Using Synopsys TCAD in high-energy physics experiments

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OUTLINE

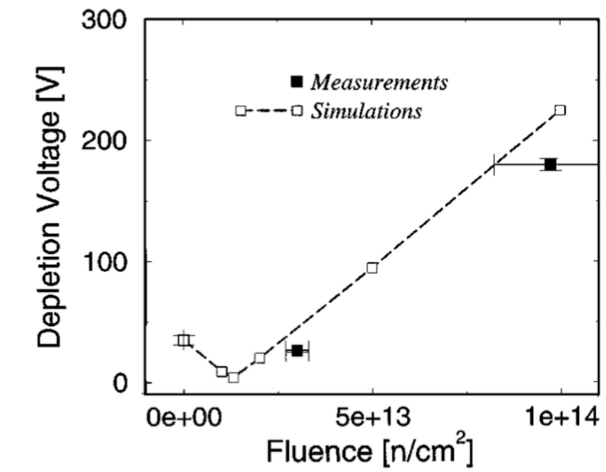
- Introduction
- Examples of process simulation
- Examples of device simulation
  - Optimisation of AGIPD pixel sensor for high X-ray doses
  - Simulation related to the investigation of the insulator layer for segmented silicon sensors
  - Development of a bulk radiation damage model
- Summary

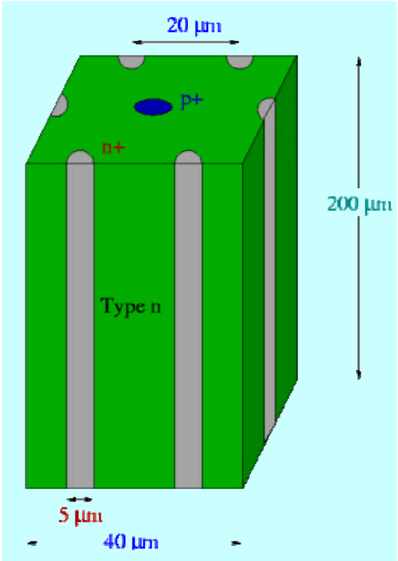
INTRODUCTION

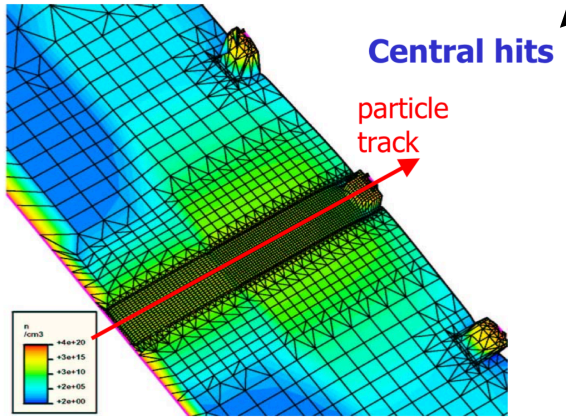
Since about 2000 Integrated Systems Engineering TCAD (acquired in 2004 by Synopsys) is used the sensor development in high-energy physics

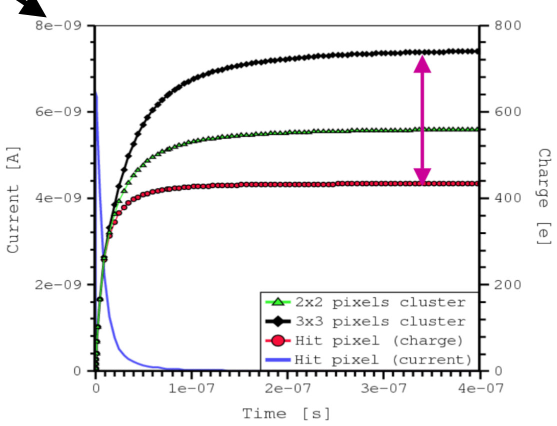
First application examples are:

- **Radiation damage simulation of diodes** (D. Passeri et al., "Comprehensive Modeling of Bulk-Damage Effects in Silicon Radiation Detectors", IEEE-TNS Vol. 48,pp. 1688 (2001))
- **Process and device simulation of 3D sensors** (P. Roy et al. , "Development of 3D detectors at the University of Glasgow", 1st RD50 Workshop, CERN 2-4 October 2002)
- **Charge collection simulation of MIMOSA sensor** (D. Contarato, et al., "Monolithic Active Pixel Sensors for the TESLA Vertex Detector ", 3rd RD50 Workshop, CERN 3-5 November 2003)









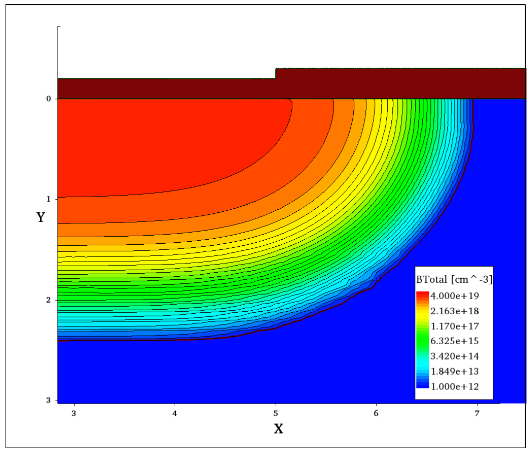
INTRODUCTION

Today's application areas and topics in HEP are:

- Process optimisation (mainly done by producers of sensors / vendors)
- Device characterisation of different kind of sensors and test structures e.g:
  - Pad diode, strip, planar and 3D pixel sensors
  - LGAD, CMOS, SiPM, HV-CMOS
  - Gate-controlled diodes, MOS capacitors and MOSFET's
- Device optimisation of sensors with respect to e.g. breakdown voltage, inter strip/ pixel capacitance, radiation hardness, charge collection etc.
- Developing of radiation damage models for bulk and surface defects
- Simulation of electric fields to be used as input for other simulation tools (Allpix^2 , PixelAV, etc)

TCAD

2D Boron profile



TCAD (Technology Computer Aided Design):

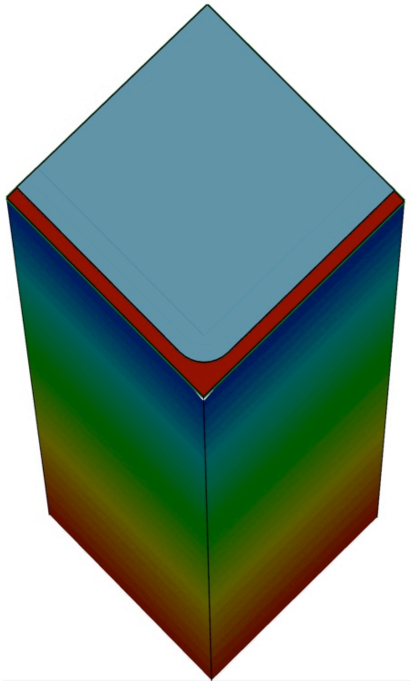
- Process simulation → doping profile
- Device simulation → electrical behaviour

- Works by modelling electrostatic potential (Poisson's equation) and carrier continuity equations
- Takes mesh, applies semiconductor equations + boundary conditions (in discrete form) and solves

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

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 $\mathbf{J}_p = qp\mu_p\mathbf{E} - qD_n\nabla p$



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

- Post-processing → Electrics fields, current density, breakdown voltage etc.

Examples of process simulation

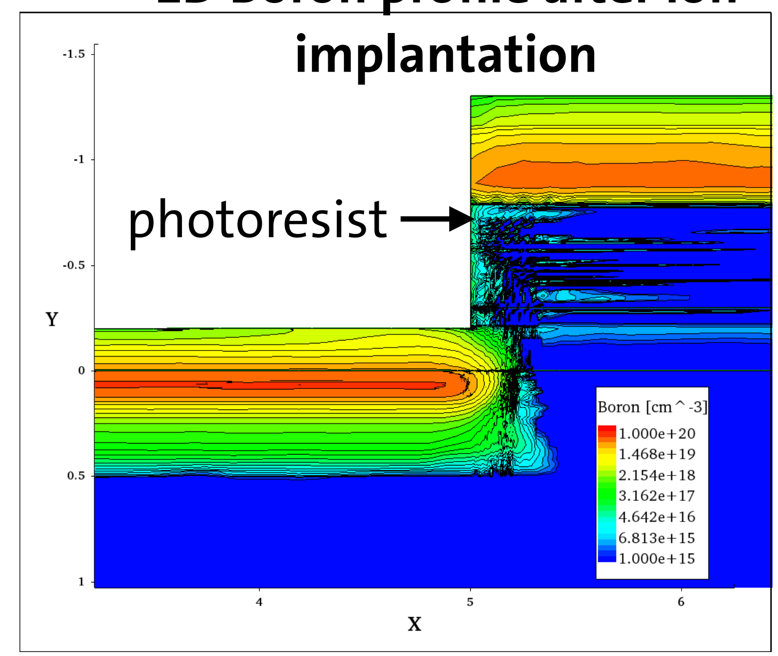
PROCESS SIMULATION

Why process simulation? Doping profiles are critical for e.g. breakdown etc.

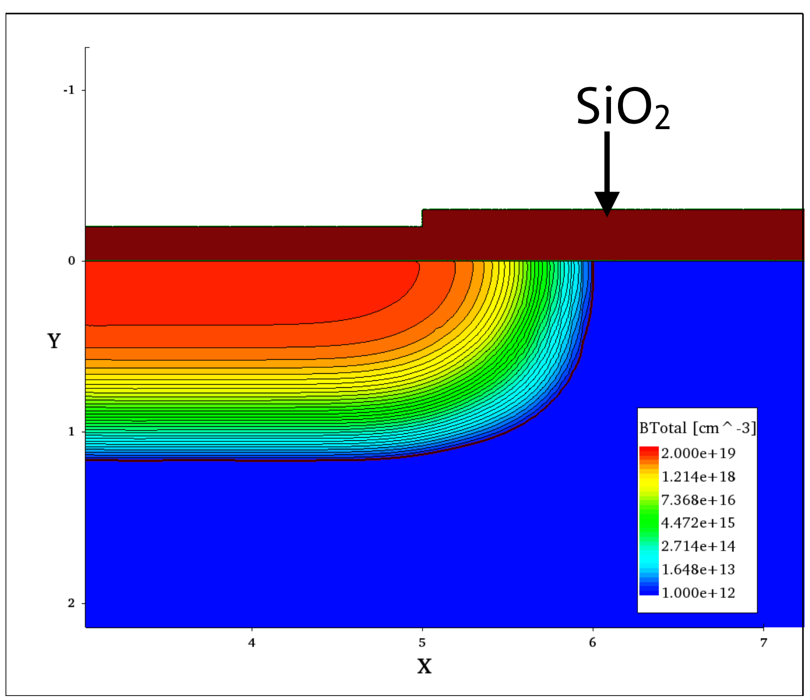
- Example: Ion implantation and drive-in for a p^+-n sensor:
  - 2D Sentaurus Process sim.
  - Simulated structure:
    - 10 µm wide , 5 µm thick Si
    - 300 nm SiO_2
    - 5 µm implant window

Doping	10^{12} [cm^{-3}] (P)
Orientation	<111>
Tilt angle	0°
Implant	Boron
Dose	1x10^{15} [ions/cm^2]
Energy	70 keV

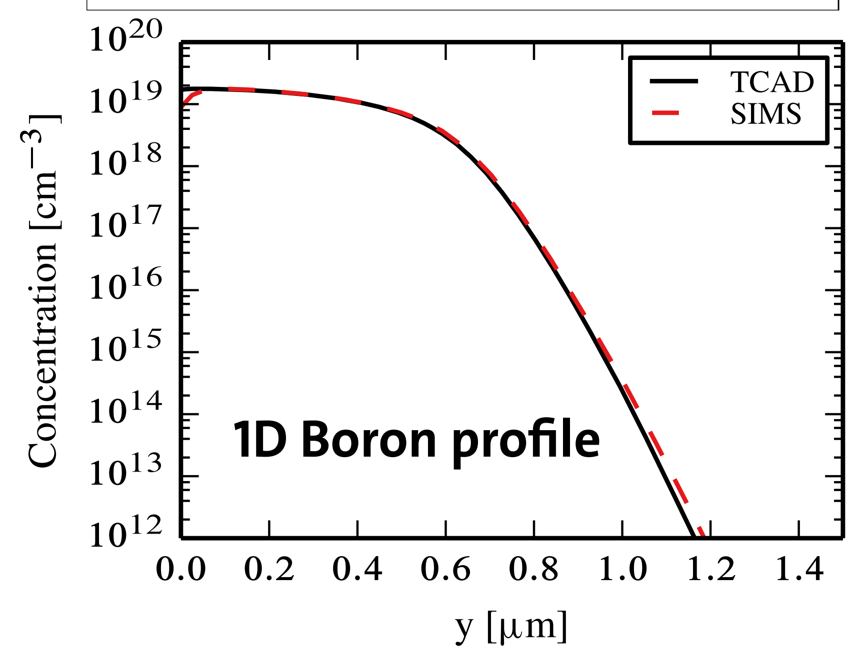
2D Boron profile after ion implantation



2D Boron profile after drive in



- Junction depth: 1.2 µm
- Lateral extension: 1 µm



Simulation has to be calibrated with SIMS or other measurement on test structures for the same process

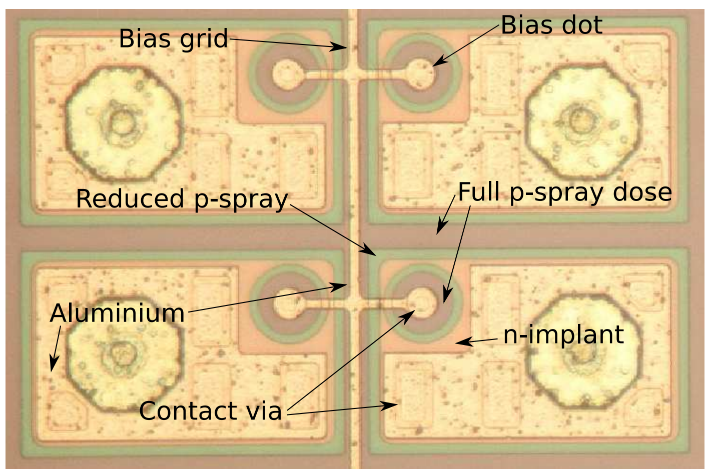
PROCESS SIMULATION

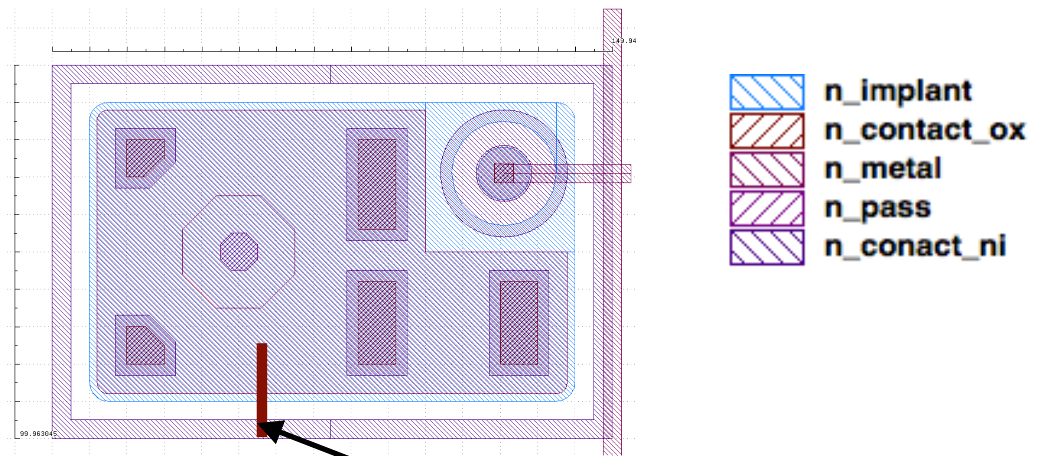
Process simulation of sensors for HEP:

- 1D, 2D and 3D simulation can be done with icwbev, sprocess and sde using GDS files
- For large structure reduce as much as possible the complexity of the simulation domain into simpler/smaller subdomains

Example:

- 285 µm thick **n⁺-n** pixel sensor with pixel size of 150 µm x 100 µm and moderated p-spray isolation + punch through





Cutline for process simulation

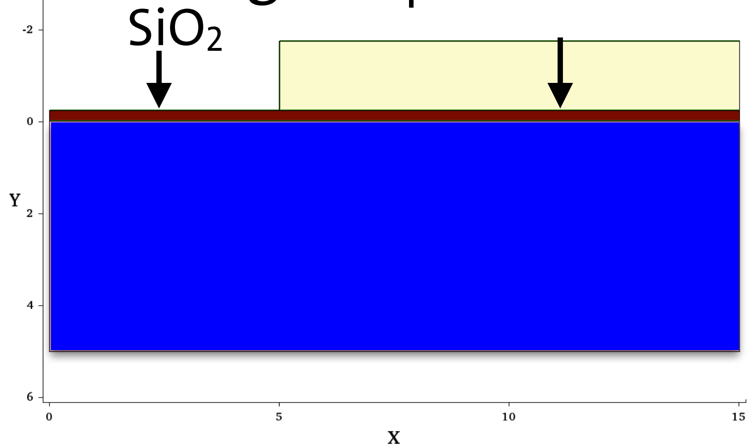
- If your simulation task allows → neglect bias dot
- Contact holes usually not import → Increase contact holes as much as possible

