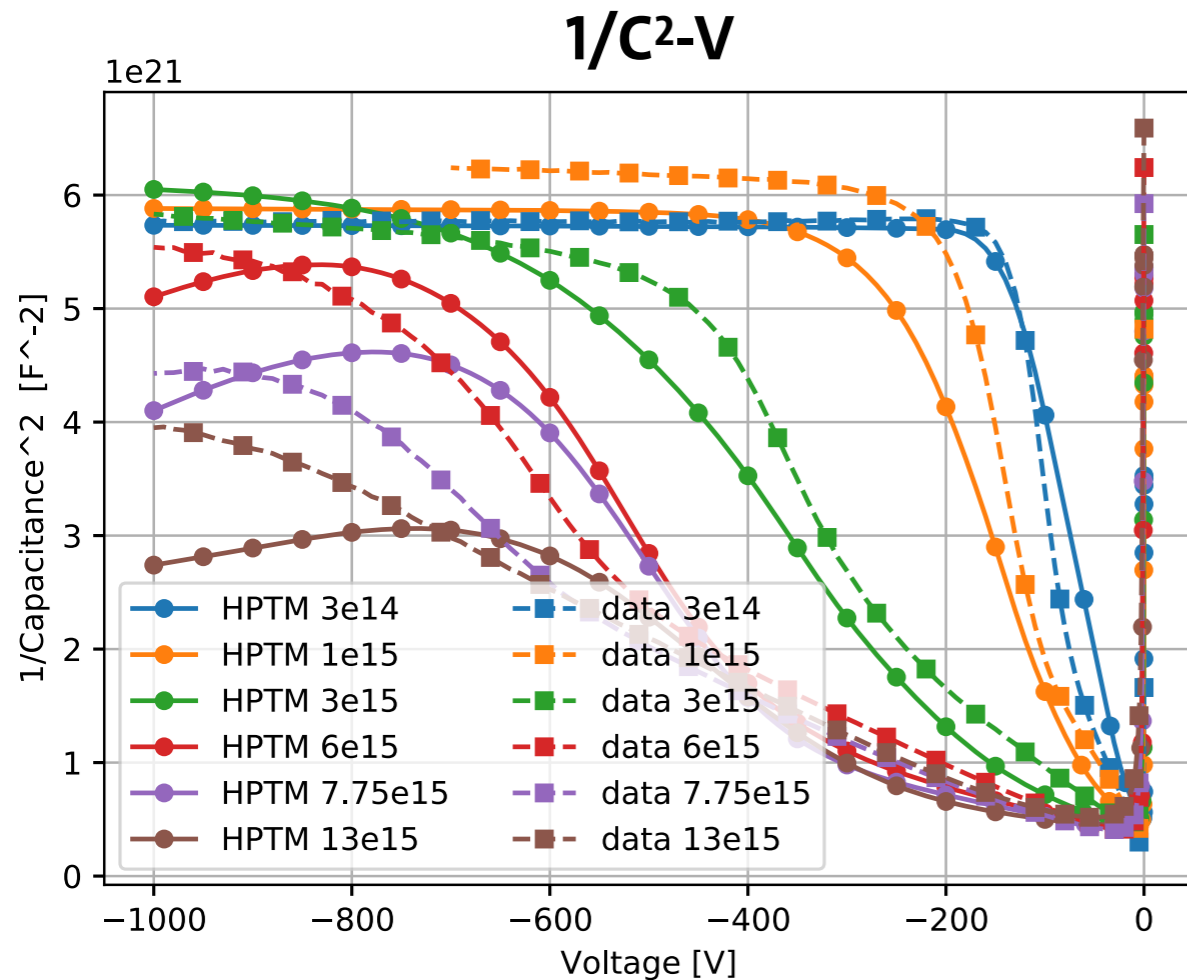
- Trap concentration of defects: $\mathbf{N} = g_{int} \cdot \Phi_{neq}$
- Simulations for the optimization have been performed at $\mathbf{T} = -20$ °C with:
 1. Slotboom band gap narrowing
 2. Impact ionisation (van Overstaeten-de Man)
 3. TAT Hurkx with tunnel mass = **0.25 m_e** (default value: 0.5 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

I-V for fluences from $0.3 - 13 \cdot 10^{15} \text{ n}_{\text{eq}}/\text{cm}^2$ at $T = -20 \text{ }^\circ\text{C}$ (for $T = -30 \text{ }^\circ\text{C}$ see backup)



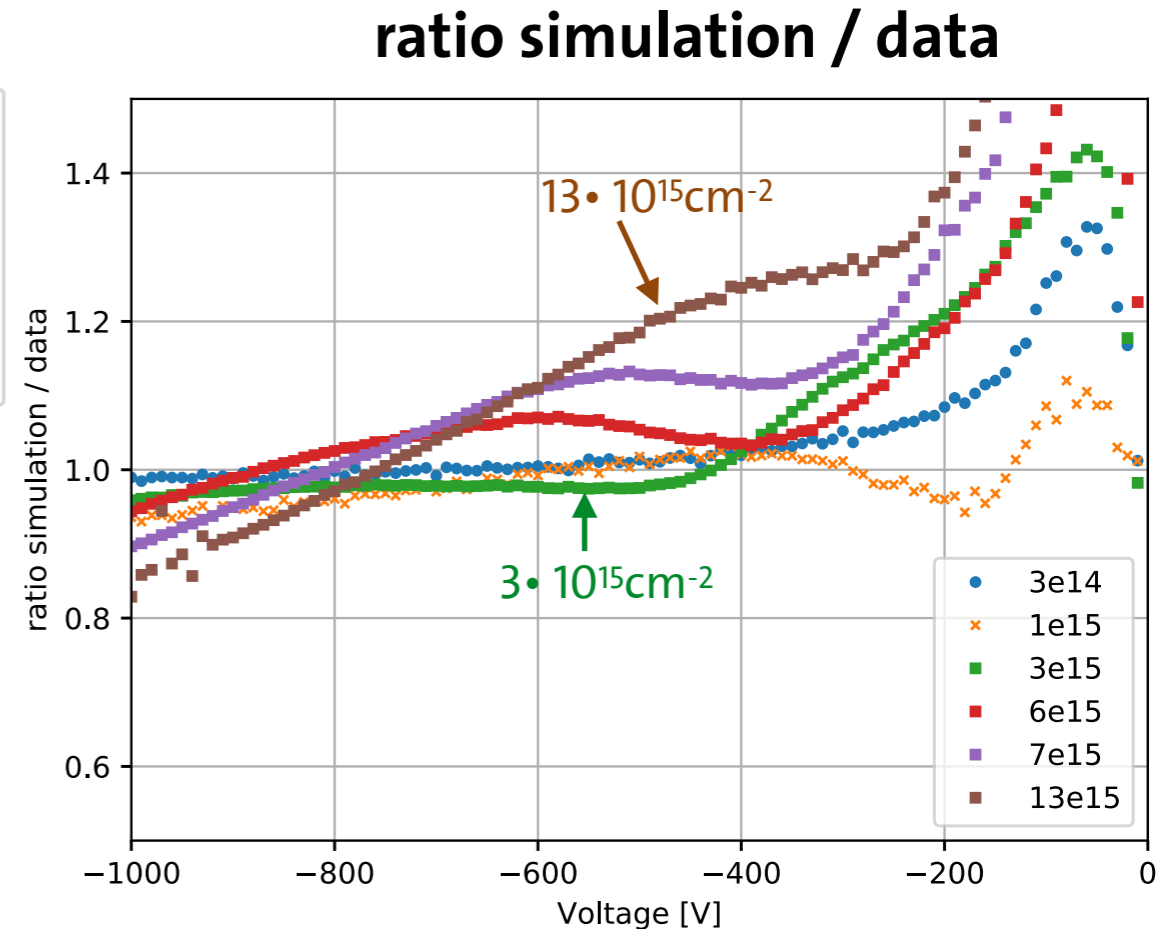
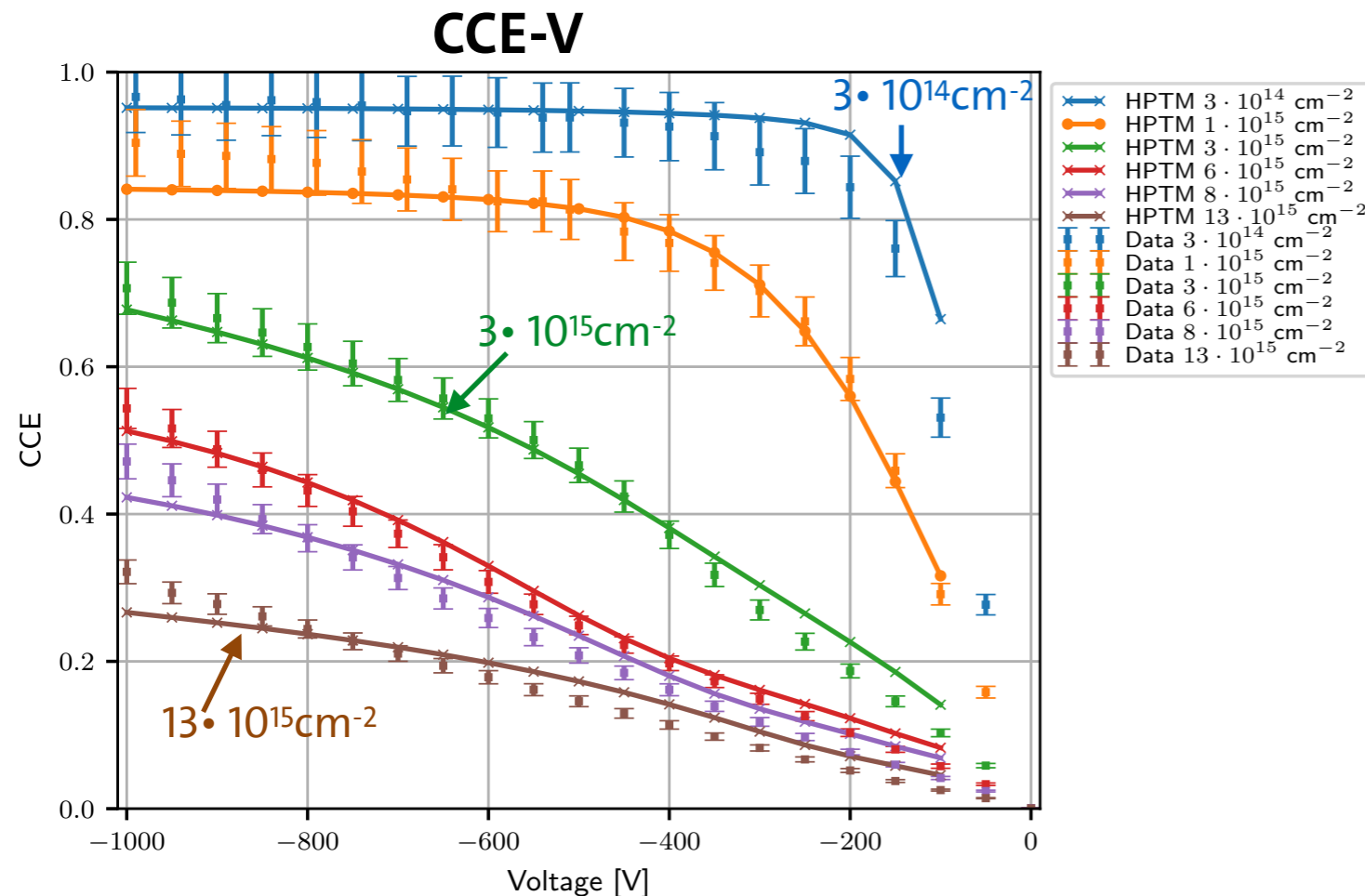
- The simulation for 0.3 and $1 \cdot 10^{15} \text{ n}_{\text{eq}}/\text{cm}^2$ are extrapolations and the $7.75 \cdot 10^{15} \text{ n}_{\text{eq}}/\text{cm}^2$ is a interpolation (not included in the optimization)
- The simulations agrees with the measurements within 20% for all fluences and voltages