➡Simulate a 2D cut

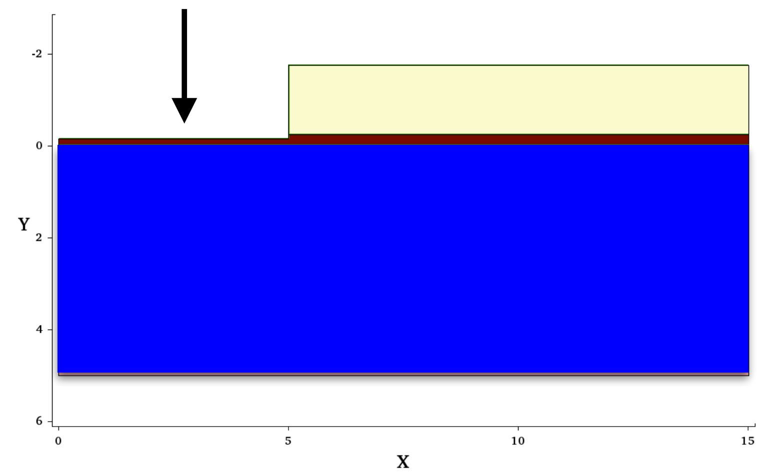
➡Sweep the 2D doping profile along the periphery of the n⁺ implant to generate a 3D profile

PROCESS SIMULATION

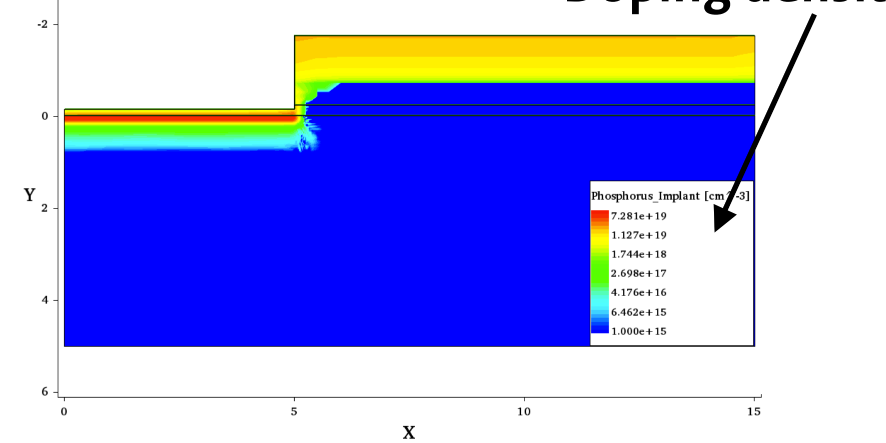
1. Oxide growth + masking



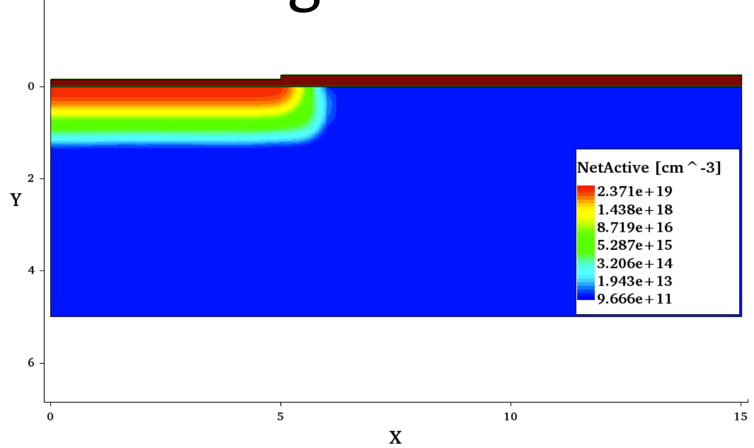
2. Etching of oxide



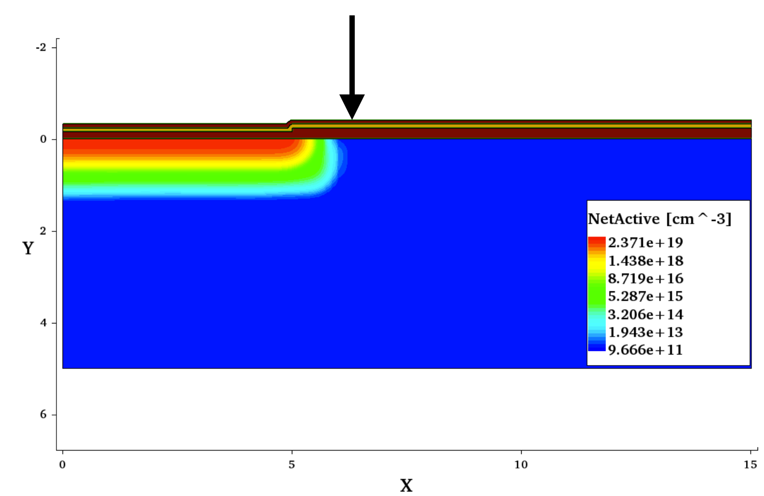
3. P implantation through oxide



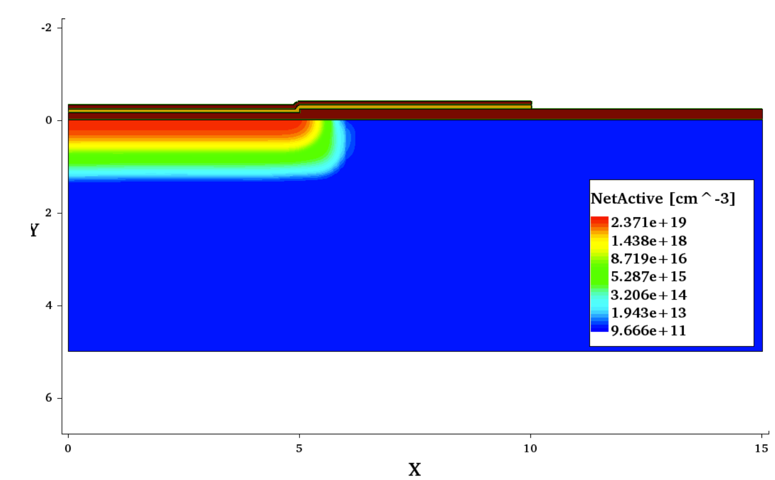
4. Backside implantation + annealing



5. Deposit of SiN + LTO

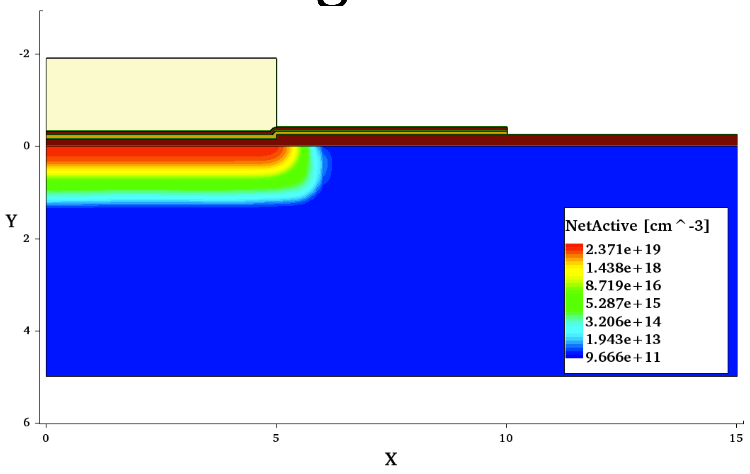


6. Etch LTO + SiN

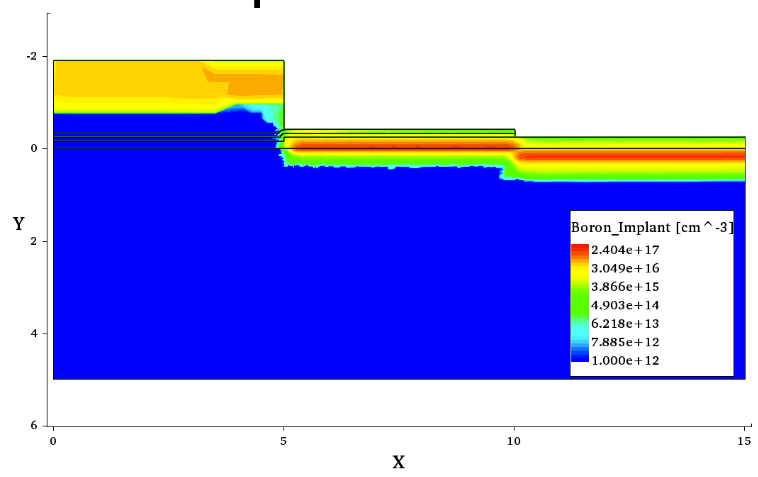


PROCESS SIMULATION

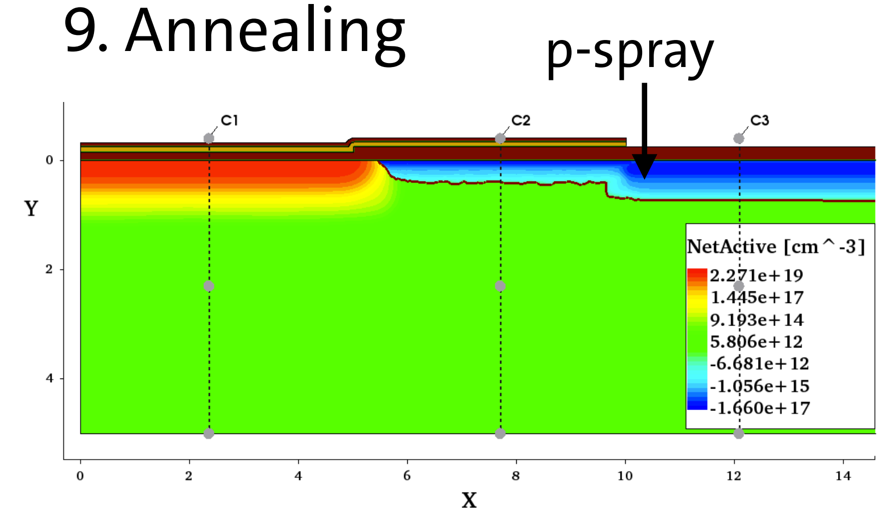
7. Masking



8. B implantation



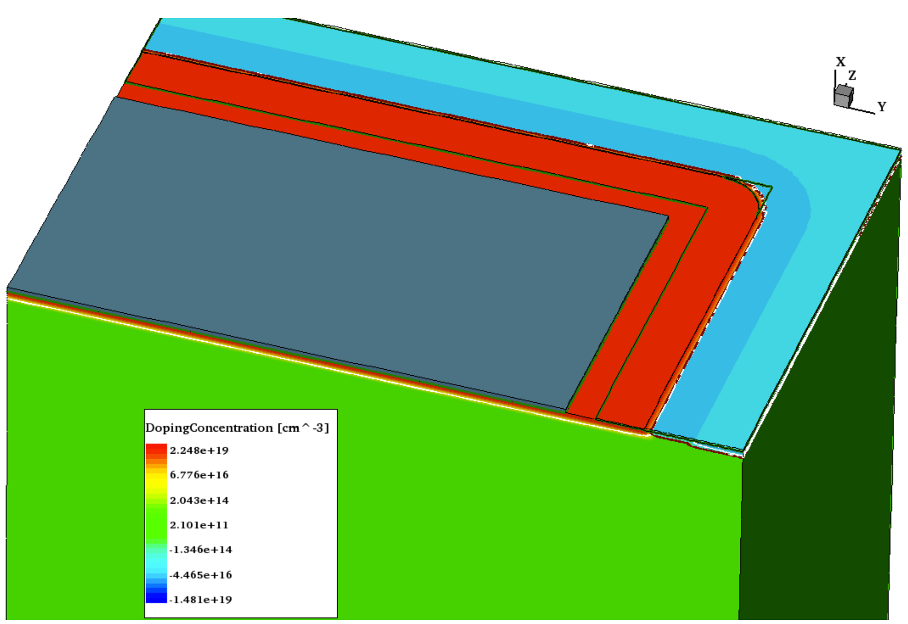
9. Annealing



10. SDE command for sweep along wire

```
(define B-Face (sdedr:define-refeval-window "RefEvalWin_P_prof1" "Rectangle"
 (position 285 0 0) (position 280 83.0 0.0)))
(define B-Wire  (sdegeo:create-polyline-wire (list
 (position 285 65.00 0.0) (position 285 65.00 35.00)
 (position 285 64.755 36.545) (position 285 64.045 37.939) (position 285 62.939 39.045)
 (position 285 61.545 39.755) (position 285 60.0 40.0) (position 285 0.0 40.0))))
(sdegeo:sweep B-Face B-Wire (sweep:options "solid" #t "rigid" #f "miter_type" "default"))
```

Doping profile



Often the process details are not know to us

➡ Start with analytical doping profiles based on best guesses

Examples of device simulations

Optimisation of AGIPD pixel sensor for high X-ray doses

SENSOR SPECIFICATION

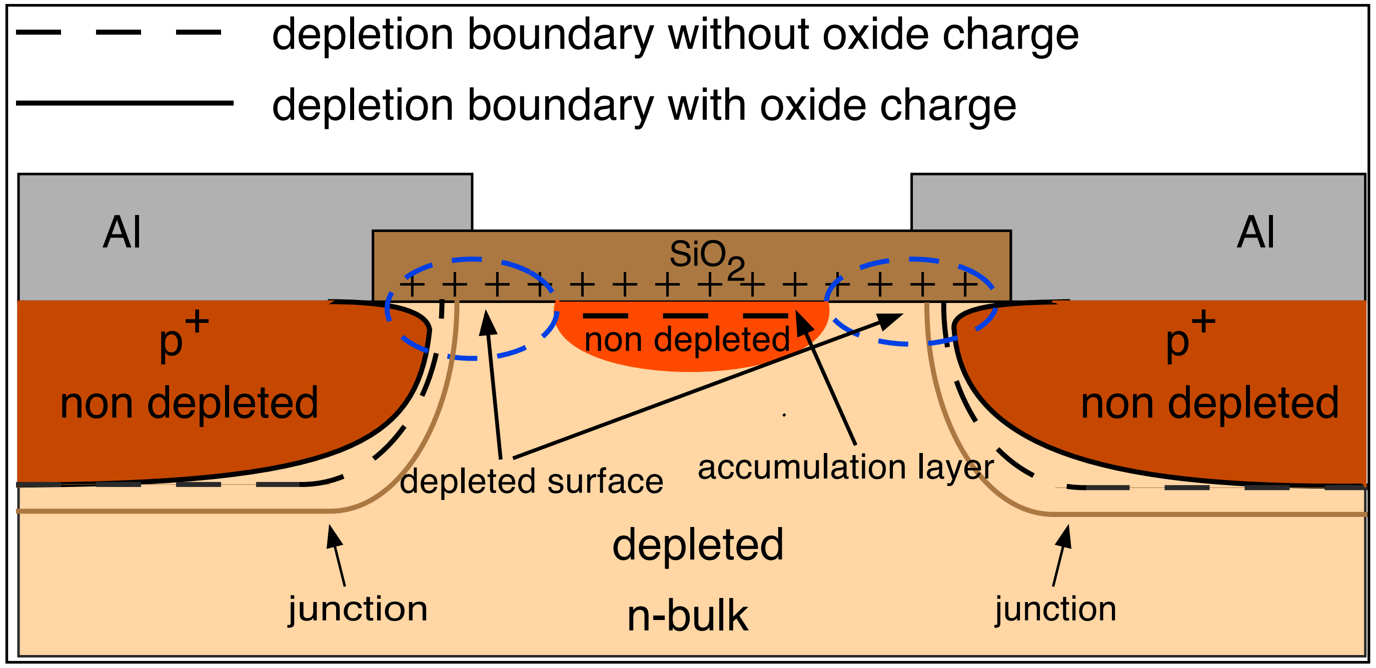
Adaptive Gain Integrating Pixel Detector a hybrid pixel detector for the European XFEL

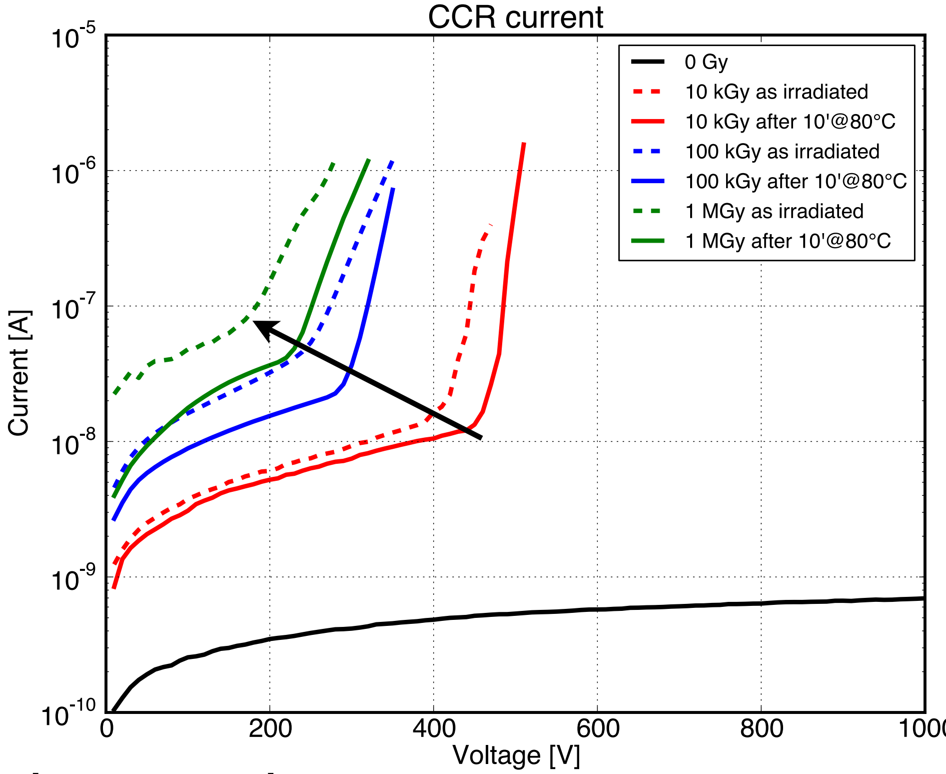
Parameter	Value
Geometry parameters	
Sensitive area	10.52 cm × 2.56 cm
Thickness	500 ± 20 µm
Pixel dimensions	200 µm × 200 µm
Deviation from flatness	< 20 µm
Distance pixel to cut edge	1200 ± 5 µm
Electrical parameters before irradiation	
Coupling	DC
n doping of Si crystal	3 – 8 kΩ·cm
n doping non-uniformity	< 10%
Dead layer n^+-side	≤ 2.5 µm
Breakdown voltage	> 900 V
Dark current of all pixels@500V	< 200 nA
Dark current of single pixel@500V	< 20 nA
Dark current of CCR@500V	< 200 nA
Electrical parameters for 0 Gy to 1 GGy	
Breakdown voltage	> 900 V
Dark current of all pixels@500V	< 50 µA
Dark current of single pixel@500V	< 50 nA
Dark current of CCR@500V	20 µA
Interpixel capacitance	500 fF

Critical parameters

X-RAY EFFECTS ON P+N SENSORS

- **Accumulation layers** form (or increase)
- **High field** regions appear reducing the breakdown voltage
- Leakage current increases due to interface states
- Depletion voltage and inter-pixel capacitances increase
- Charge losses close to the Si-SiO_2 interface occur (increase)





- Details depend on sensor geometry, technology and boundary conditions
- For the optimisation of the sensor:

Knowledge of the oxide-charge density and surface-current density is sufficient

- For a detailed comparison of simulations with measurements:

Oxide-charge density, interface-trap density distribution + their cross sections have to be known

SENSOR DESIGN: PARAMETERS

Parameters to be optimised using TCAD:

1. Geometry of pixel:

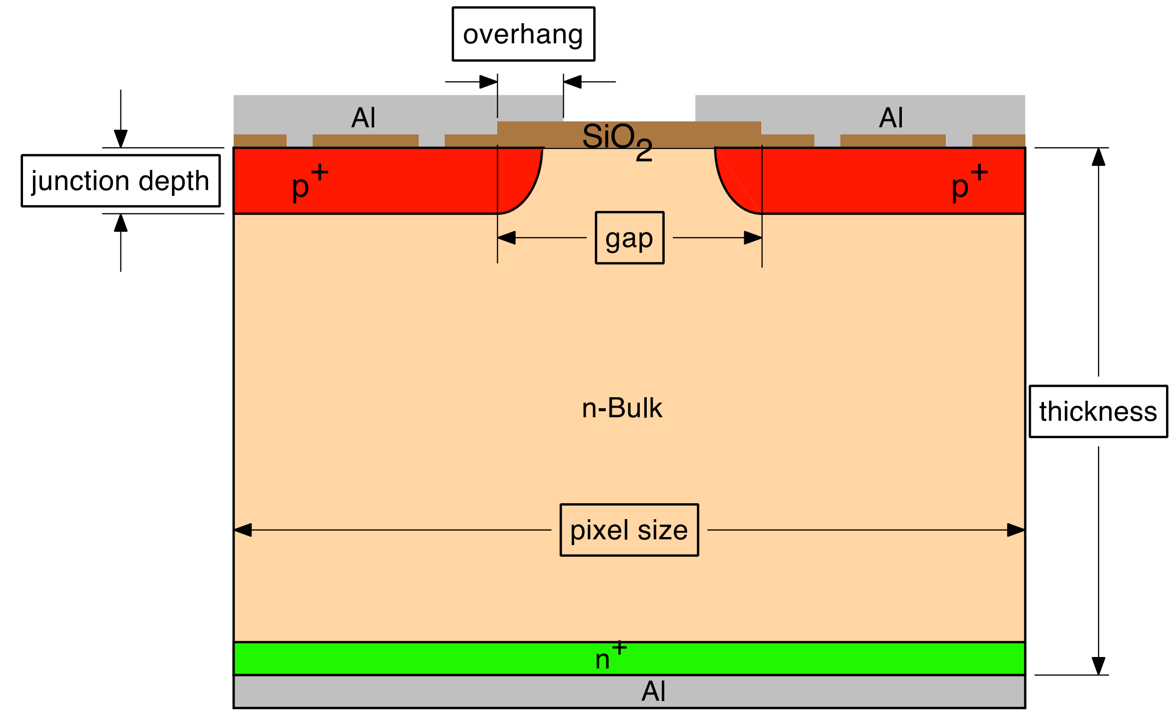
- Gap
- Al overhang
- Radius of implant and Al at corners

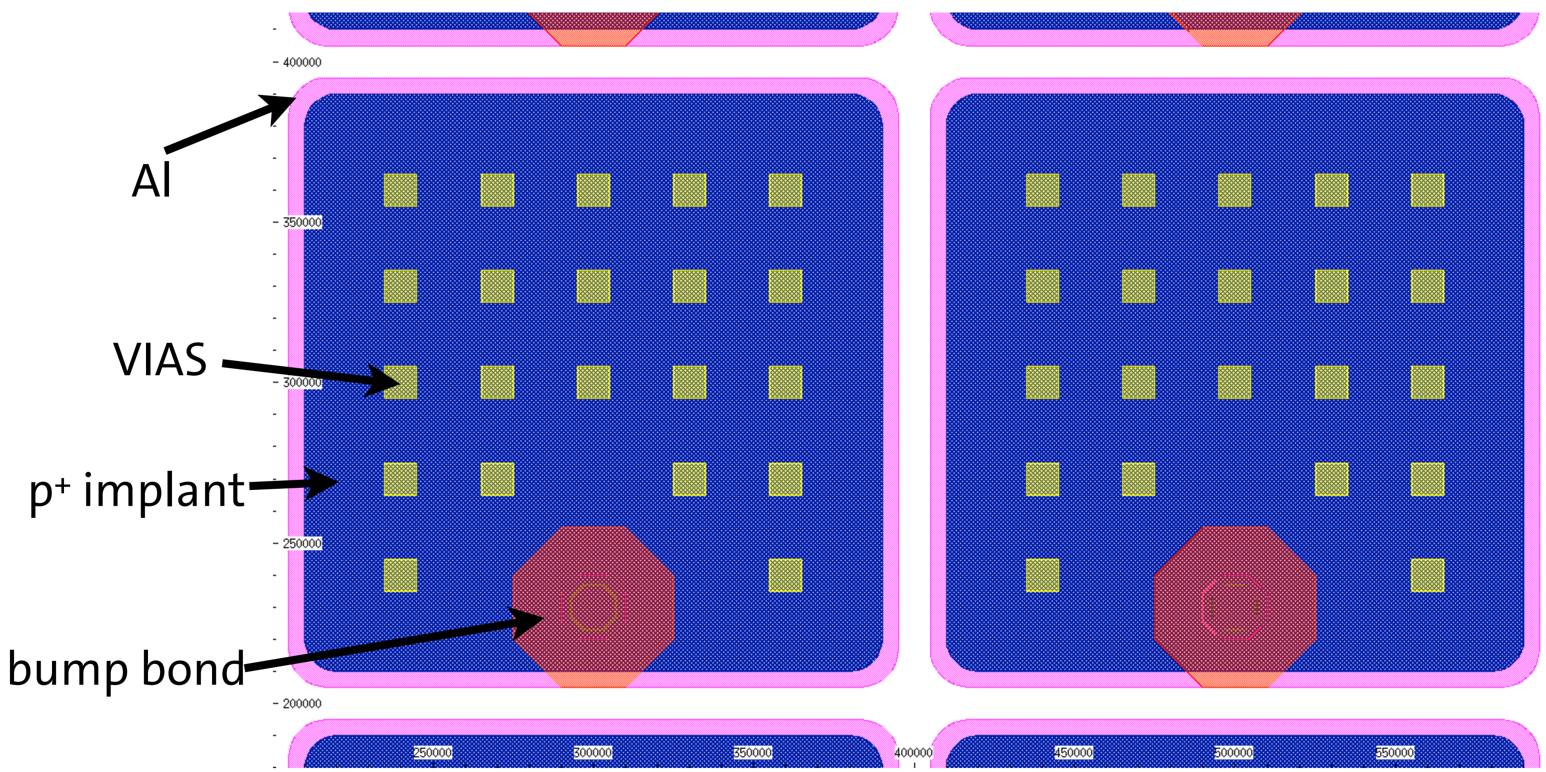
2. Geometry of guard-ring structure

- Number of rings
- Implantation width
- Spacing
- Al overhangs
- Radii

3. Process parameters:

- Junction depth
- Oxide thickness





OPTIMISATION FOR X-RAY HARDNESS

Specifications to be achieved for doses between 0 and 1 GGy non-uniform:

- **Pixel:**
  1. Breakdown voltage ↑ (> 900V)
  2. Surface current ↓ (< 1nA/pixel)
  3. Inter-pixel capacitance ↓ (< 500 fF)
- **Guardrings:**
  1. V_{bias} (900 V) over 1.2 mm
  2. Bulk not depleted at scribe line (no leakage current from the cut edge)

Strategy of guard-ring (GR) optimisation (2D in cartesian and cylindrical coordinates):

- 0 GR: Study breakdown behaviour of 0 GR (CCR [*]) only) for different oxide charges as function of oxide thickness and Al overhang
- Estimate number of floating GRs for 1000 V
- Vary spacing between rings, implant width and overhang to achieve maximum V_{bd} →max E-field between individual GRs the same
- Minimise space

Strategy of pixel optimisation (2D „strip sensor“ calculation used):

- Optimise oxide thickness, Al overhang, gap and implantation depth with respect to breakdown voltage, dark current and capacitance for different N_{ox}
- Extrapolate dark current and capacitances to „3D numbers“
- Check breakdown voltage + dark current with 3D simulation (only 1/4 pixel used due huge number of grid points)

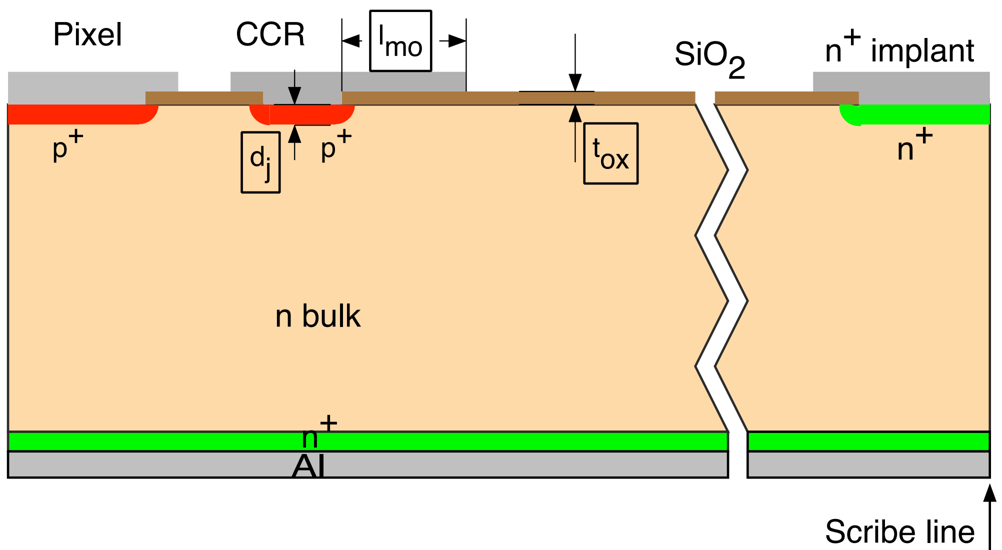
Optimisation requires detailed TCAD simulations

[*]) CCR = Current Collection Ring

GUARD RING: 0 GR

Structure used for simulations:

1. Gap between pixel and CCR: 20 µm
2. CCR implant width: 30 µm
3. n-bulk: doping: 5.1 kOhm·cm (P)
4. Right Al overhang CCR: 0 - 20 µm
5. Oxide thickness: 180 - 1000 nm

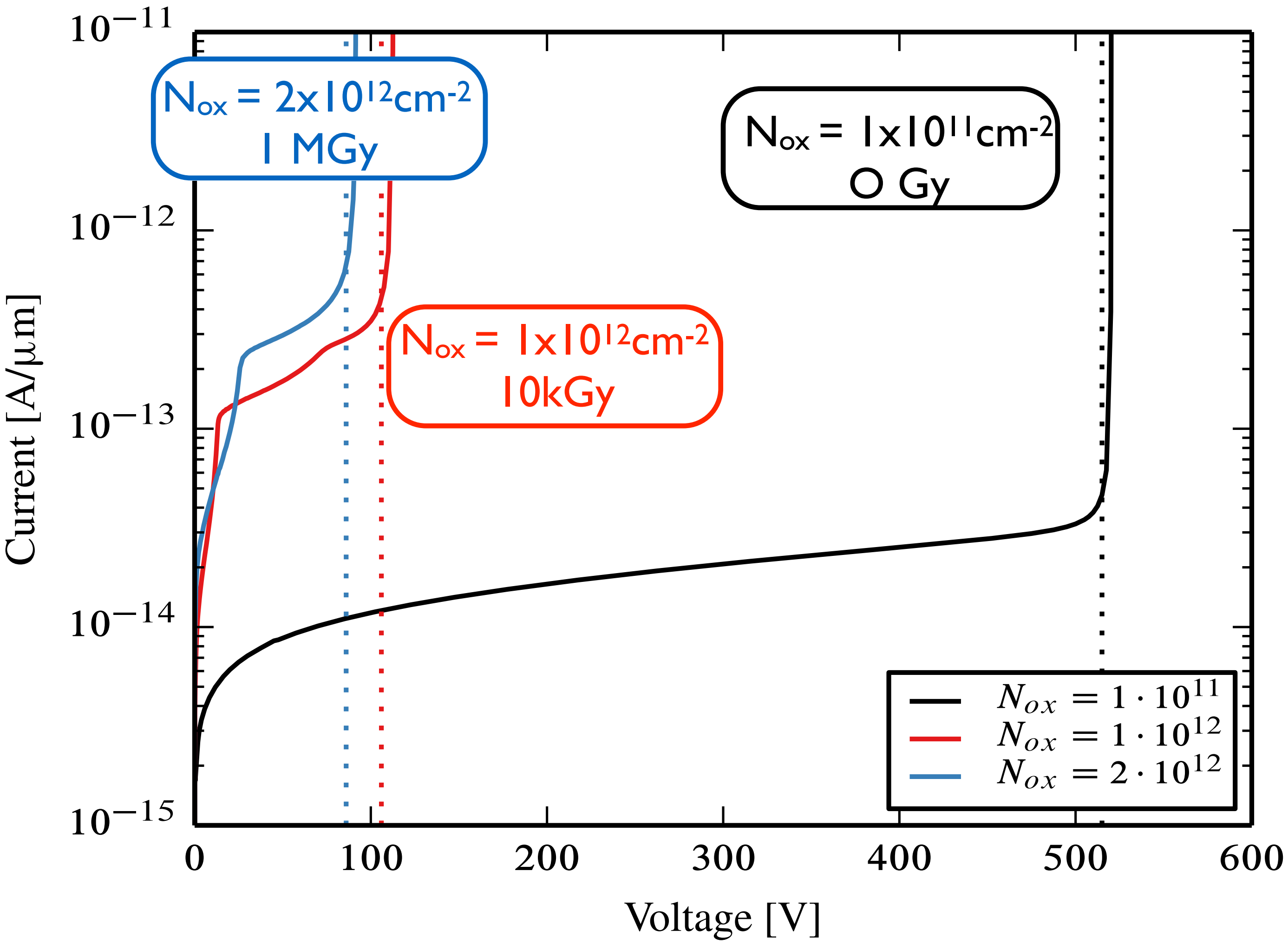


N_{ox} used in TCAD simulations:

1×10^{11} cm^{-2}	← 0 Gy
1×10^{12} cm^{-2}	← 10 kGy
2×10^{12} cm^{-2}	← 1 MGy
3×10^{12} cm^{-2}	← 10 MGy

Surface-recombination velocity s_0:

8 cm/s	← 10 nA/cm²	← 0 Gy
3580 cm/s	← 2 µA/cm²	← 10 kGy
7500 cm/s	← 5 µA/cm²	← 1 MGy
12040 cm/s	← 8 µA/cm²	← 10 MGy

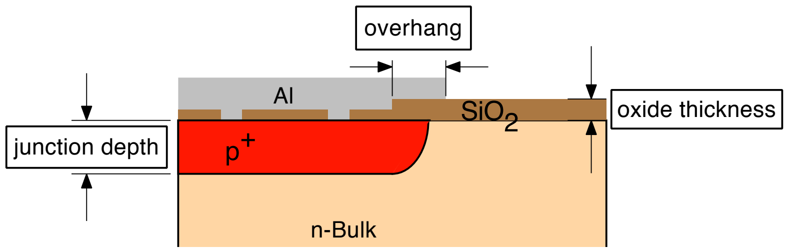


N_{ox} is assumed to be uniformly distributed at the Si-SiO_2 interface!