C-V for fluences from $0.3 - 13 \cdot 10^{15} n_{eq}/cm^2$ at 455 Hz and $T = -20^\circ C$ (for $T = -30^\circ C$ see backup)



- The simulation for 0.3 and $1 \cdot 10^{15} n_{eq}/cm^2$ are extrapolations and the $7.75 \cdot 10^{15} n_{eq}/cm^2$ is a interpolation (not included in the optimization)
- The simulations agrees with the measurements within 20% for all fluences and voltages
- Deviation at highest fluence and voltage maybe due to impact ionization
- A better agreement between simulations and measurements is achieved at 1 kHz

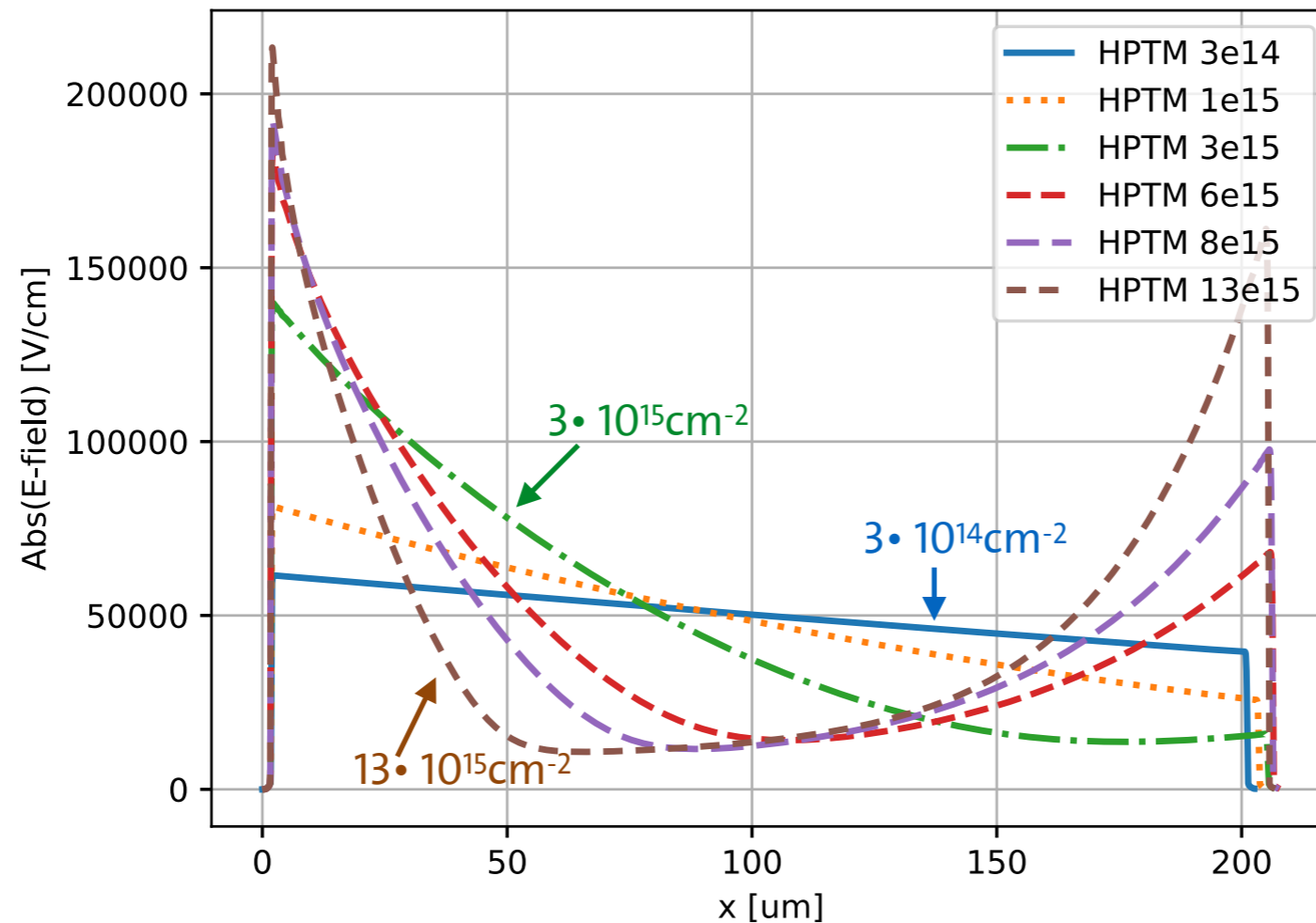
CCE vs. V for fluences from $0.3 - 13 \cdot 10^{15} \text{ n}_{\text{eq}}/\text{cm}^2$ with infrared laser and $T = -20 \text{ }^\circ\text{C}$ (for $T = -30 \text{ }^\circ\text{C}$ see backup)