Breakdown criterium: $\frac{\Delta I}{\Delta V} / \frac{I}{V} = 10$

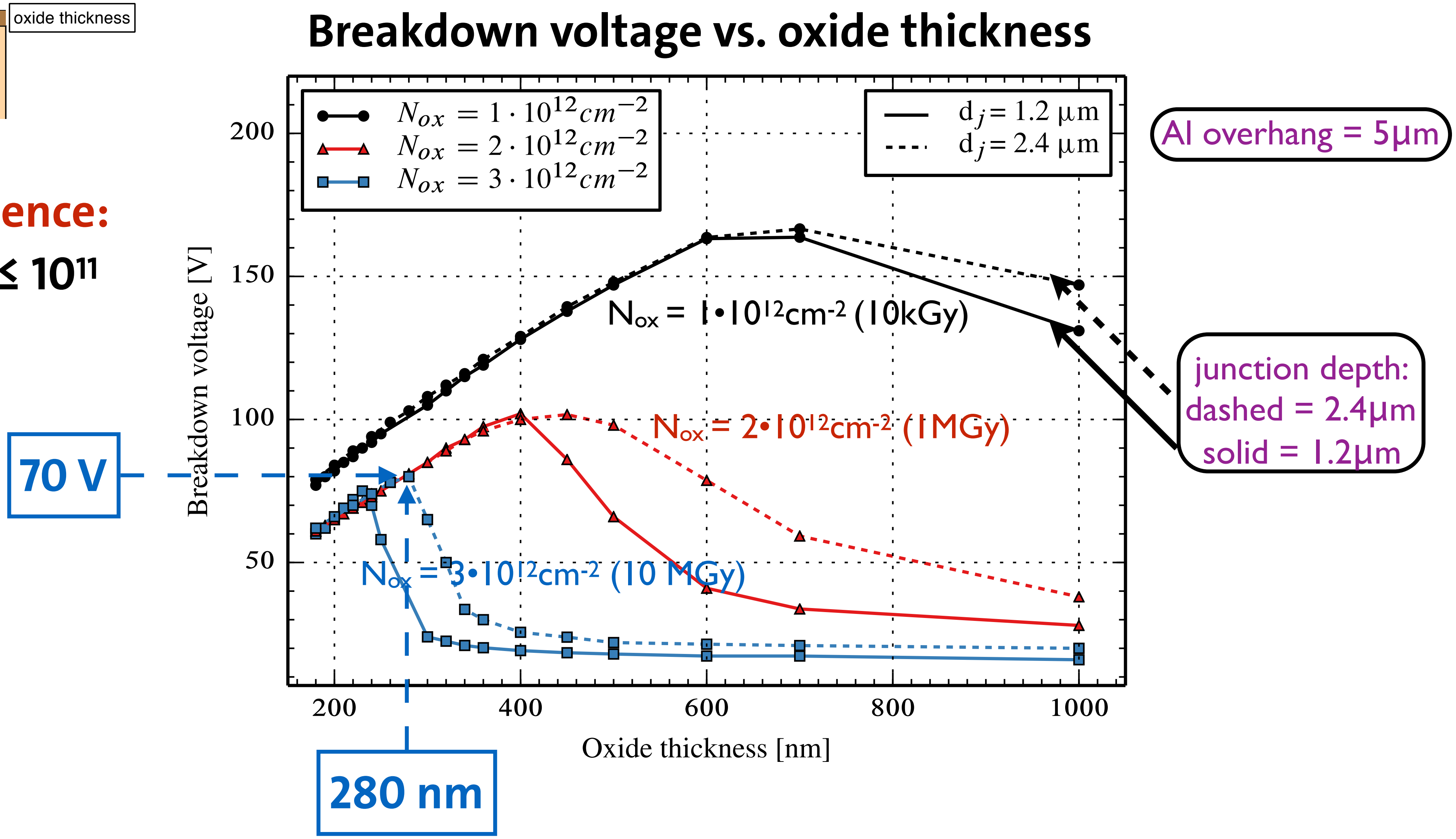
0 GUARD RING

2D simulations in cartesian coordinates (for 0 guard rings - 0 GR)



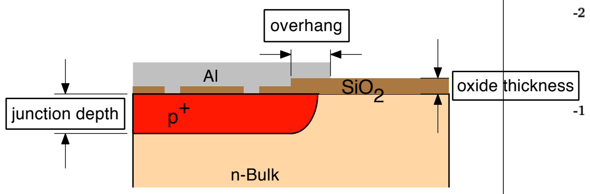
Strong dose dependence:

(V_{bd} > 400 V for $N_{ox} \leq 10^{11}$ cm^{-2})



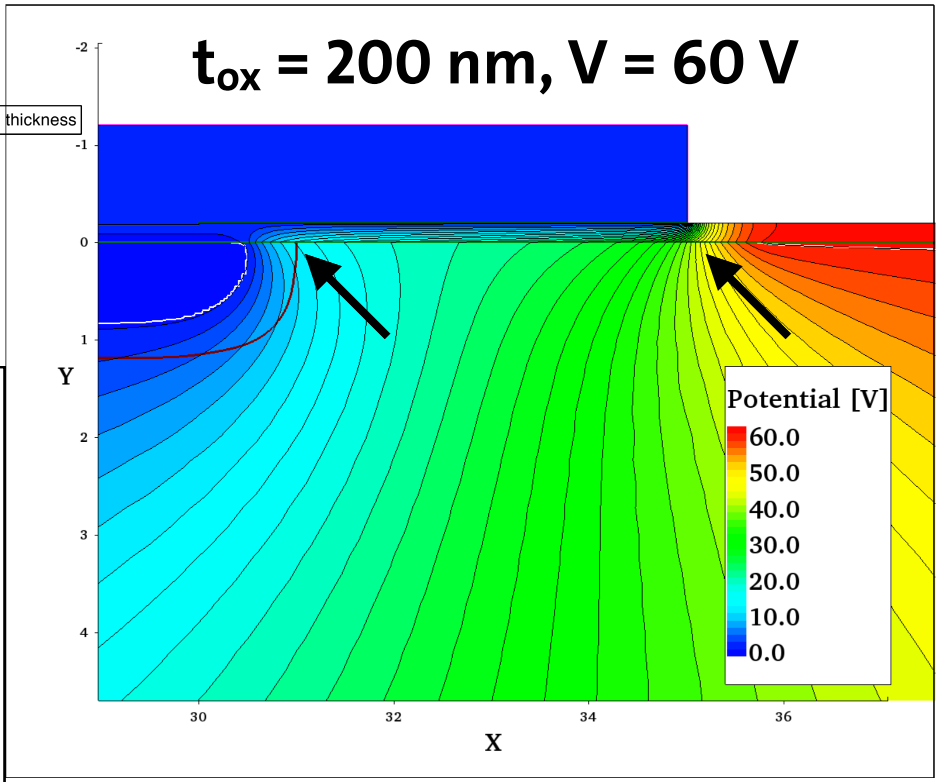
Optimum thickness: breakdown at edge of implant and edge of metal simultaneously

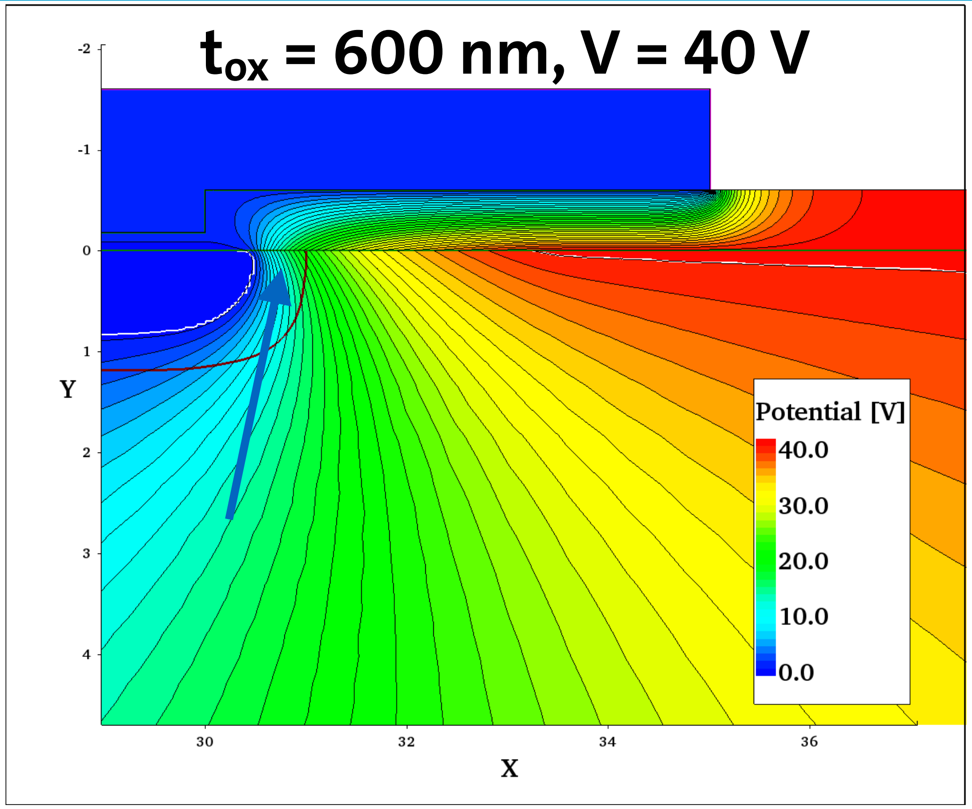
ELECTRIC FIELDS FOR GRO N_{ox} = 2E12

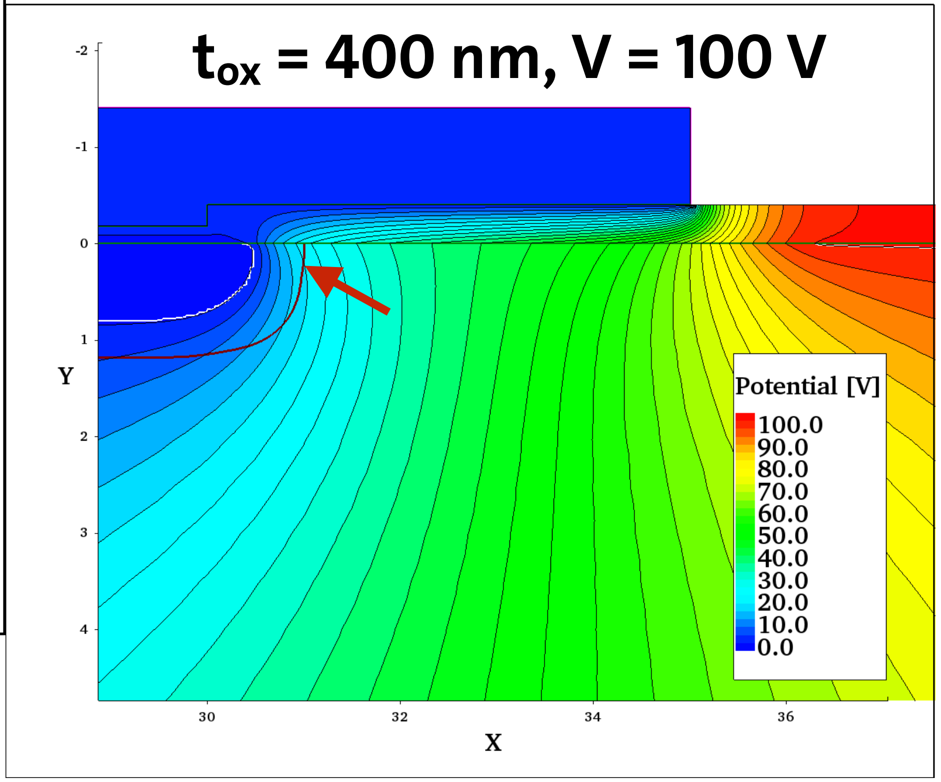


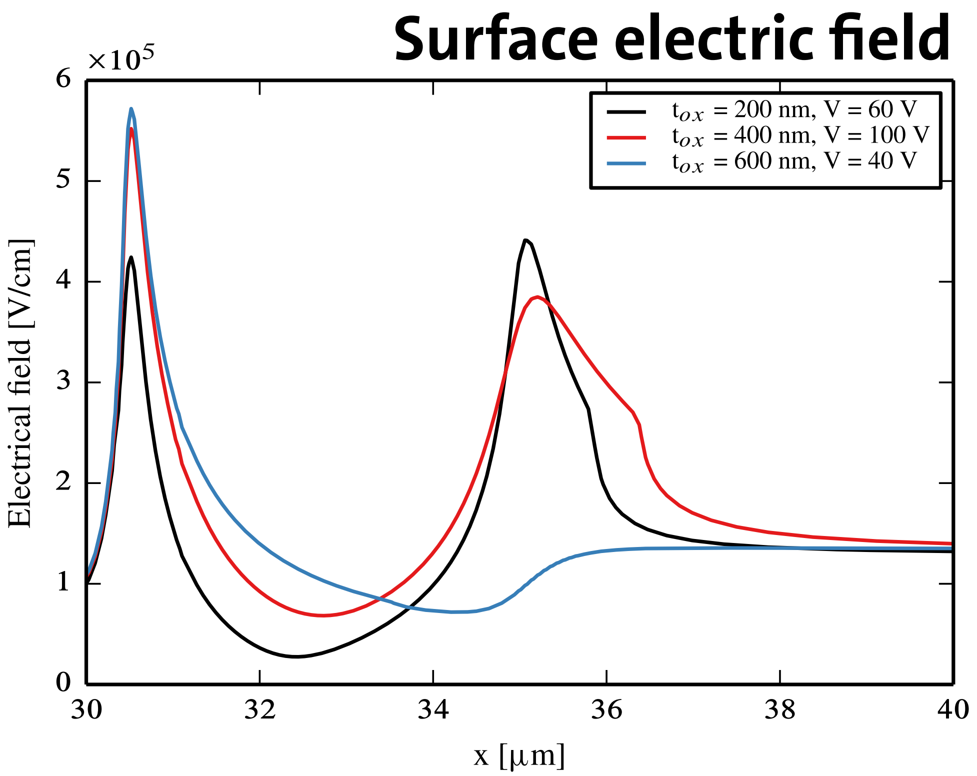
Oxide thickness dependence of V_{bd} at high oxide-charge densities:

- Thin oxide: breakdown at edge of metal overhang
- Thick oxide: breakdown at edge of implant
- Optimum thickness: breakdown at edge of implant and edge of metal simultaneously









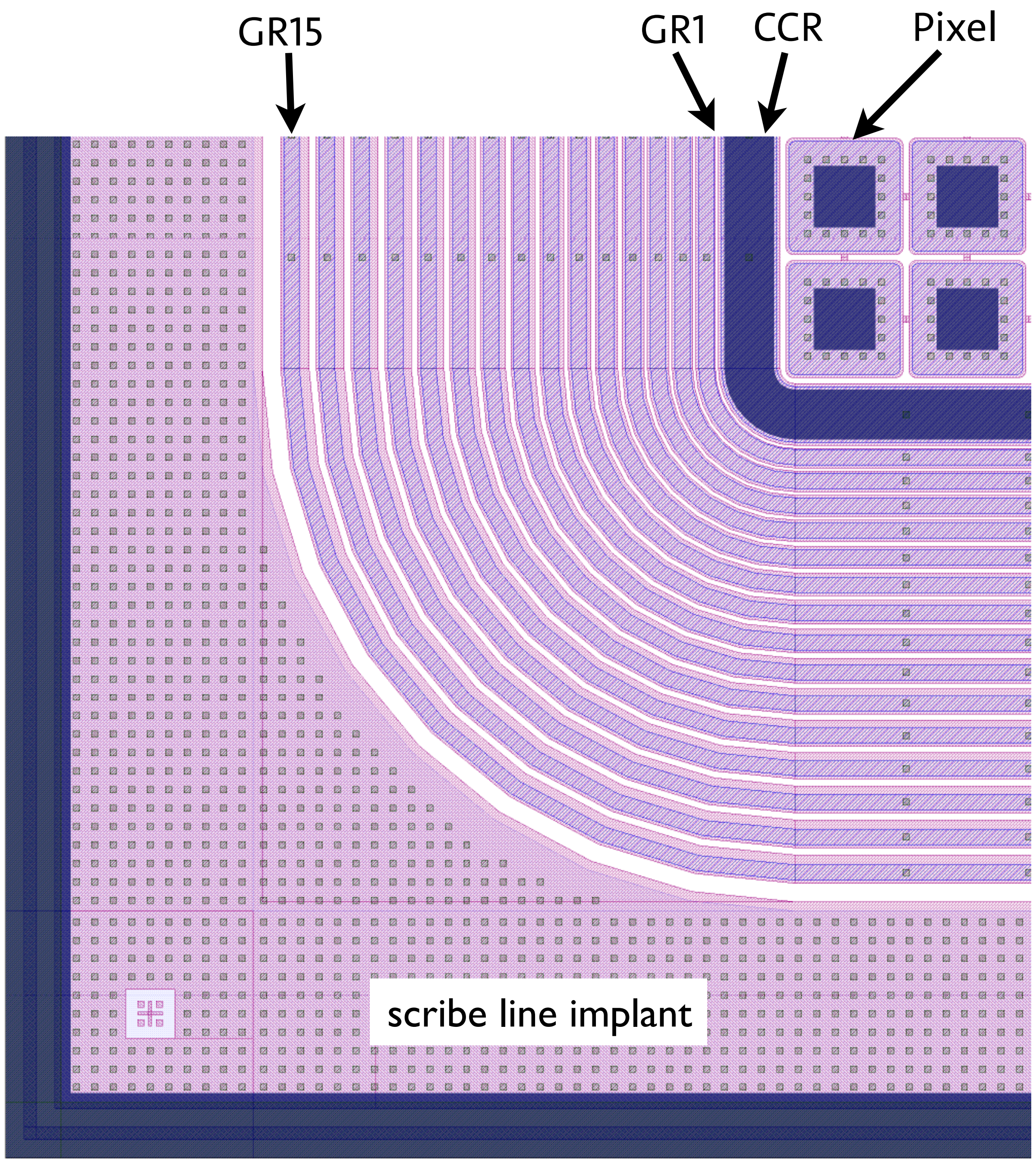
GR OPTIMISATION RESULTS

Optimised design for 250 nm oxide thickness and 2.4 µm junction depth

- Breakdown voltage for **0 GR** with **N_{ox} = 3x10^{12} cm^{-2}** ≘ 10 May : ≅ **70 V**
- Ideally **16 rings** (1 CCR + floating 15 GRs) needed for > **1000 V** (16 × 70 V = 1120 V)

Geometry of guard ring structure:

- Gap pixel to CCR: 20 µm
- Width implantation window CCR: 90 µm
- Al overhang CCR: 5 µm
- Gap CCR to 1st guard ring (GR): 12 µm
- Width of implantation window GR 25 µm
- Al overhang left (towards pixel) of GR 1, 2, … 15: 2, 3, … 16 µm
- Al overhang right (away from pixel) of GR 1 – 15: 5 µm
- Gap between GR 1-2, 2-3, … 14-15: 12, 13.5, … 33 µm



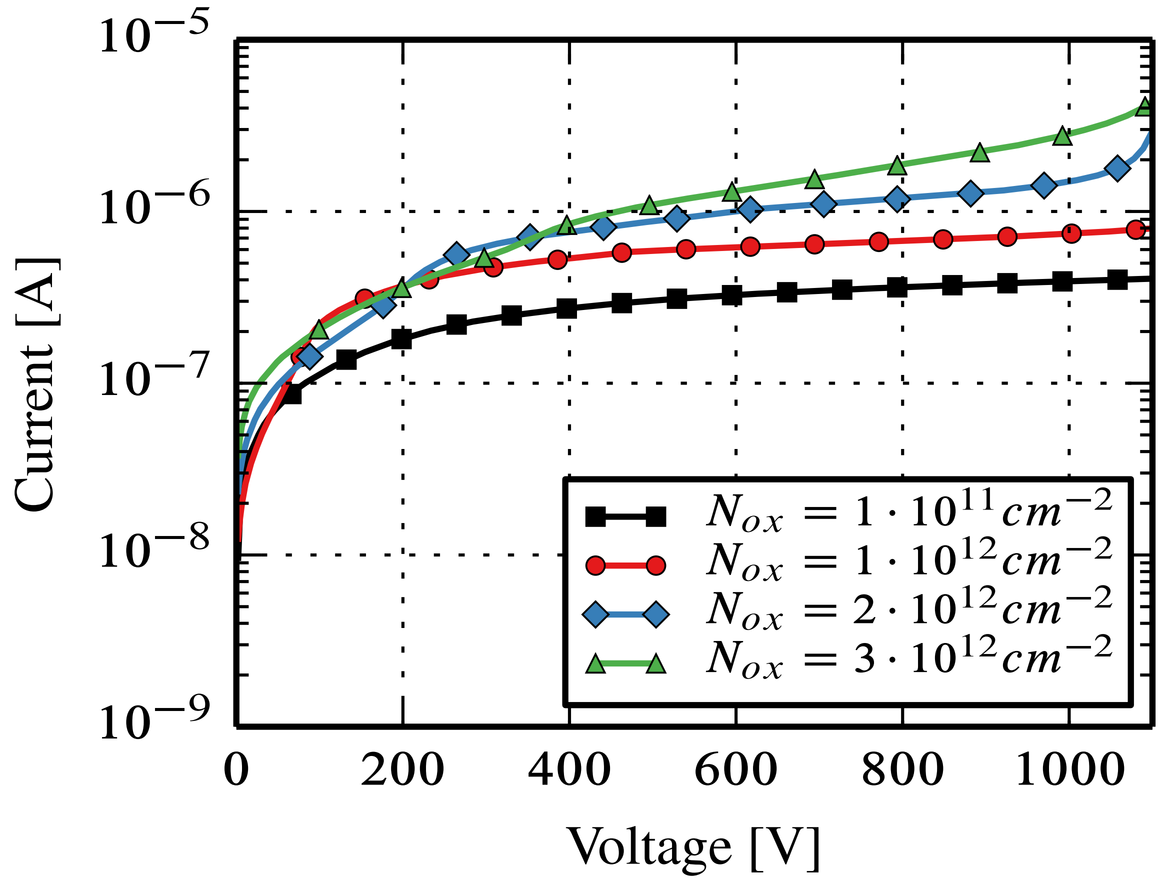
Bulk resistivity:

- 5.1 kΩ·cm (3 and 8 kΩ·cm to check depletion towards cut edge)

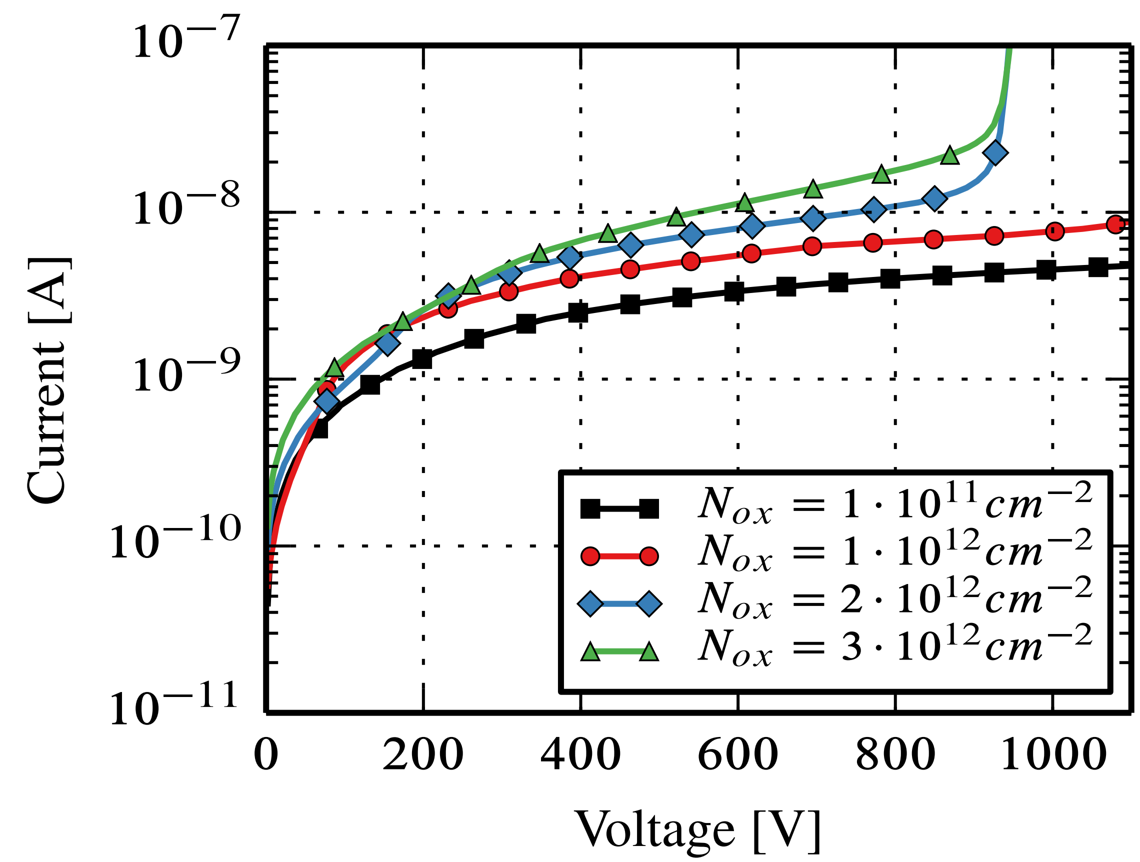
GR OPTIMISATION RESULTS

CCR current for optimised design (5.1 kΩ·cm)

2D Cartesian



2D cylindrical



- CCR current ~ 3 µA at 900 V and $N_{ox} = 3x10^{12}$ cm^{-2}

Breakdown voltage at corners ~ 900 V for $N_{ox} = 3x10^{12}$ cm^{-2}

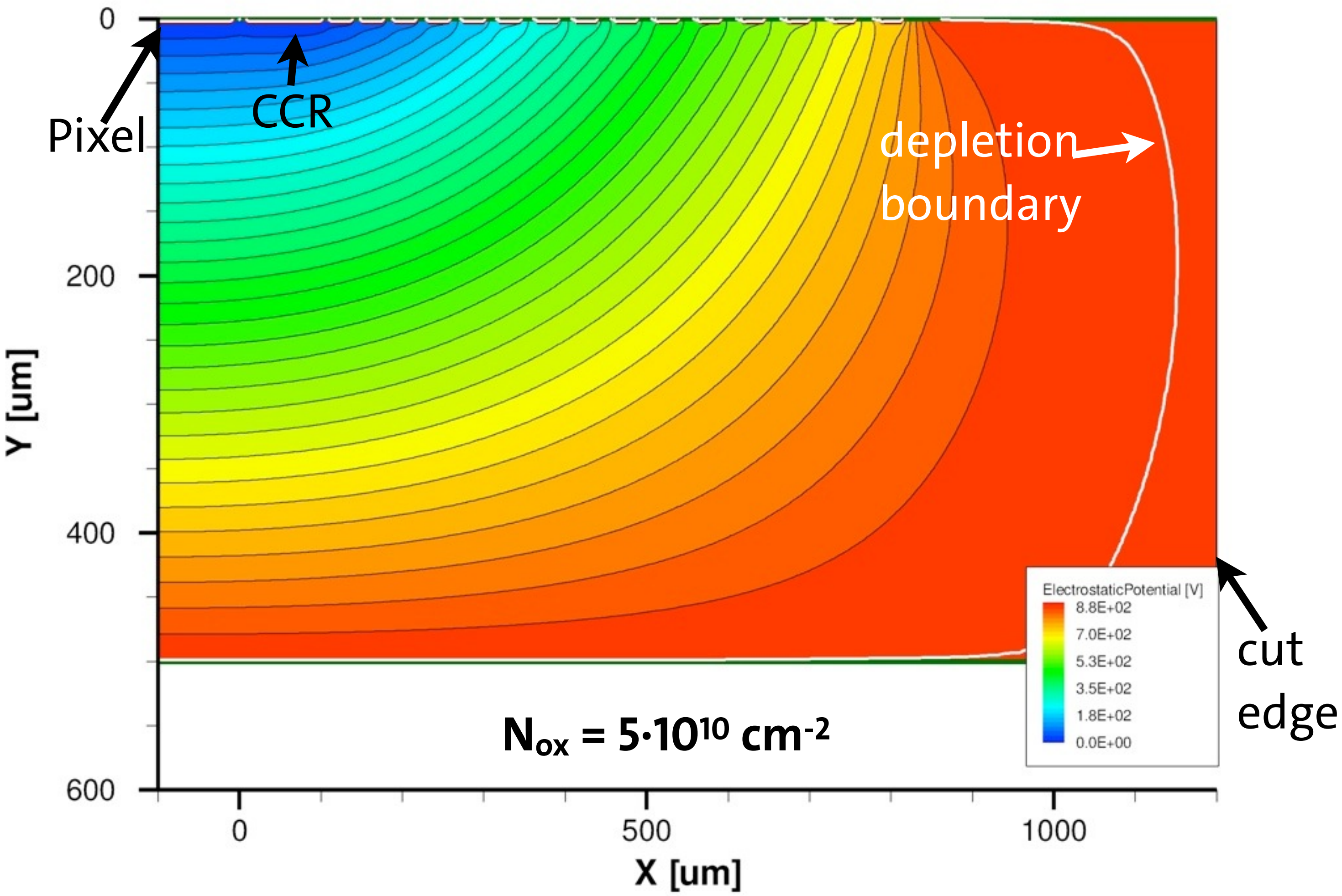
Breakdown voltage as function of resistivity						
	3 kΩ·cm		5.1 kΩ·cm		8 kΩ·cm	
N_{ox} [cm^{-2}]	2D (x,y)	2D (r,z)	2D (x,y)	2D (r,z)	2D (x,y)	2D (r,z)
$1x10^{12}$	>1100 V	1060 V	>1100 V	>1100 V	>1100 V	>1100 V
$2x10^{12}$	1000 V	830 V	1080 V	910 V	950 V	950 V
$3x10^{12}$	1010 V	840 V	>1100 V	910V	1000 V	960 V

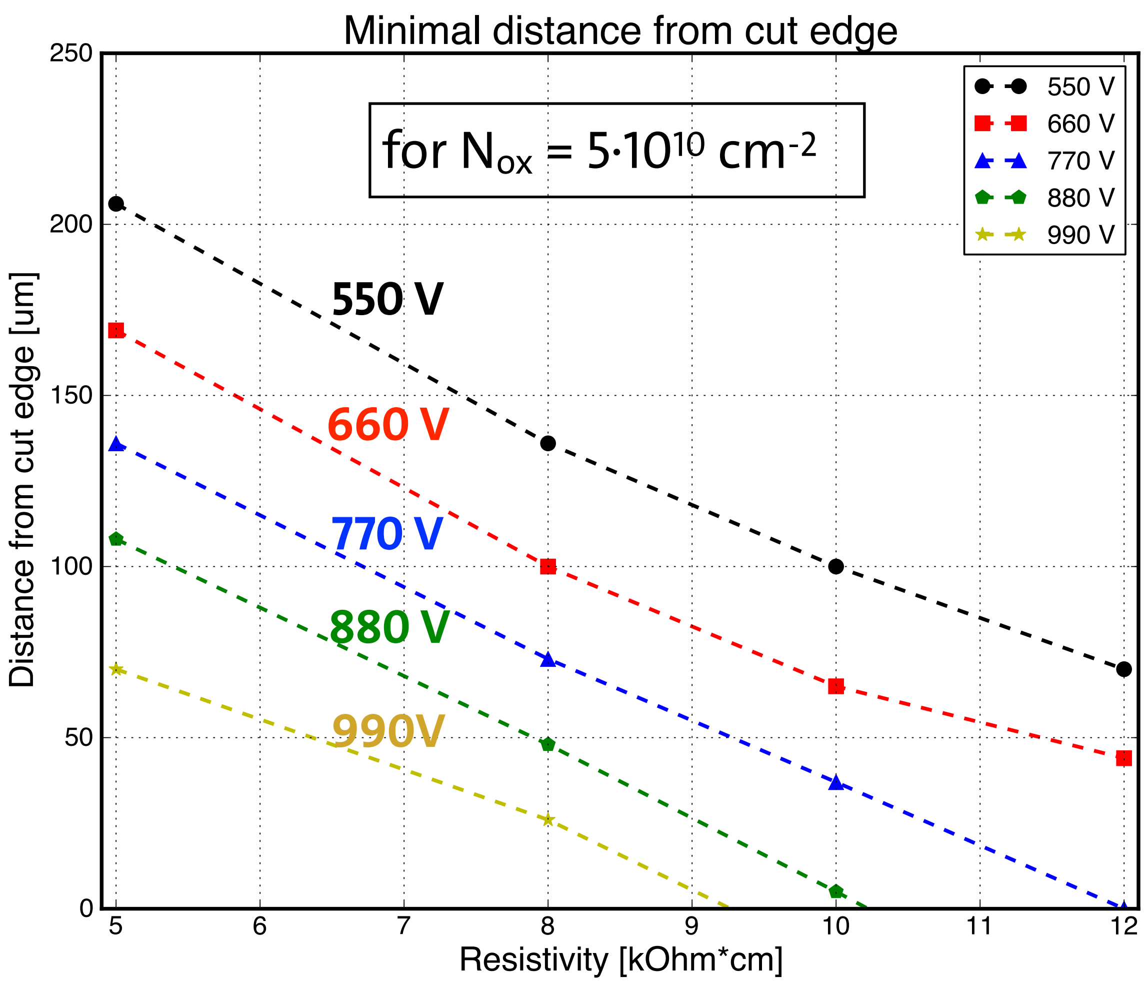
Resistivity range

Effects of resistivity on shape of depleted region close to the cut edge:

- High resistivity → risk of depletion region touching the edge at low oxide charge → increased leakage current due to defects at the cut edge

Potential distribution at 880 V for 8 kΩ·cm





Minimal distance form cut edge at 880 V and 8.0 kΩ·cm:

- N_{ox} = 5·10^{10} cm^{-2} : 50 µm
- N_{ox} = 1·10^{10} cm^{-2} : 25 µm

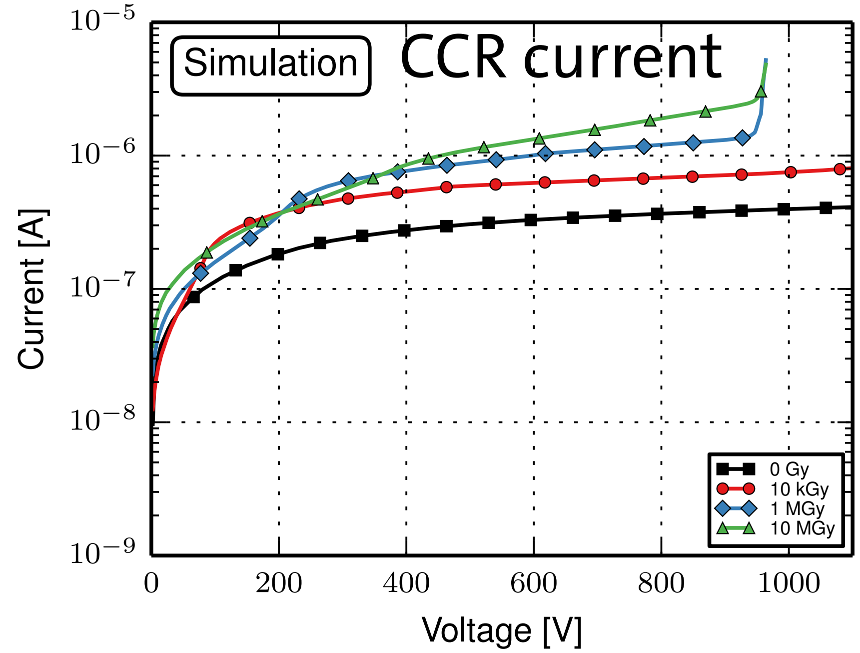
50 µm should be safe → resistivity ≤ 8.0 kΩ·cm