- In the optimization only the voltages -200, -400, -600, -800 and -1000V were used
- For all fluences the voltage dependence is good reproduced
- At high voltages the simulations agrees with the measurements within 20% for all fluences

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

E-field vs position

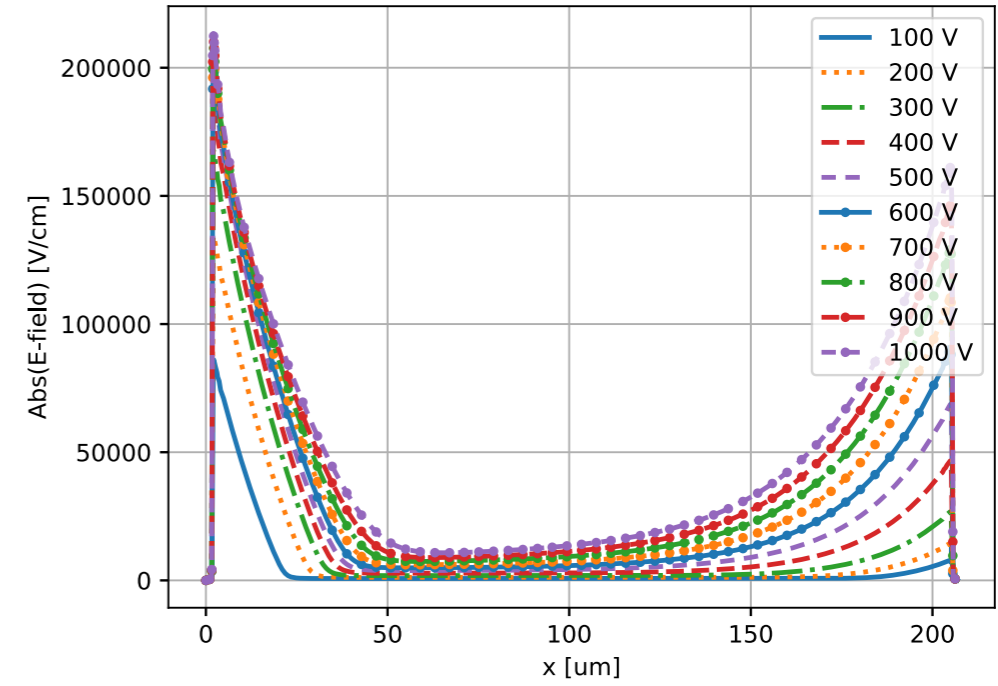
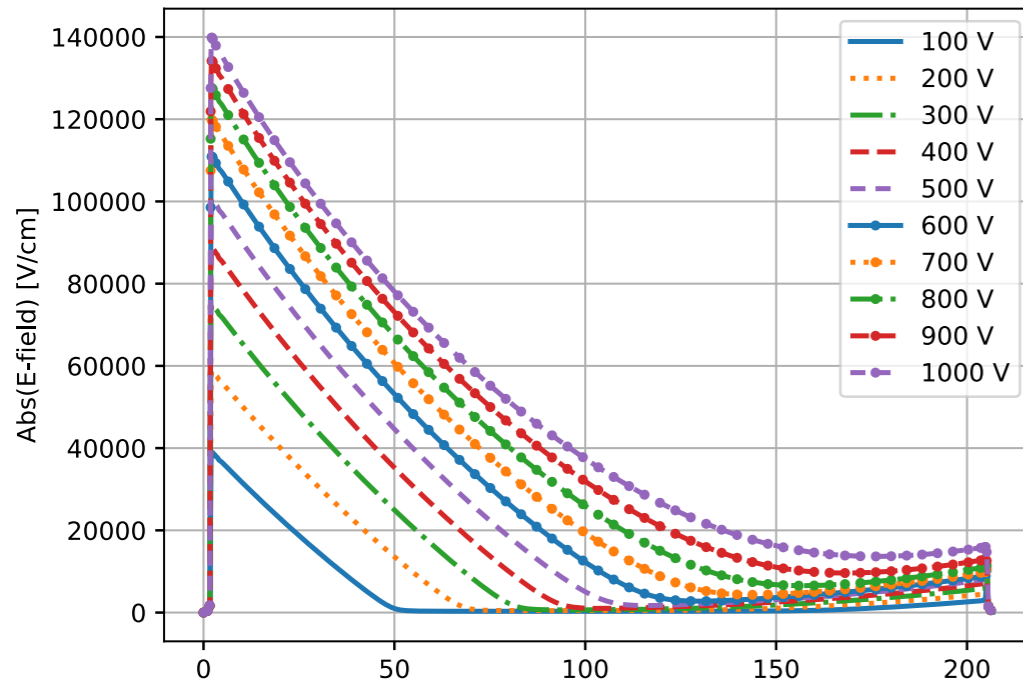


- Double peak structure for fluences $\geq 3 \cdot 10^{15} n_{eq}/cm^2$ clearly visible
- Peak field of $\approx 2 \cdot 10^5$ V/cm at the highest fluence \rightarrow impact ionisation

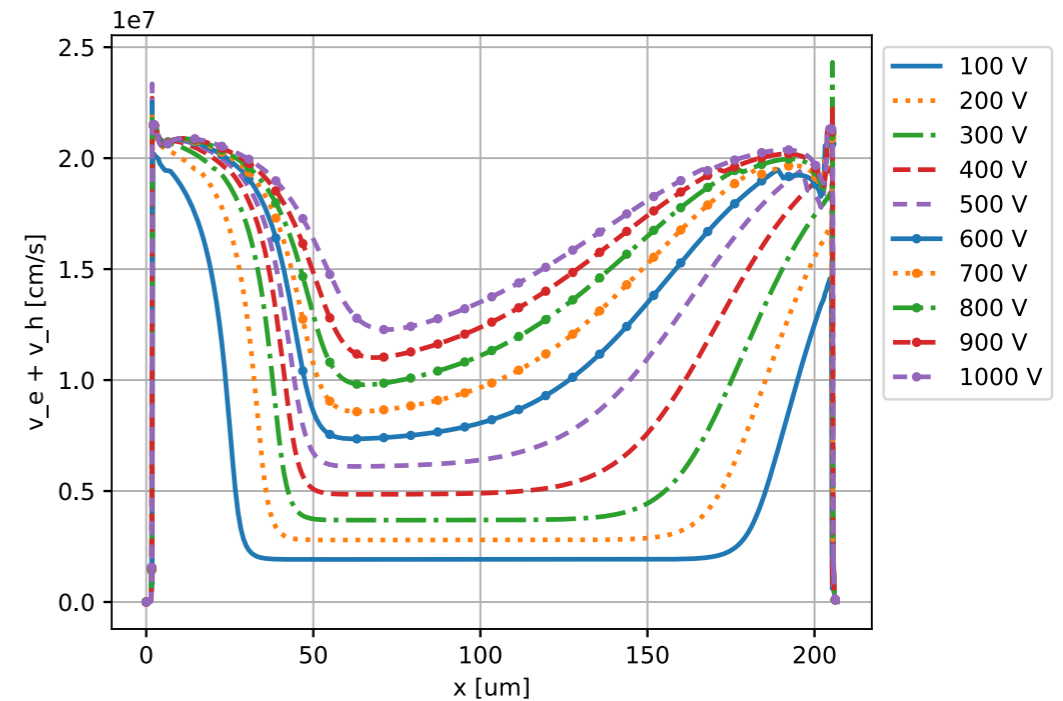
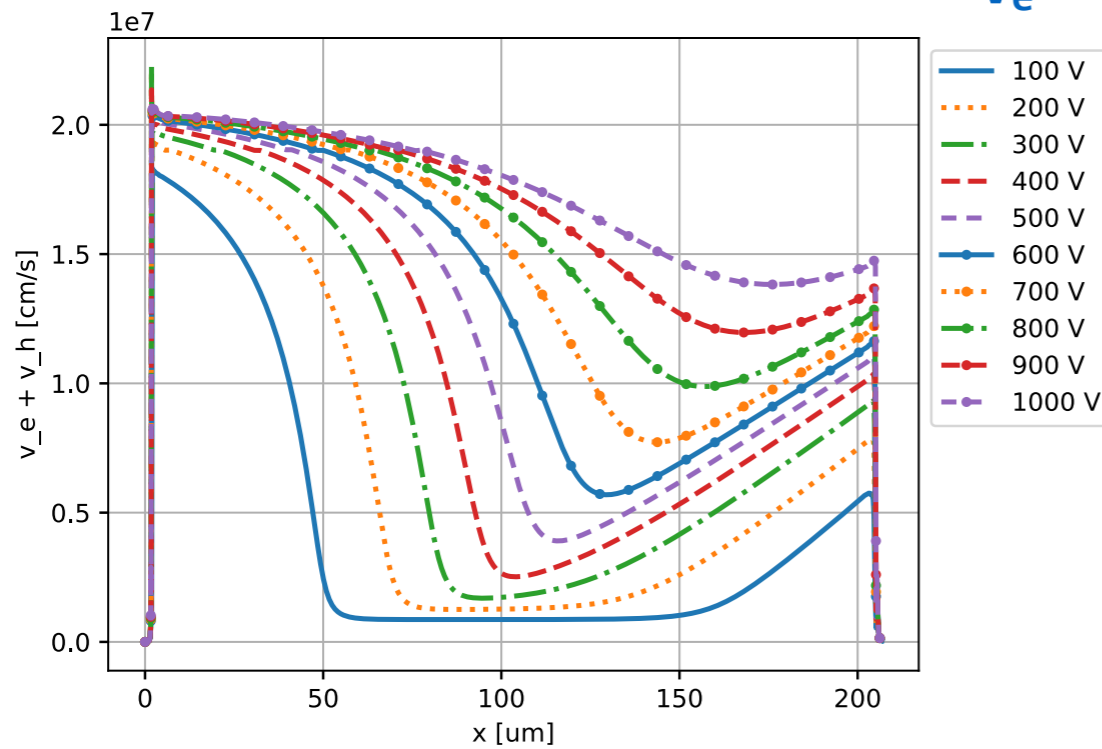
$3 \cdot 10^{15} n_{eq}/cm^2$