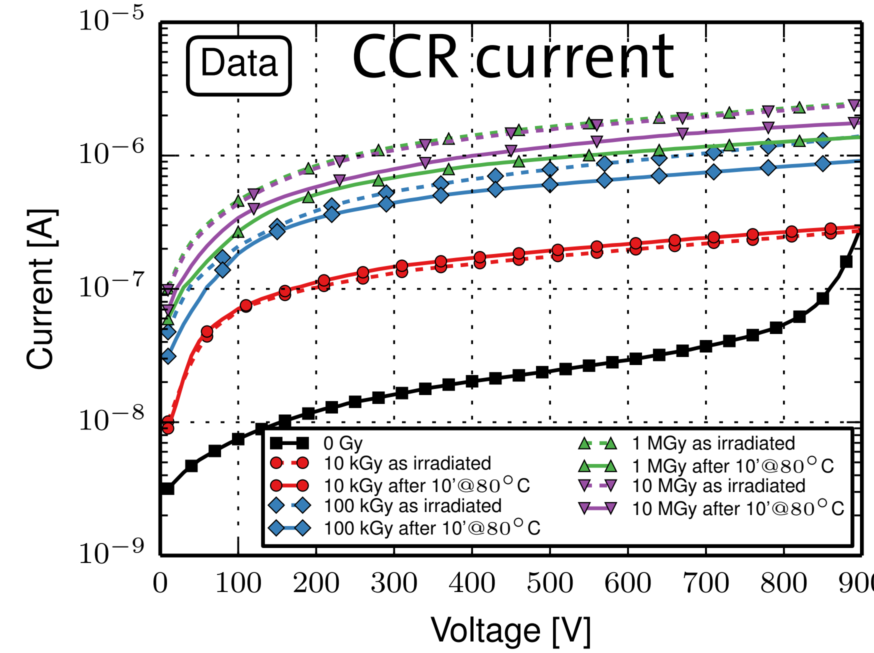
COMPARISON SIM. TO MEASUREMENTS

Optimised sensor fabricated by SINTEF

CCR current:

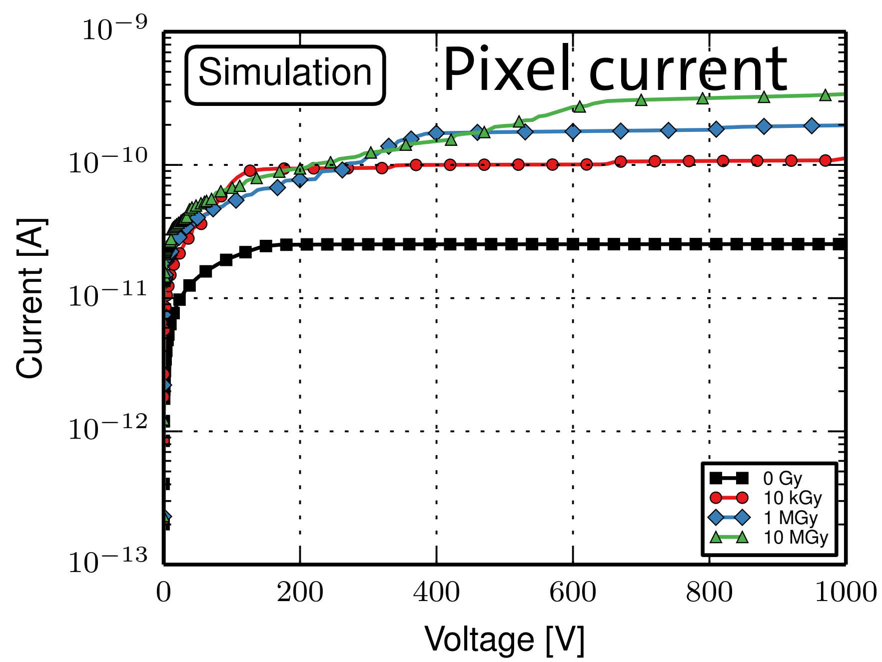
- Specifications:
  V_{bd} > 900 V
  I(500V) < 20 µA
- Measured:
  V_{bd} > 900 V
  I(500V) < 2 µA

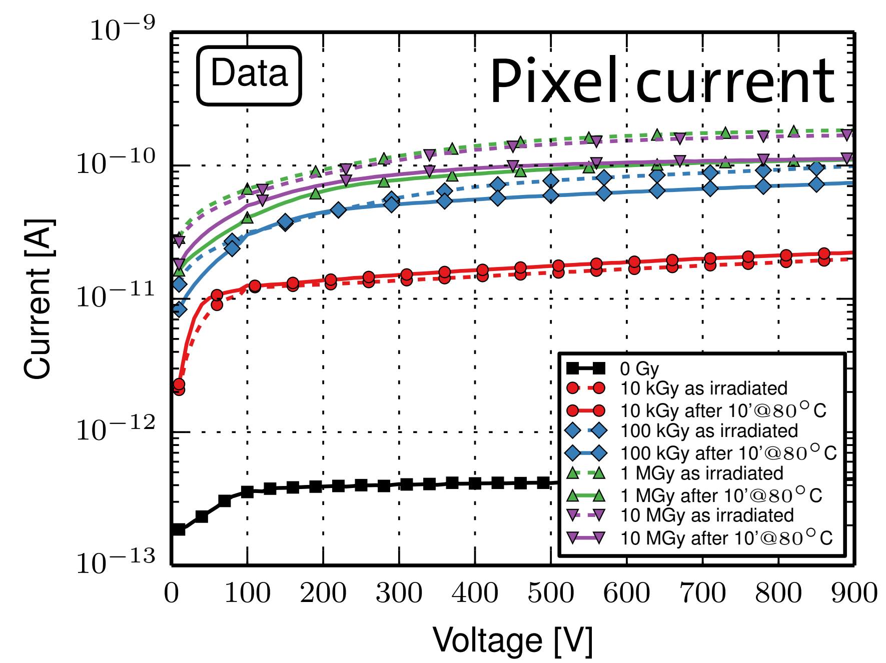




Pixel current:

- Specifications:
  V_{bd} > 900 V
  I_{mean} (500V) < 1 nA
  I_{max} (500V) < 50 nA
- Measured:
  V_{bd} > 900 V
  I(500V) < 0.2 nA





Optimisation successful: simulations ≈ measurement results

Examples of device simulations

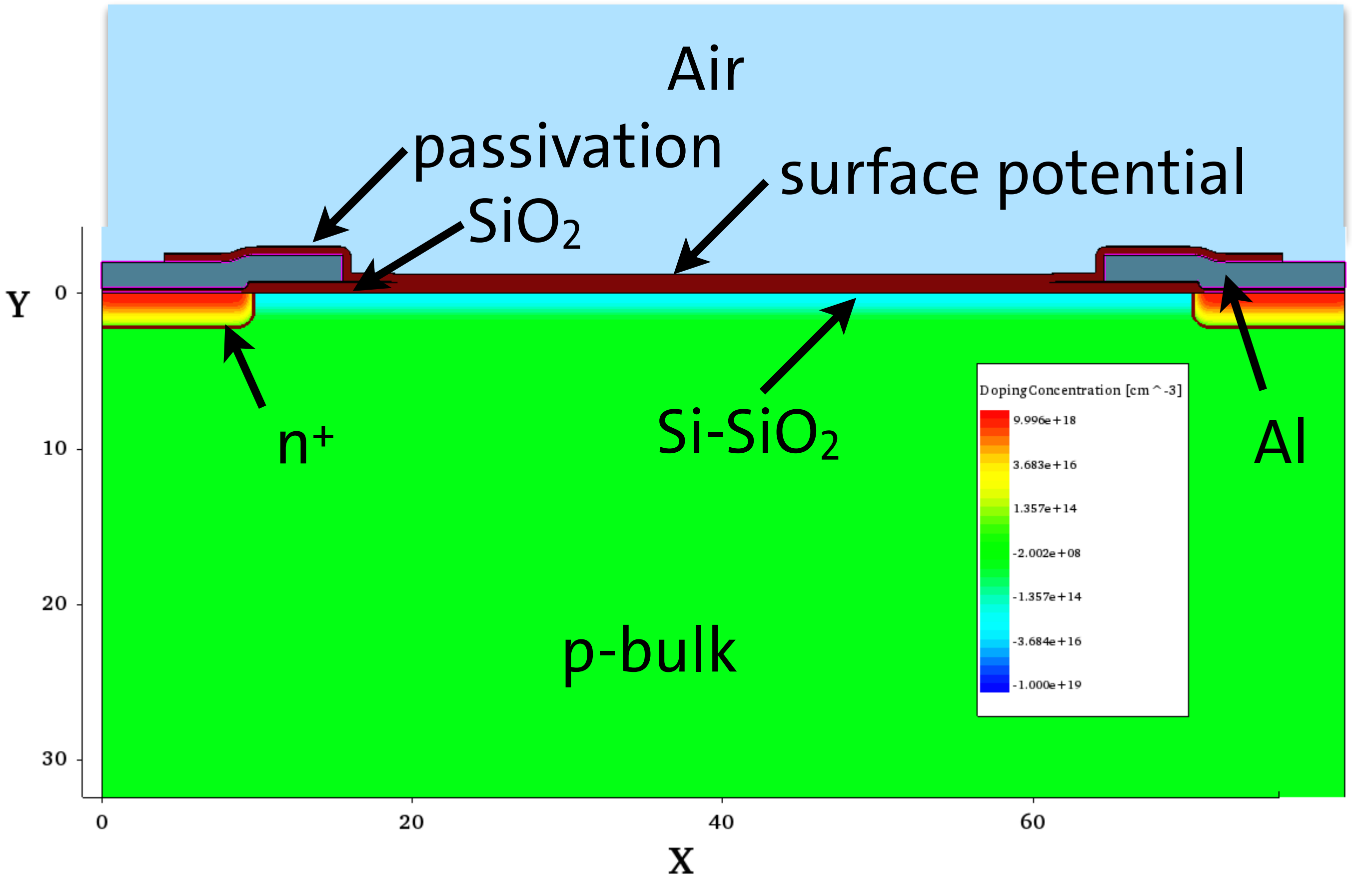
Simulation related to the investigation of the insulator layer for segmented silicon sensors

MOTIVATION

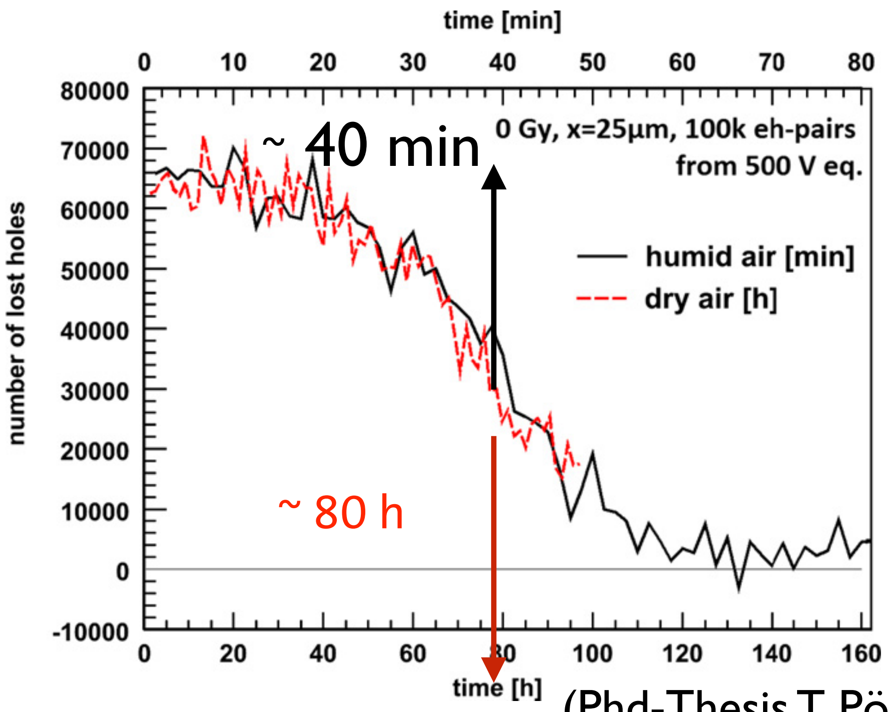
Instabilities of segmented silicon sensors have been observed which can be depend on environment and time e.g:

- Dependence of the **breakdown voltage** on **humidity** and ramping speed
- Dependence of **leakage current** on **humidity**
- Dependence of **charge sharing** and **charge loss** on **humidity**

Instabilities caused by changes of the potential distribution on the sensor surface and of the charge distribution at the Si-SiO_2 interface



Hole losses vs. time after changing bias voltage from 500 V to 200 V: 0 Gy, 600nm laser, 100k e-h paris injected



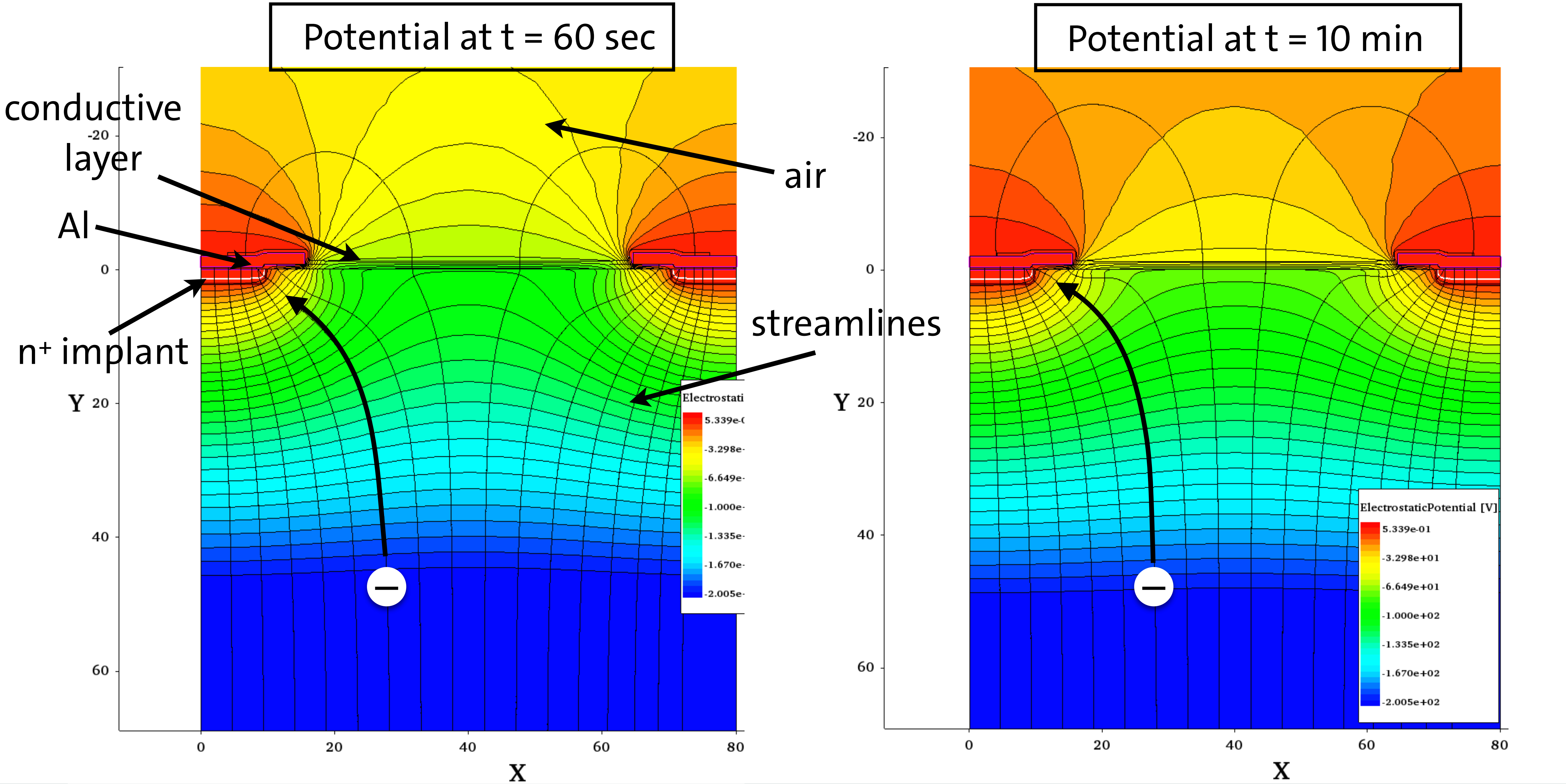
(Phd-Thesis T. Pöhlsen)

Effects of surface potential

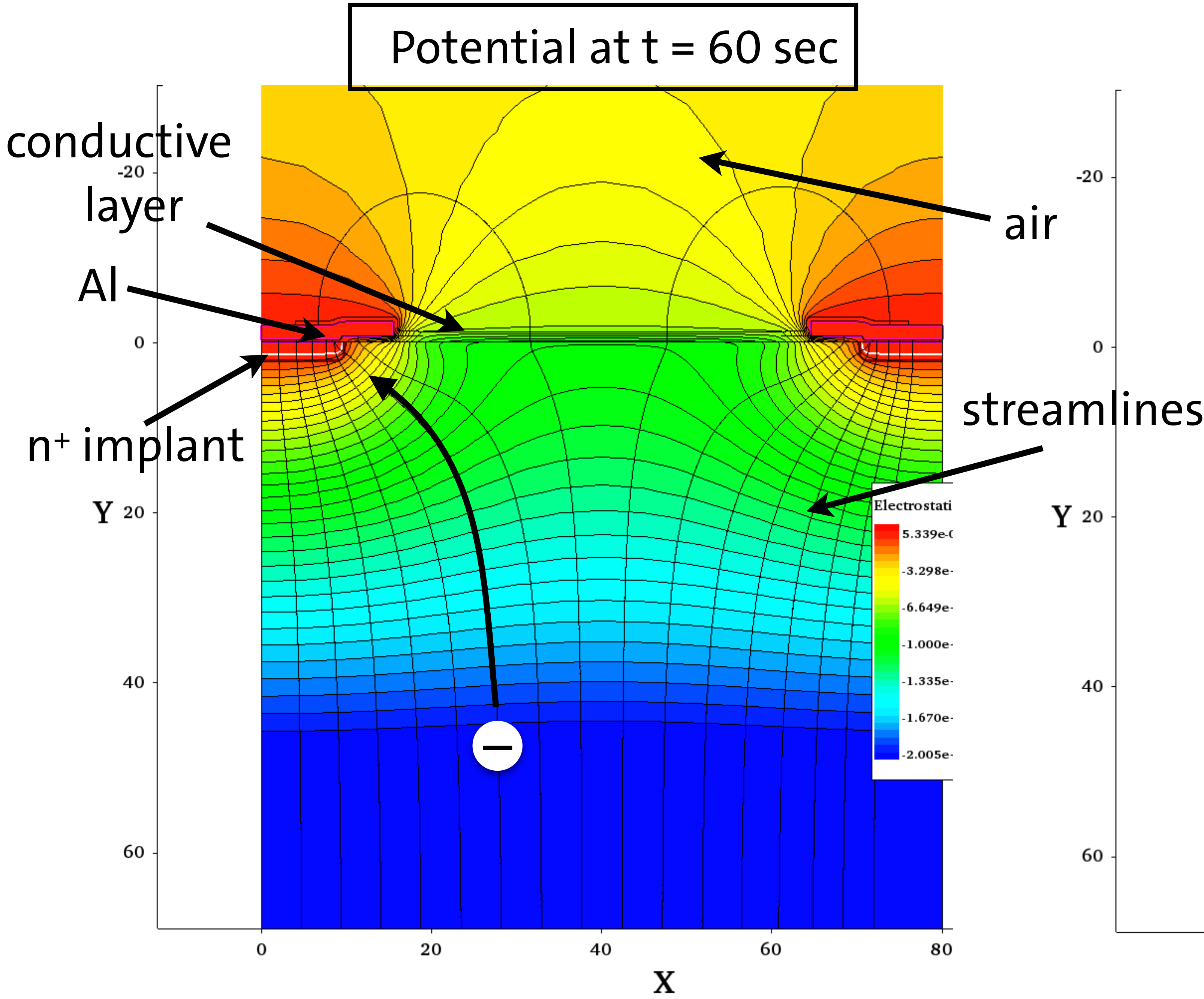
Simulation example of time dependent surface potential

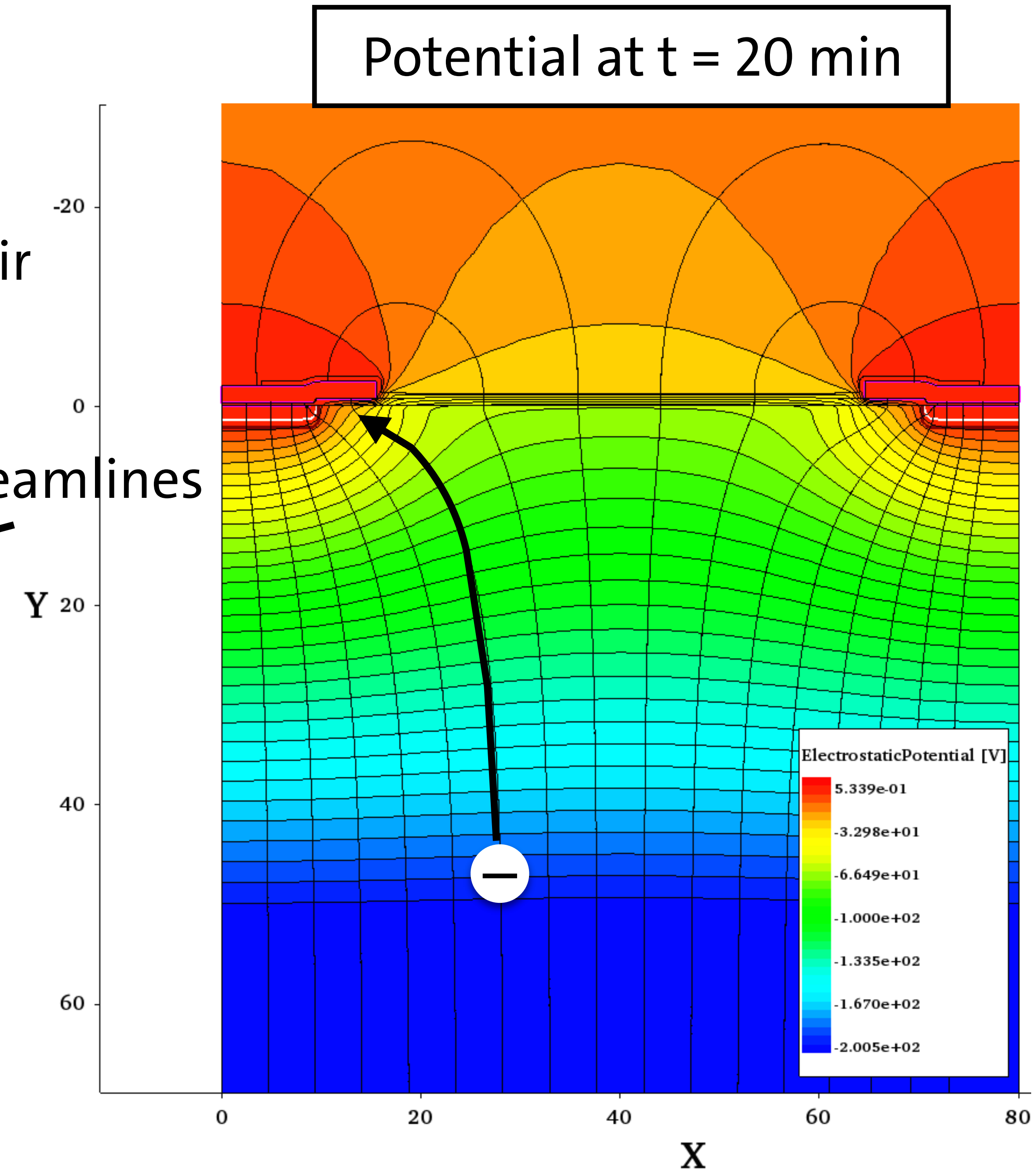
- AC coupled n⁺-p sensor with p-spray ($N_{p\text{-spray}} = 5{\bullet}10^{11}\ cm^{-2}$), $N_{ox} = 1{\bullet}10^{10}\ cm^{-2}$
- Conductive layer of 10 nm on top of passivation with $R_\square \approx 7{\bullet}10^{14}\ \Omega$
- Voltage ramp: -10 V/s up to -600 V and than constant -600 V

- pitch 80 µm
- width 18 µm
- thickness 200 µm
- $N_A = 3.4{\bullet}10^{12}\ cm^{-3}$