E-field vs. voltage

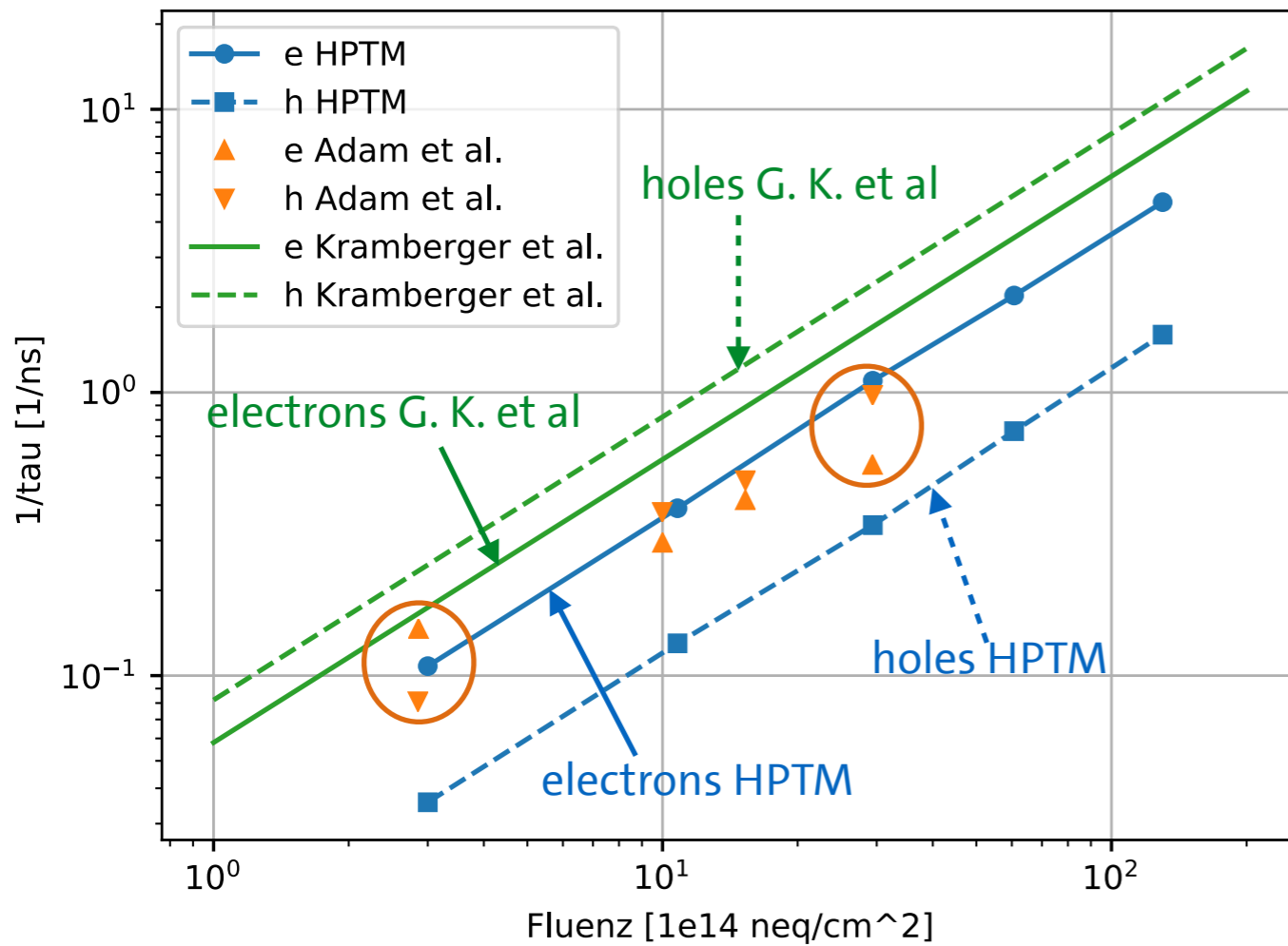
$1.3 \cdot 10^{16} n_{eq}/cm^2$



$v_e + v_h$ vs. voltage



Trapping rates:



- For HPTM the trapping probability of electrons a factor 3 higher than for holes
- Similar to old alpha TCT measurements but different to new red laser TCT measurements
- Effect known since Brodbeck et al NIMA 2000, but not investigated further

Kraner et al NIMA 1993

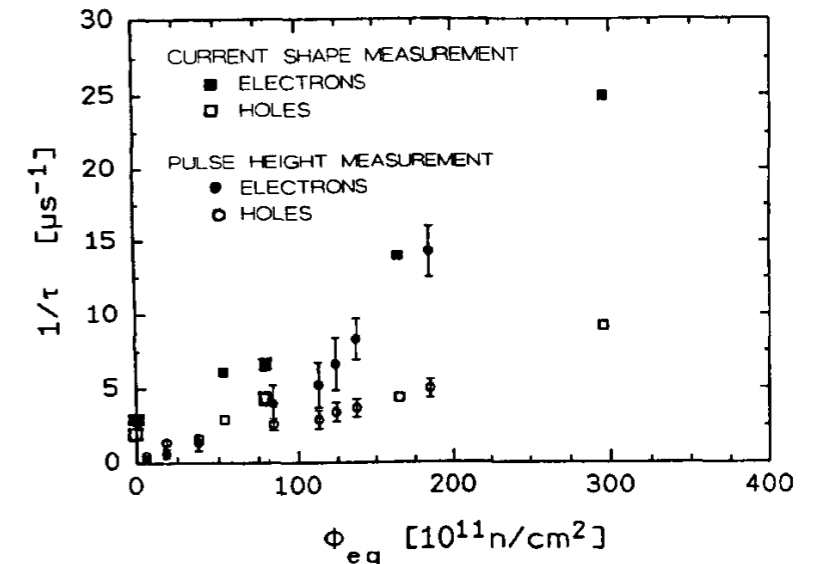
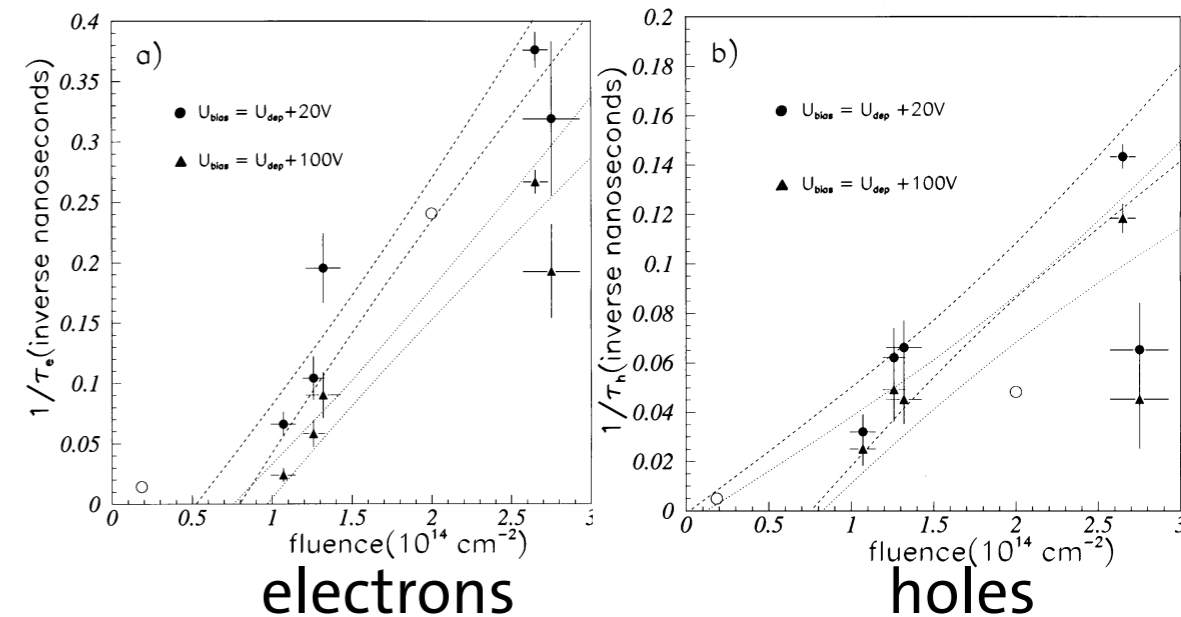


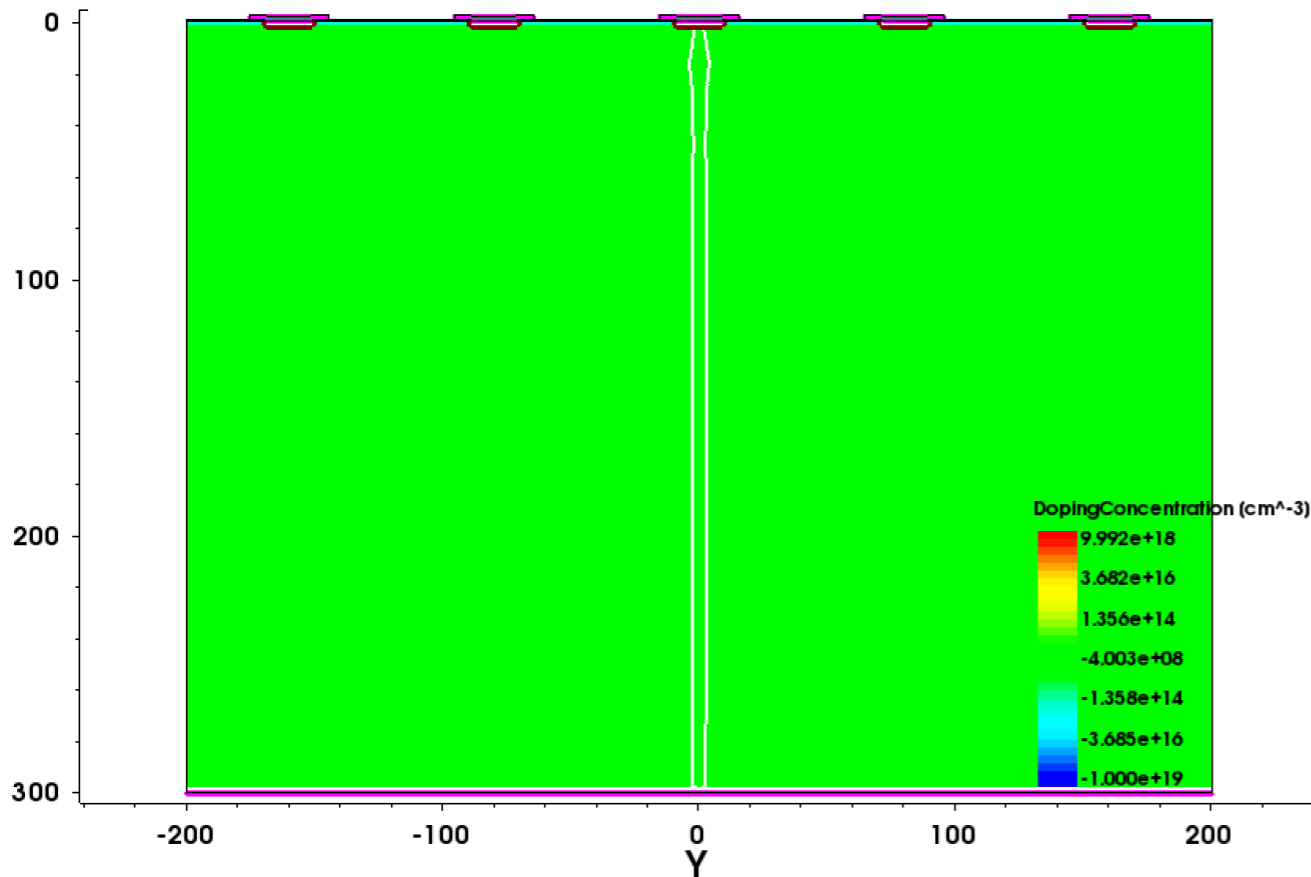
Fig. 9. Trapping probabilities, $1/\tau$, for both holes and electrons as a function of fast neutron fluence as measured by the observed pulse width (squares) and the calculated charge collection time (circles).

Beatie et al NIMA 1999



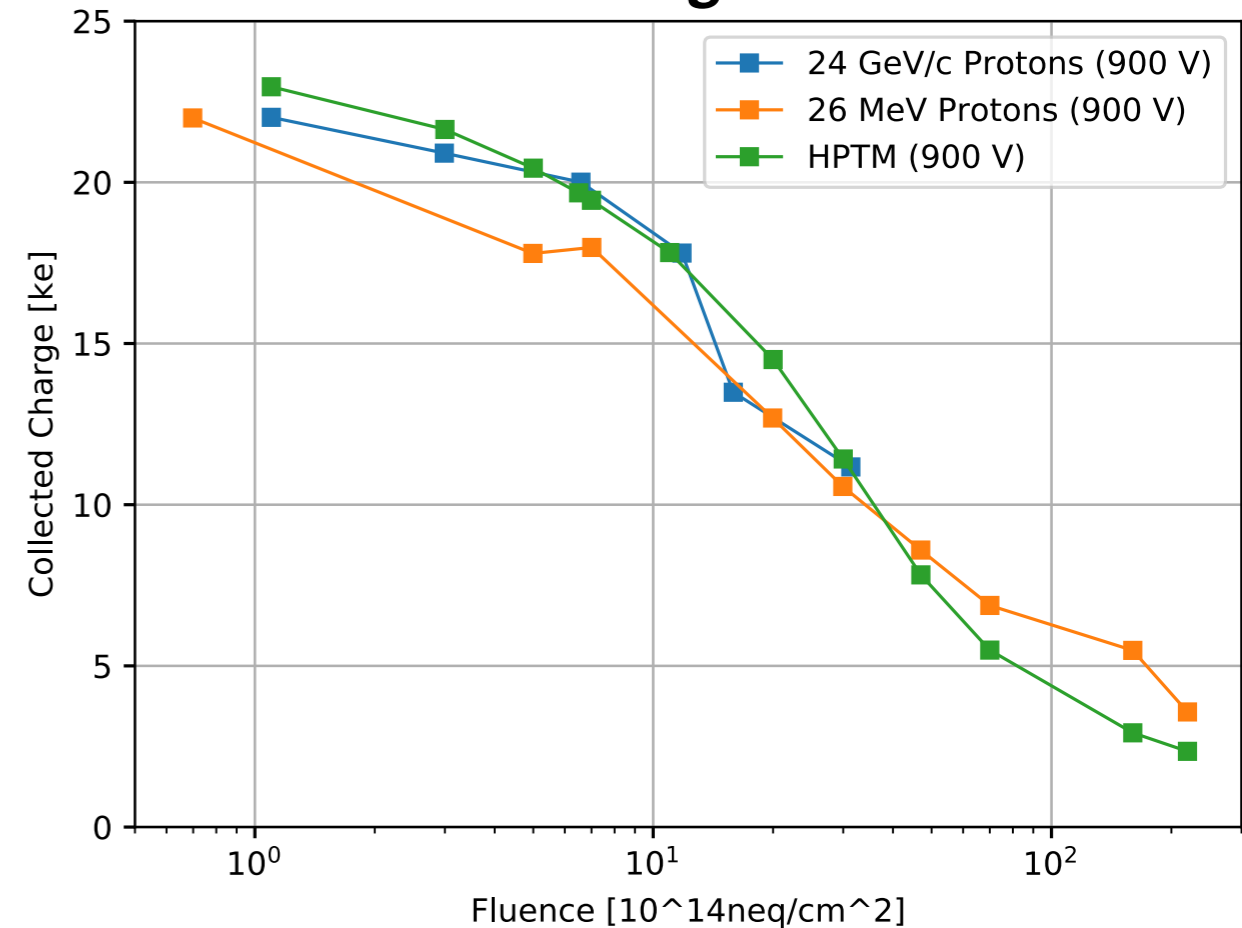
Charge collection measured with strip sensors (data from Affolder et al NIMA 2010)

Simulated structure

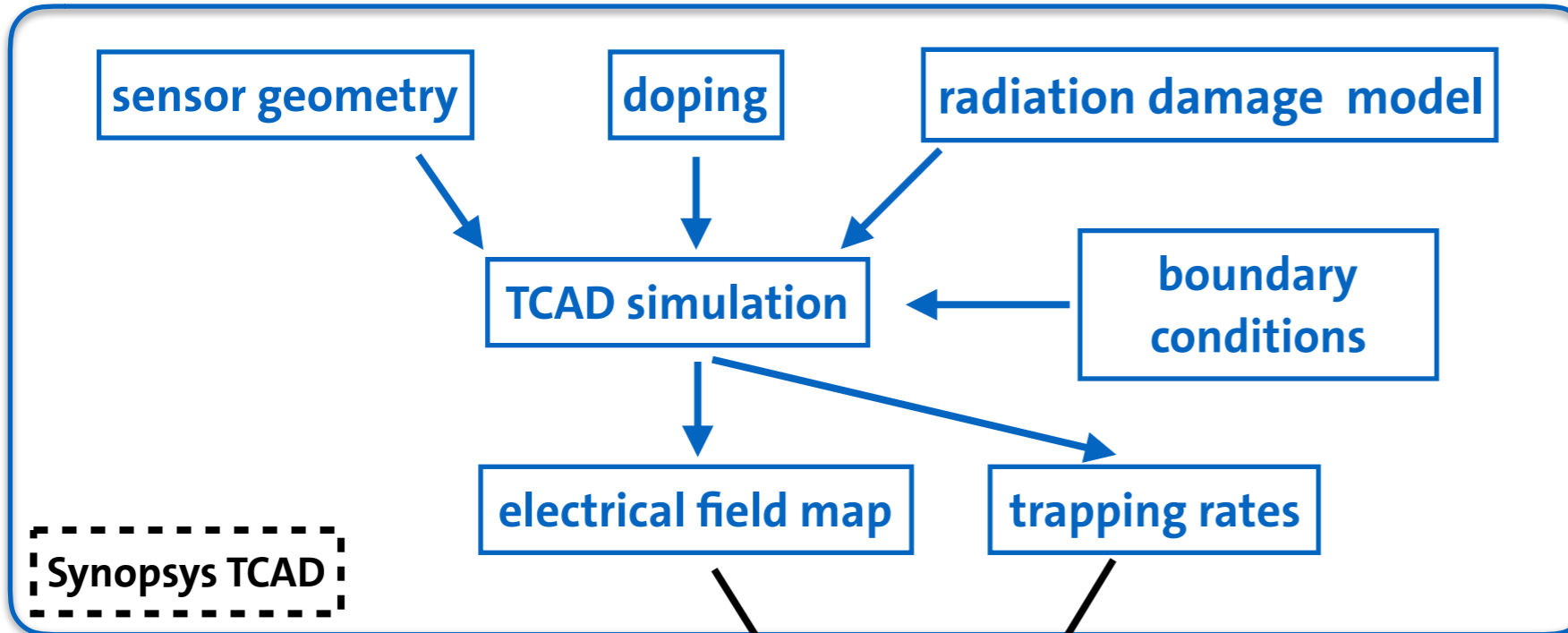


- 5 AC coupled strips simulated
- 80 e-h/um generated

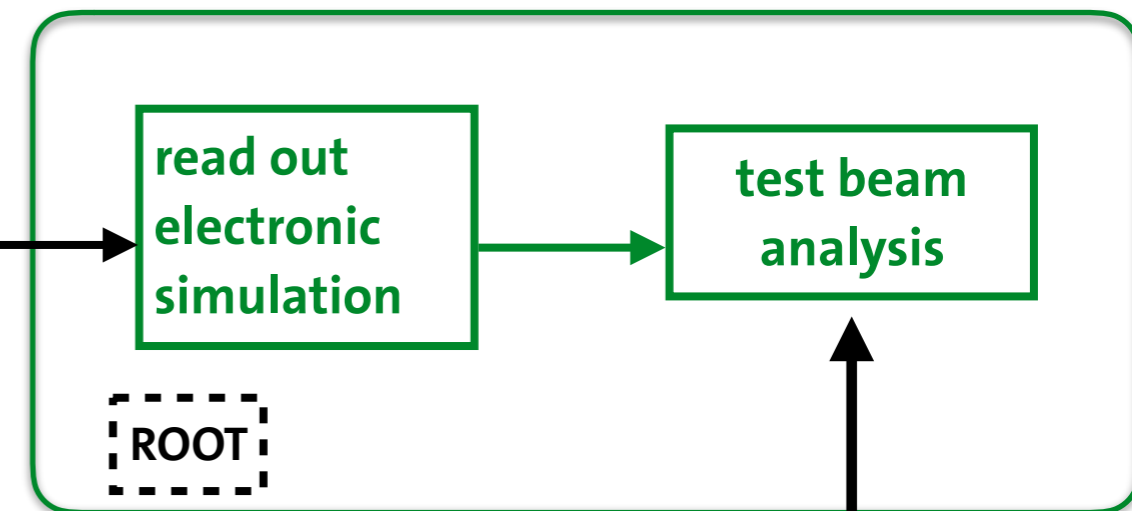
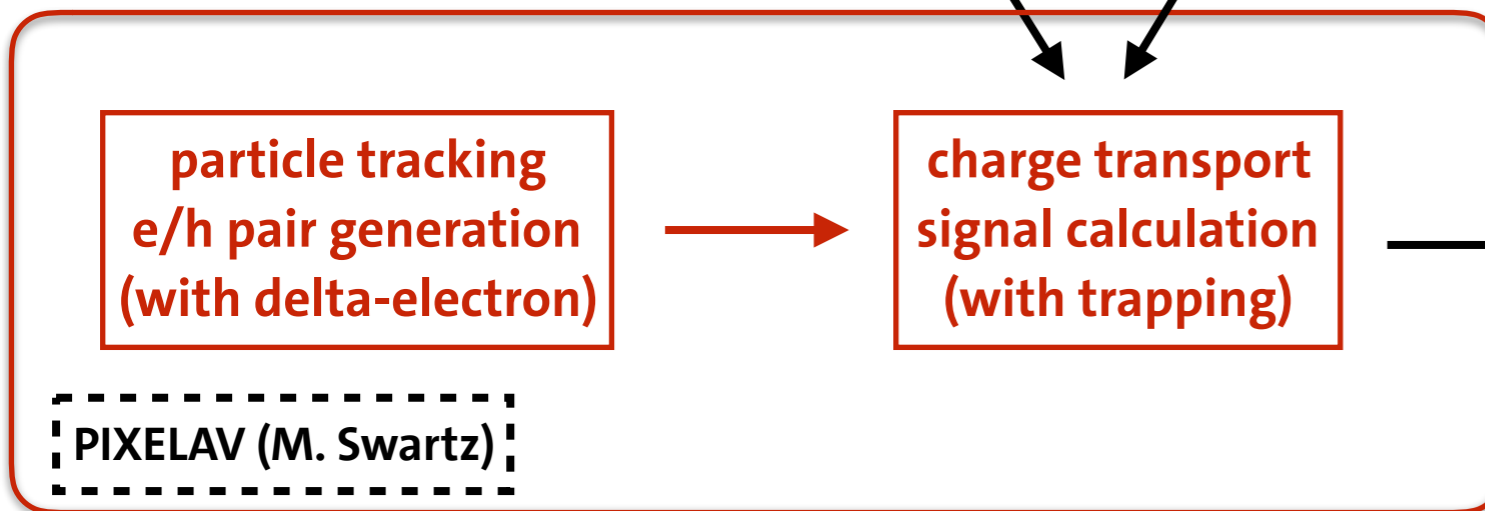
Collected charge vs. fluence



- Float zone silicon
- 300 um thick sensors
- 80 um pitch
- T = -25 °C
- ^{90}Sr source

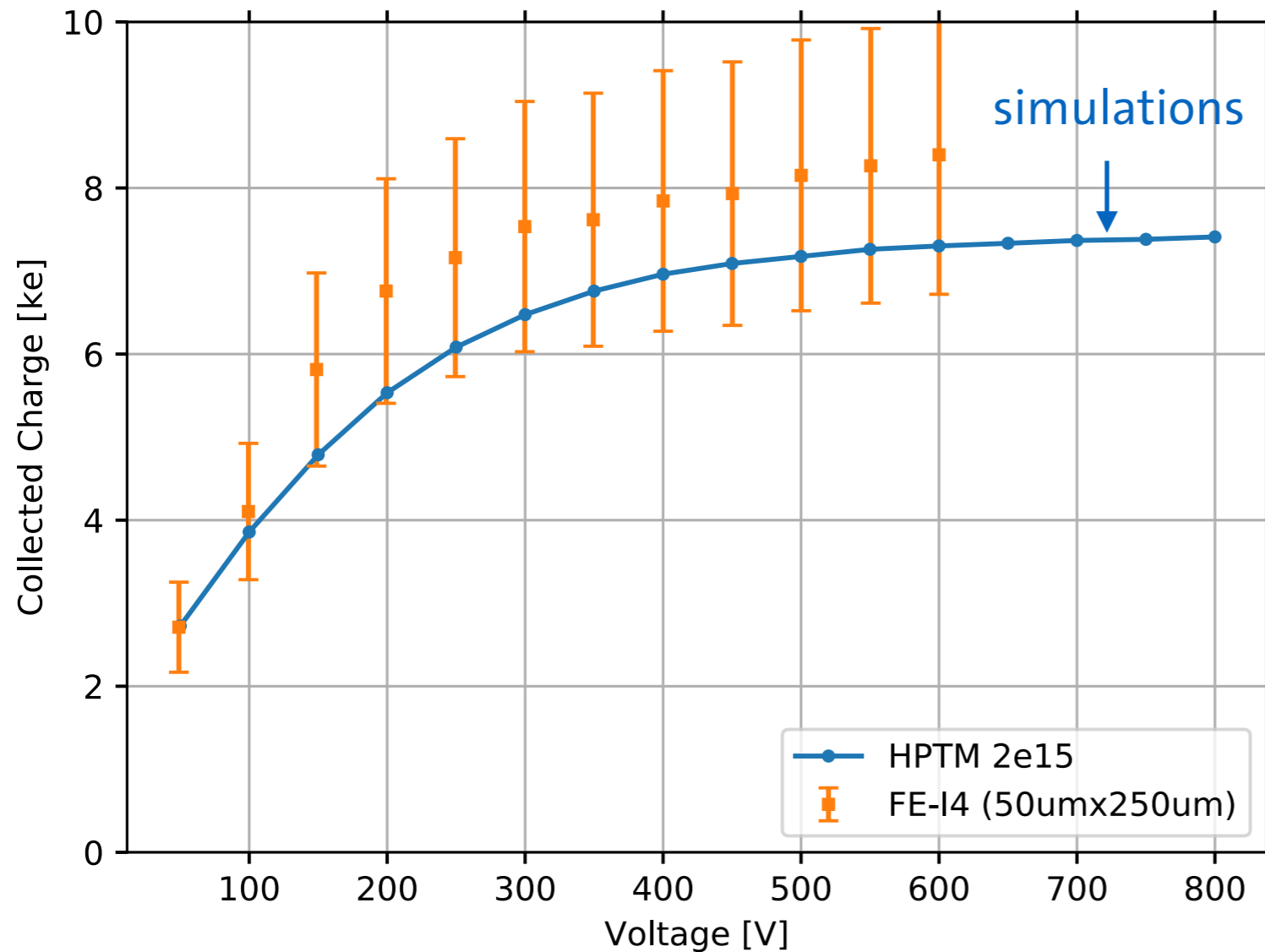


C++ / Python program



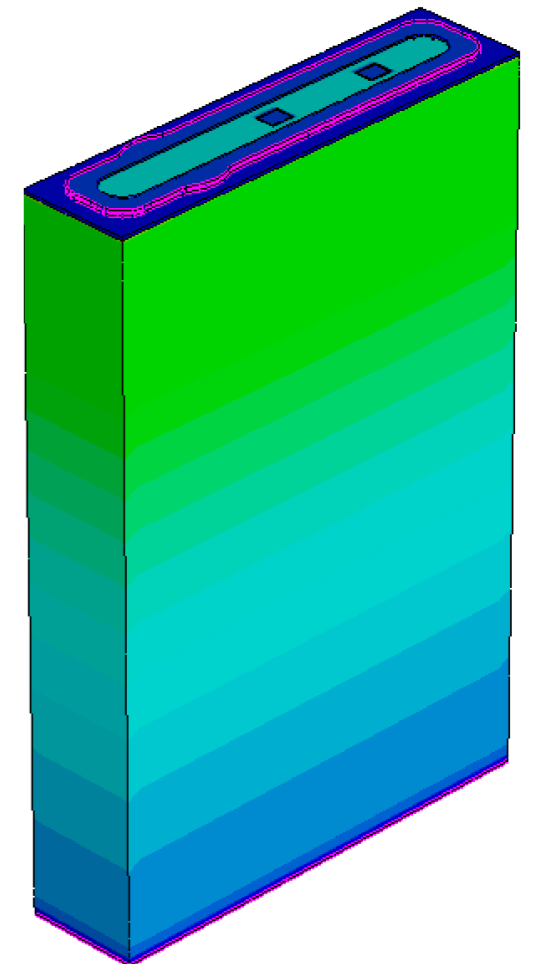
test beam data

Collected charge vs voltage for $2 \cdot 10^{15} \text{ n}_{\text{eq}}/\text{cm}^2$ and 150 μm thick sensors



Simulations:

- $T = -15 \text{ }^\circ\text{C}$
- Noise: 170 e
- Threshold: 1000 e



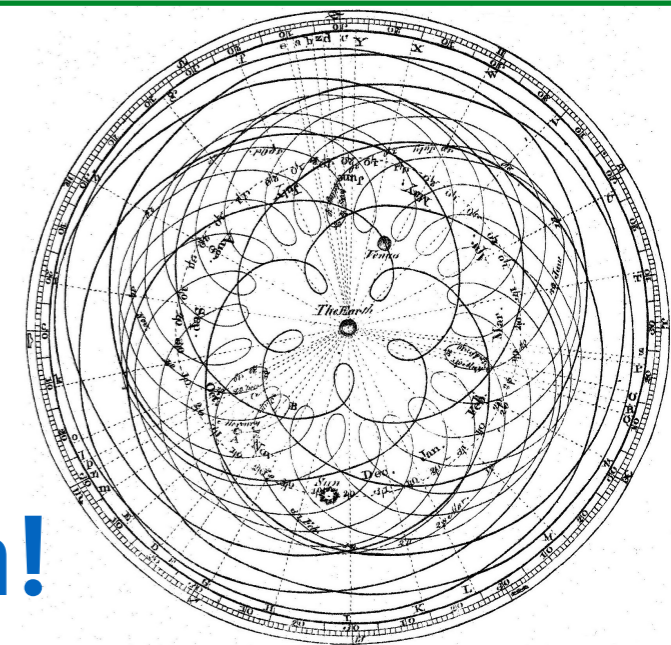
- FE-I4 data from S. Terzo Phd thesis 2015
- Data from non-annealed sensors

- New measurements (IV, CV, CCE) on highly irradiated diodes are available
- A comparison of the measurements with TCAD simulations using the Perugia trap parameters shows a large disagreement
- Attempts are made to develop a new model by fitting I-V, C-V and CCE measurements using the optimizer of TCAD
- The **Hamburg Penta Trap Model** gives a **significantly better** and **consistent** description of a **large set of measurements** of pad diodes irradiated with protons in the fluence range from $3 \cdot 10^{14} n_{eq}/cm^2$ to $1.3 \cdot 10^{16} n_{eq}/cm^2$
- First application of HPTM in strip sensor simulations and to pixel sensors in combination with PIXELAV are encouraging

To do:

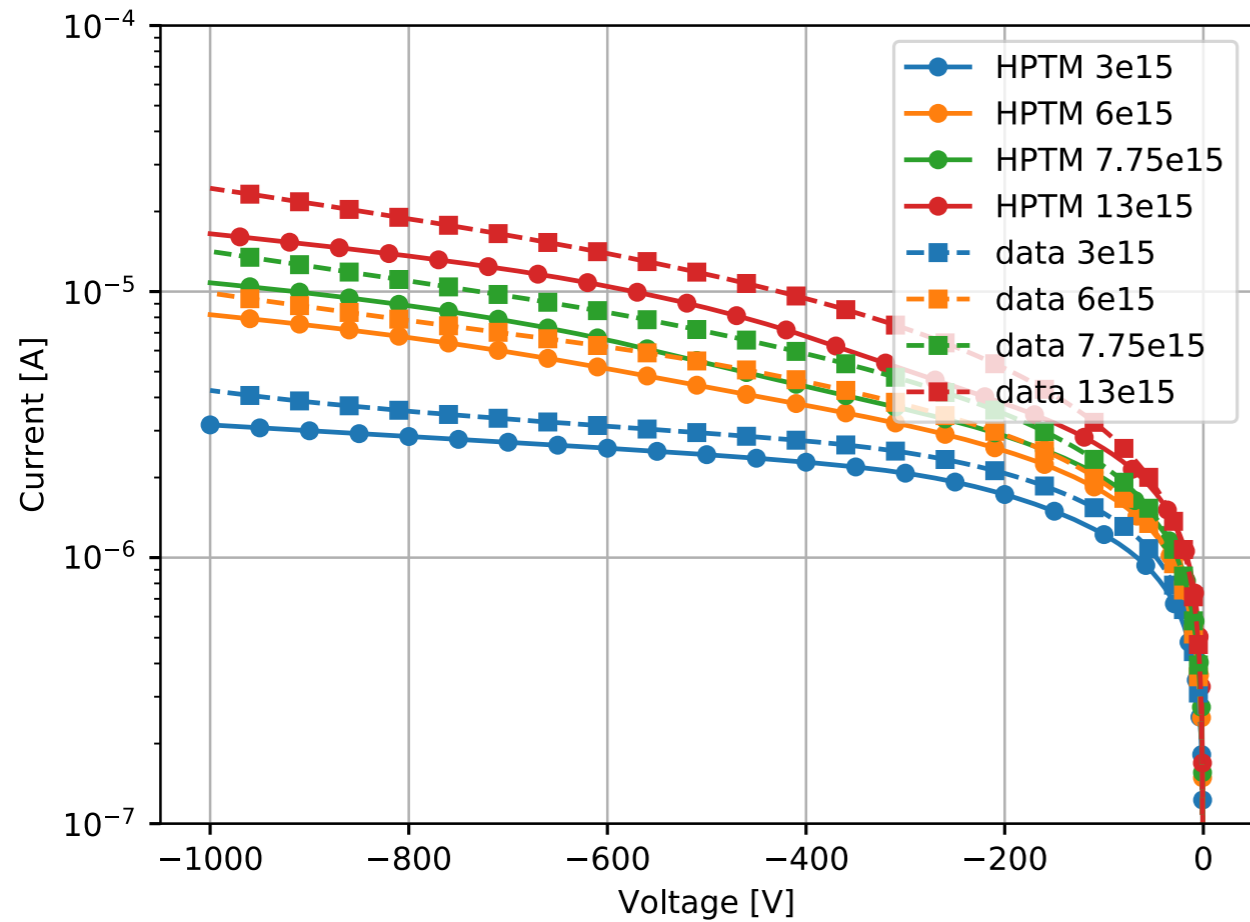
- Improve temperature dependence of HPTM by introduction of temperature depending cross sections for I_p
- Reduction from 5 to 4 defects? There are indication that H220 is not needed.
- Differences in trapping rates by red laser and alpha particles

End of the epicycles?

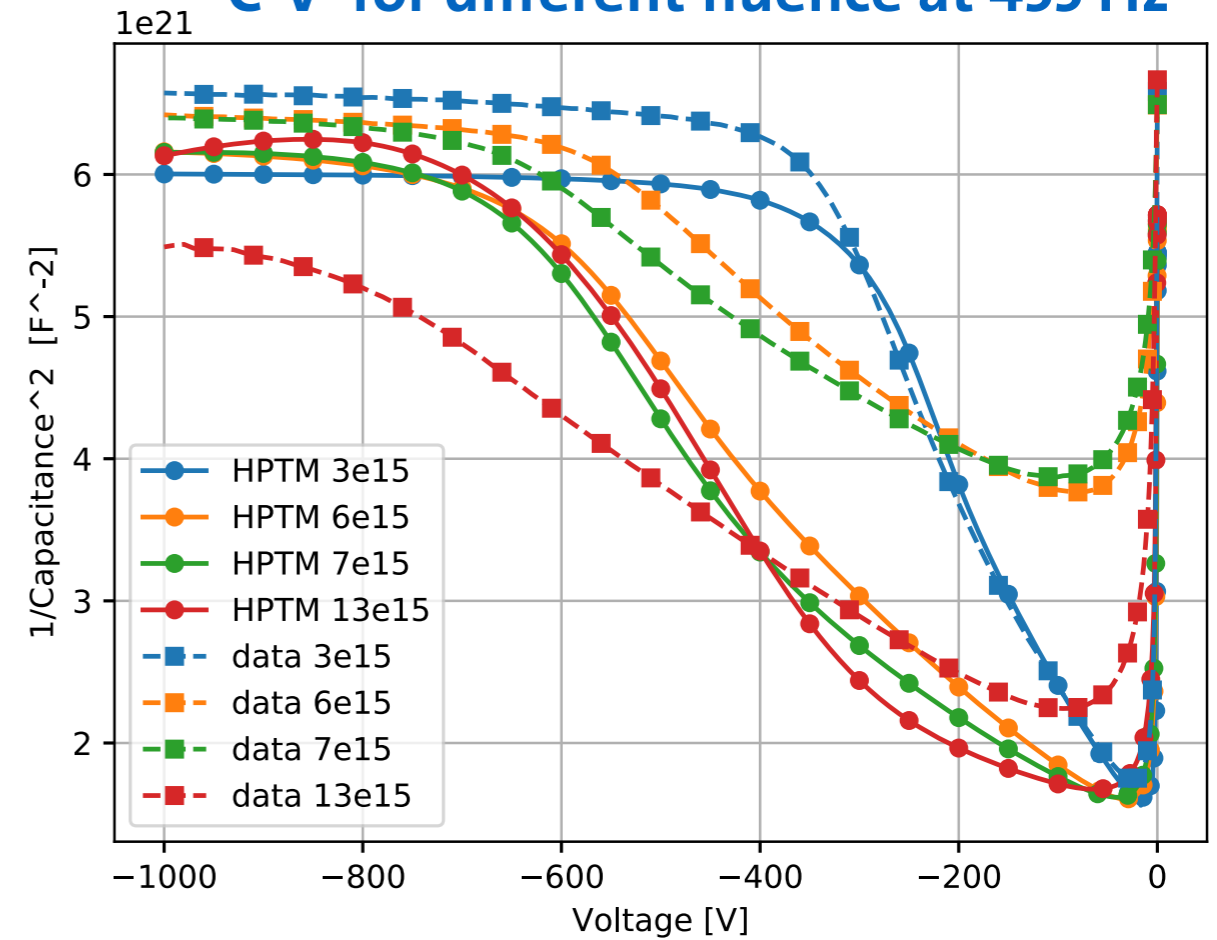


Thank you for your attention!

I-V



C-V for different fluence at 455 Hz



CCE-V for different fluence (infrared) at T = -30 °C