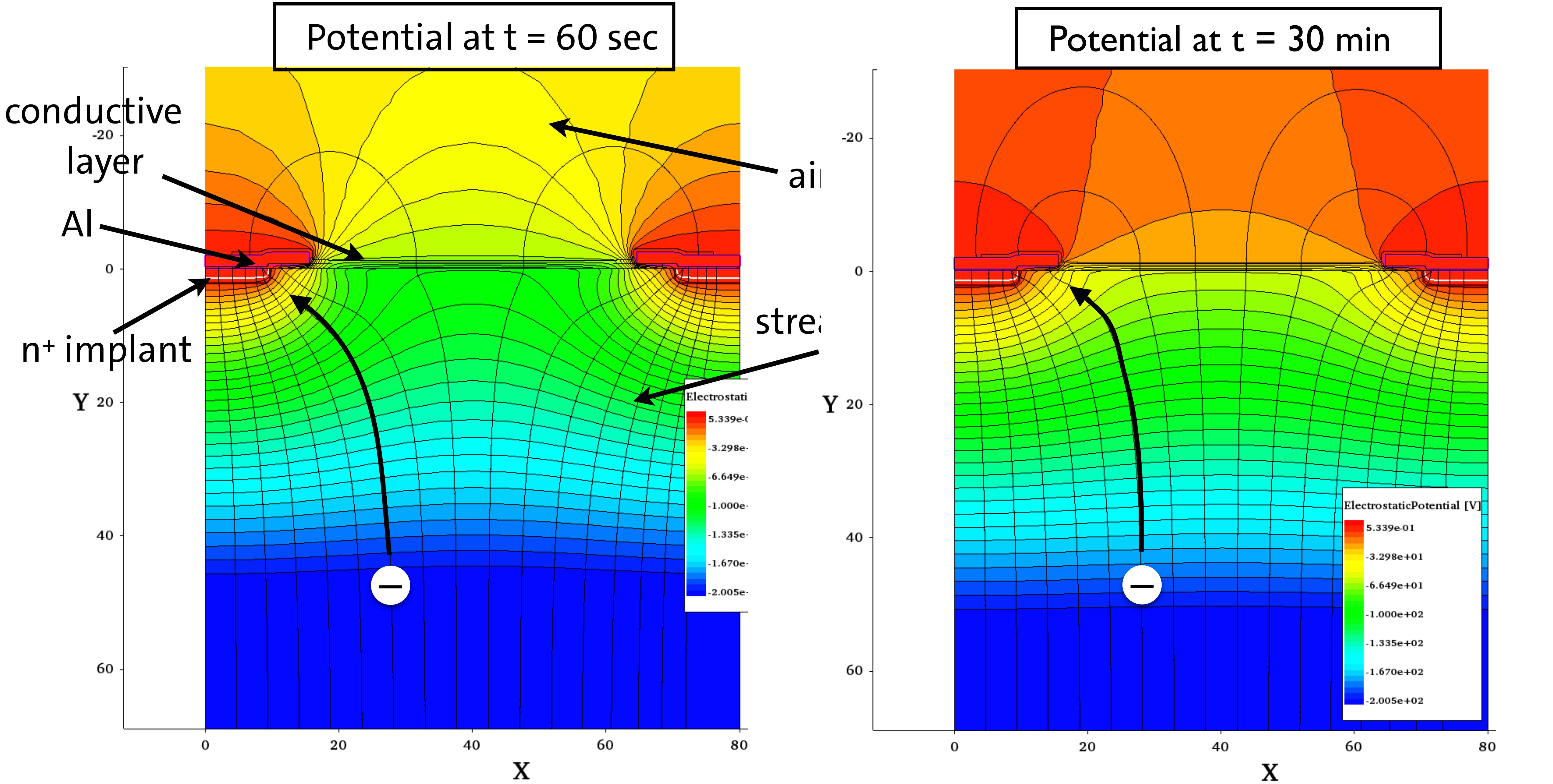


EFFECTS OF SURFACE POTENTIAL

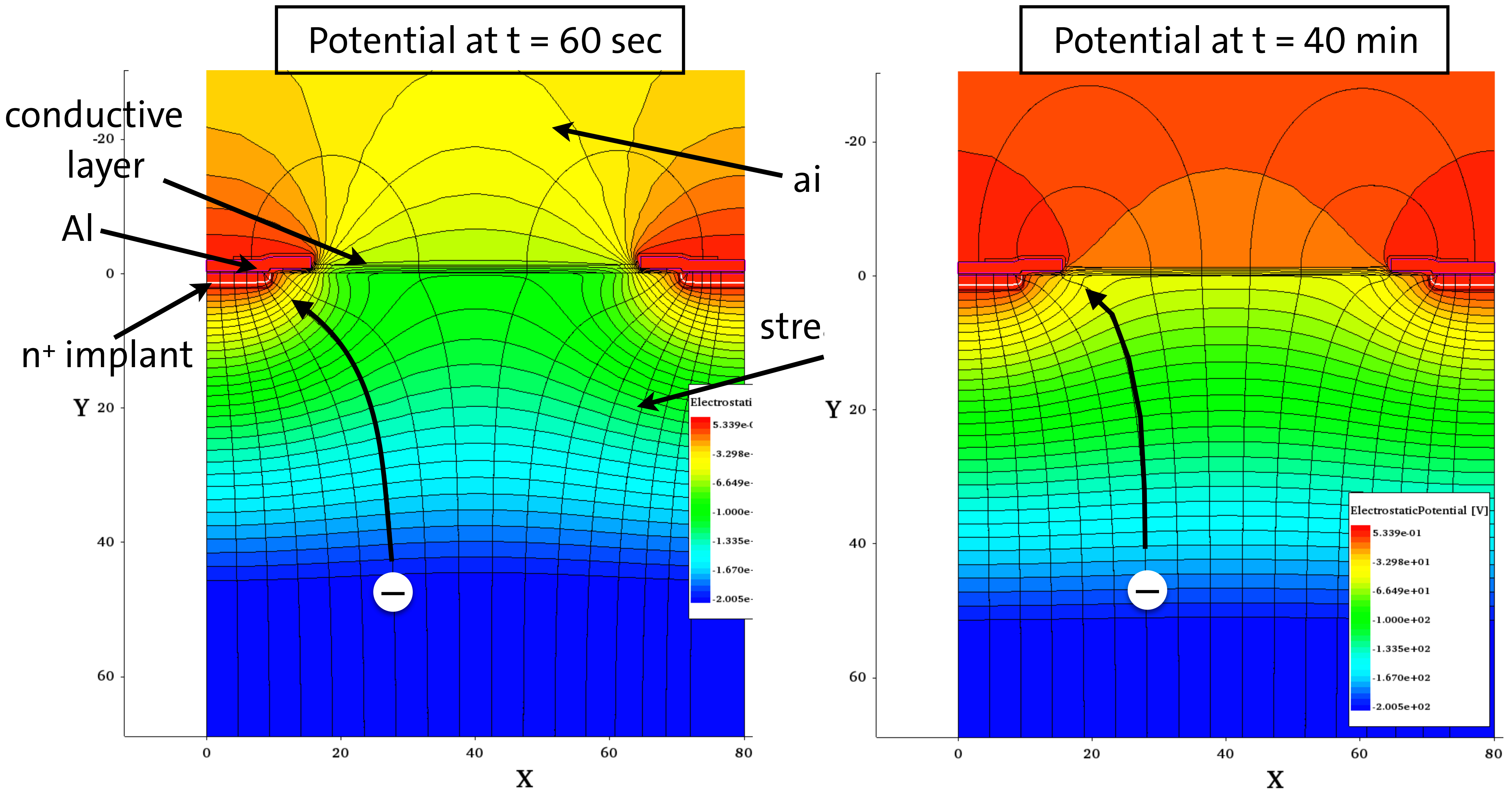




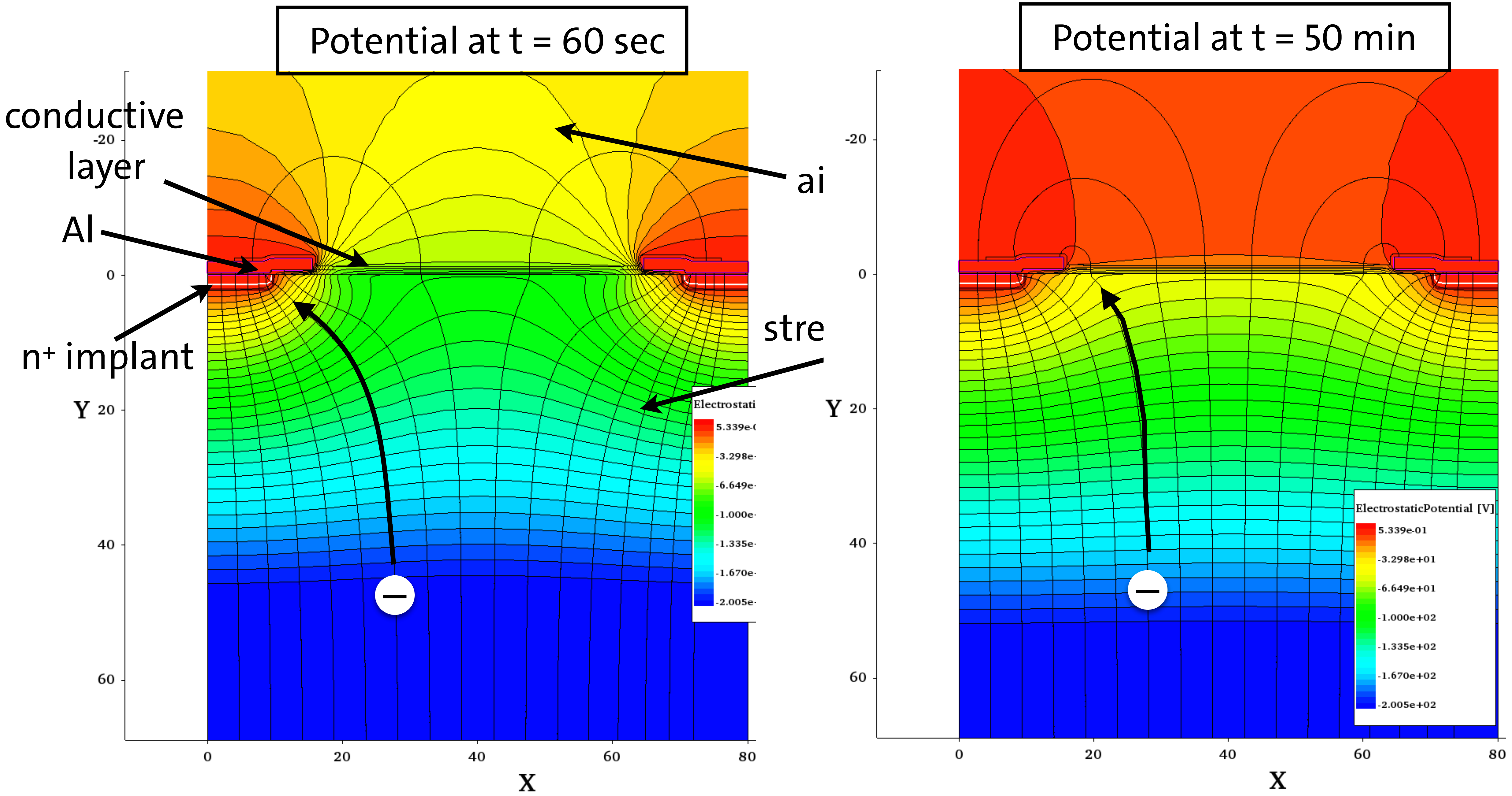
EFFECTS OF SURFACE POTENTIAL



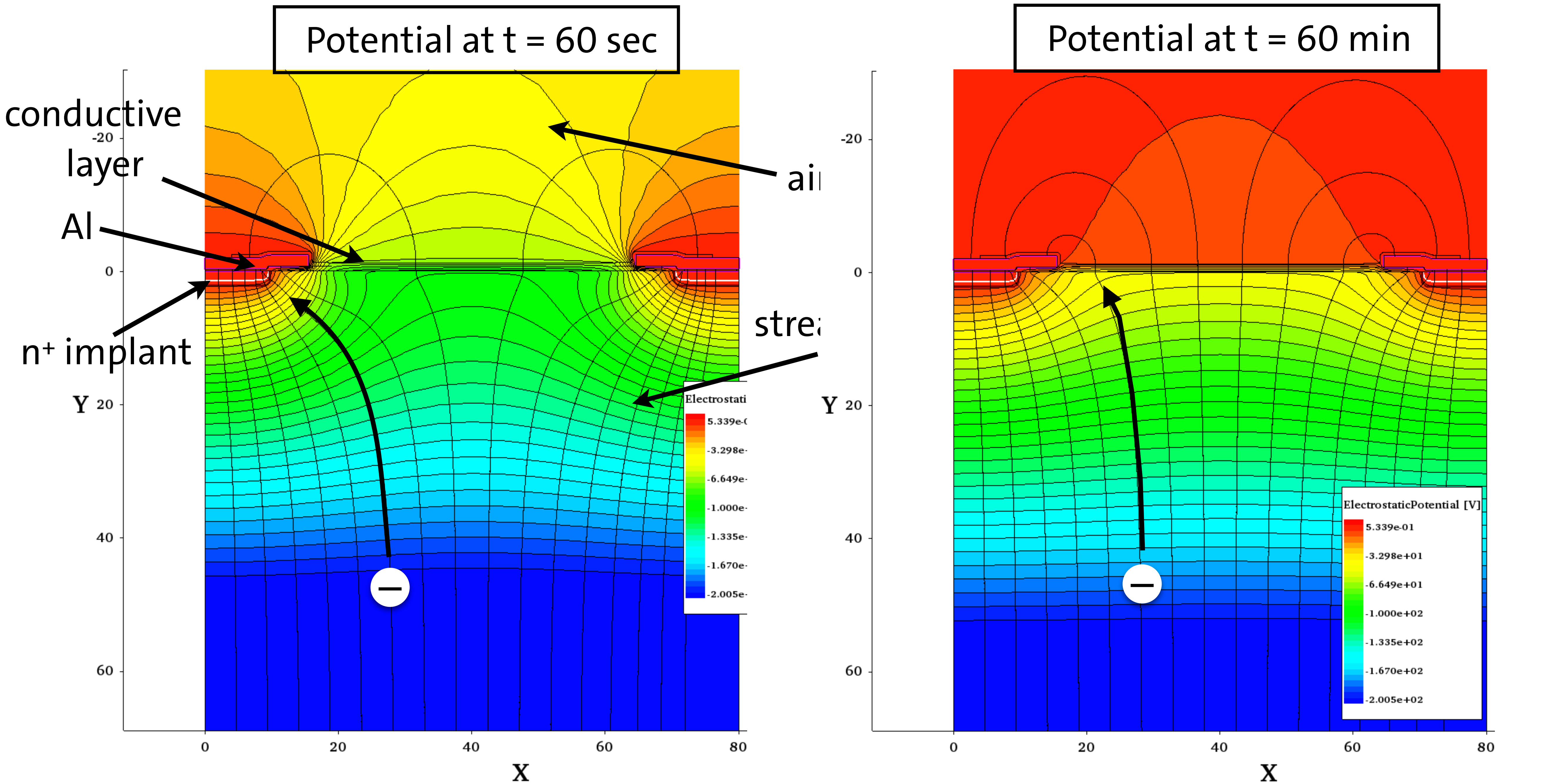
EFFECTS OF SURFACE POTENTIAL



EFFECTS OF SURFACE POTENTIAL

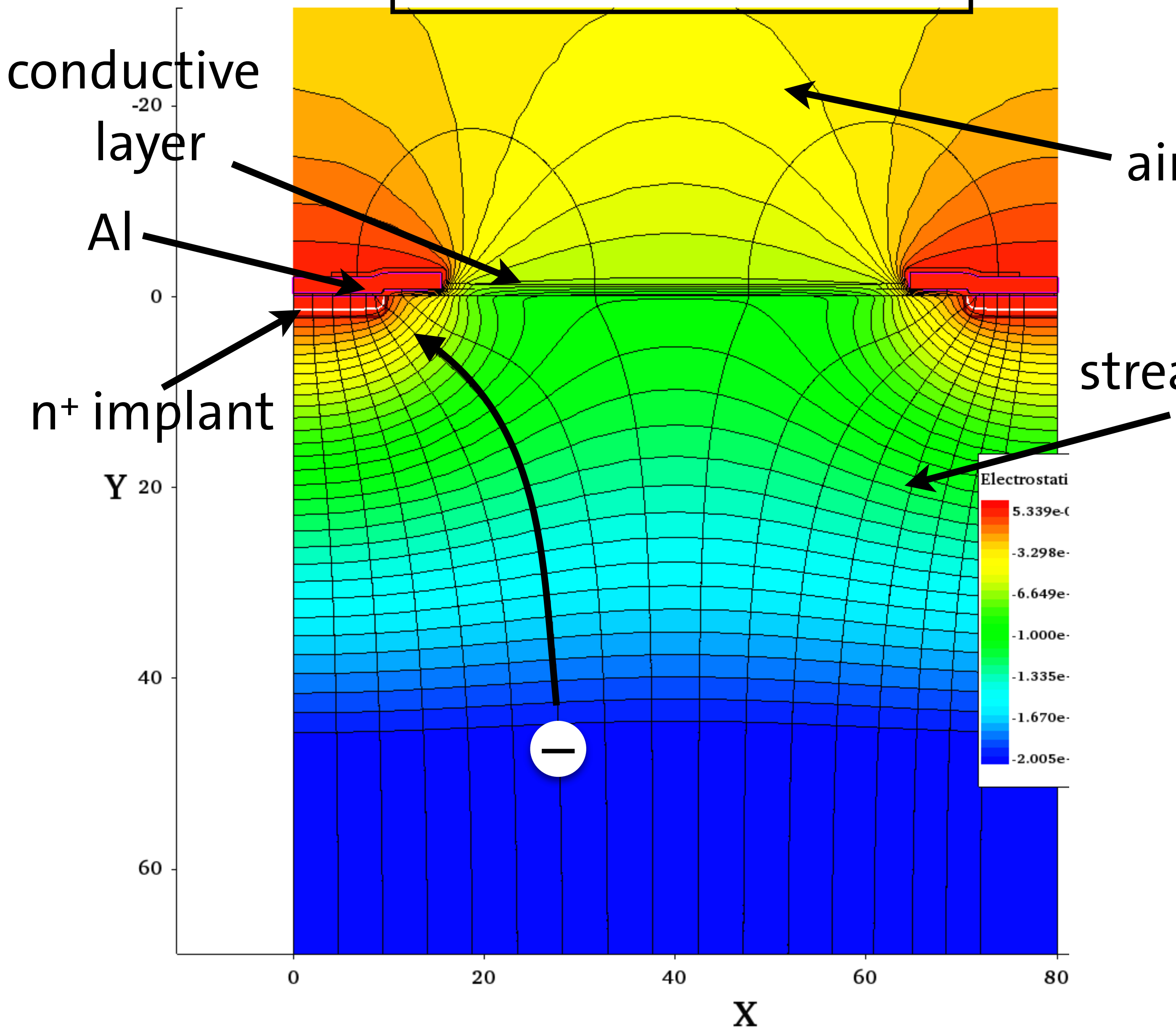


EFFECTS OF SURFACE POTENTIAL

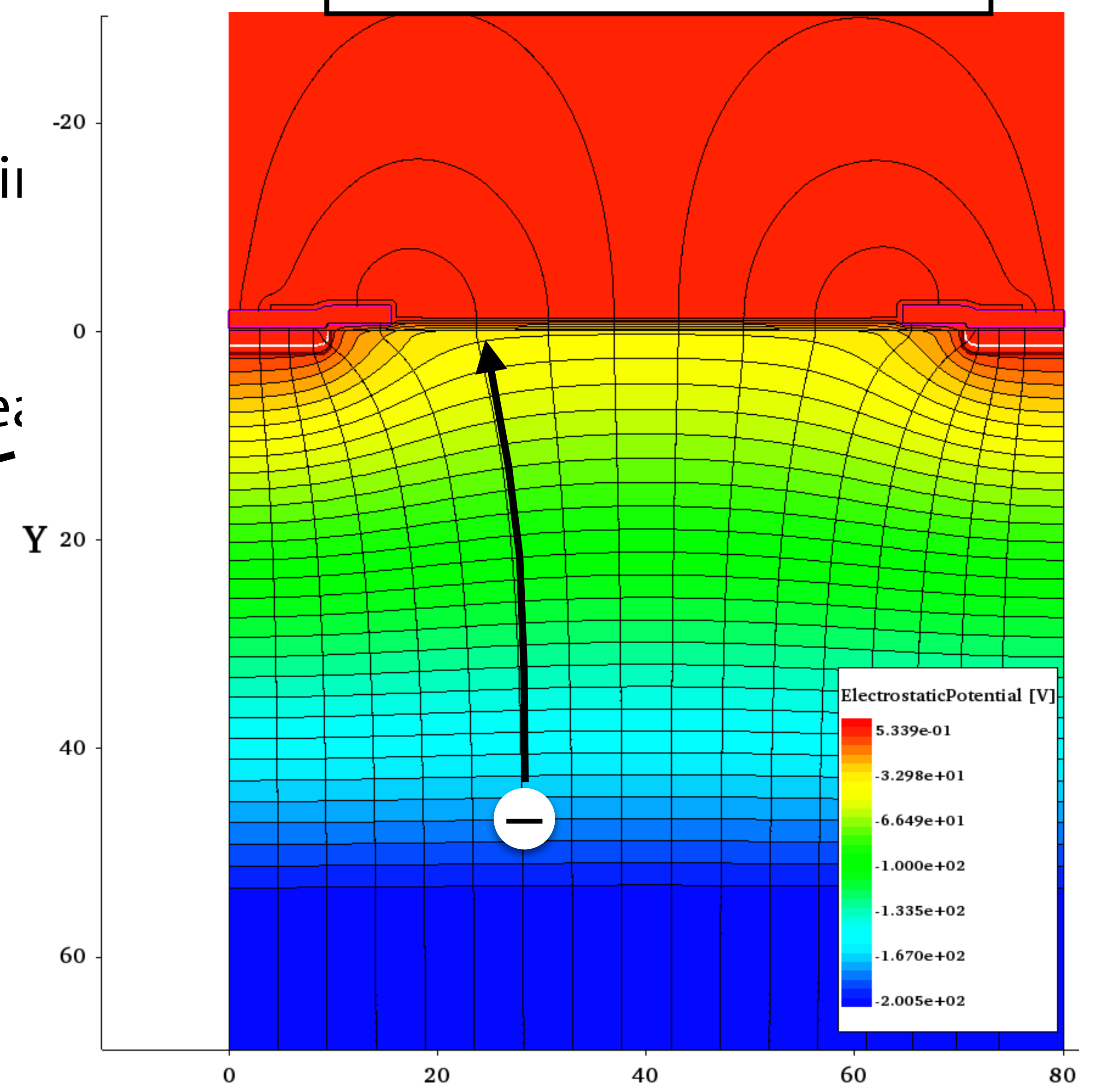


EFFECTS OF SURFACE POTENTIAL

Potential at t = 60 sec



Potential at t = 120 min



- Most streamlines end at implant
- Many streamlines ending at interface
  ➡ charge sharing, charge losses

➜ **E-field in the silicon sensitive to surface conditions**

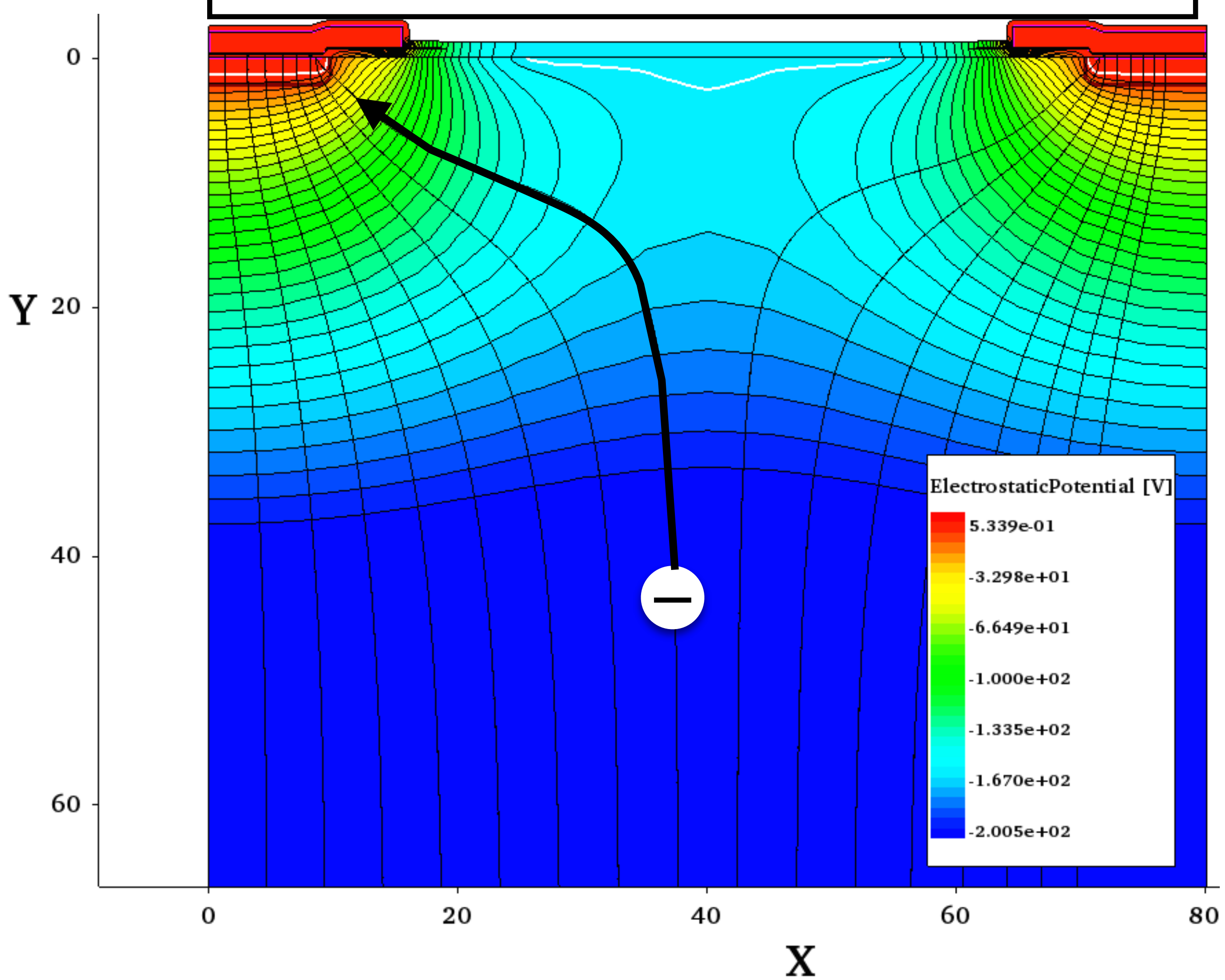
EFFECTS OF N_{OX}

Simulation example oxide charge dependence

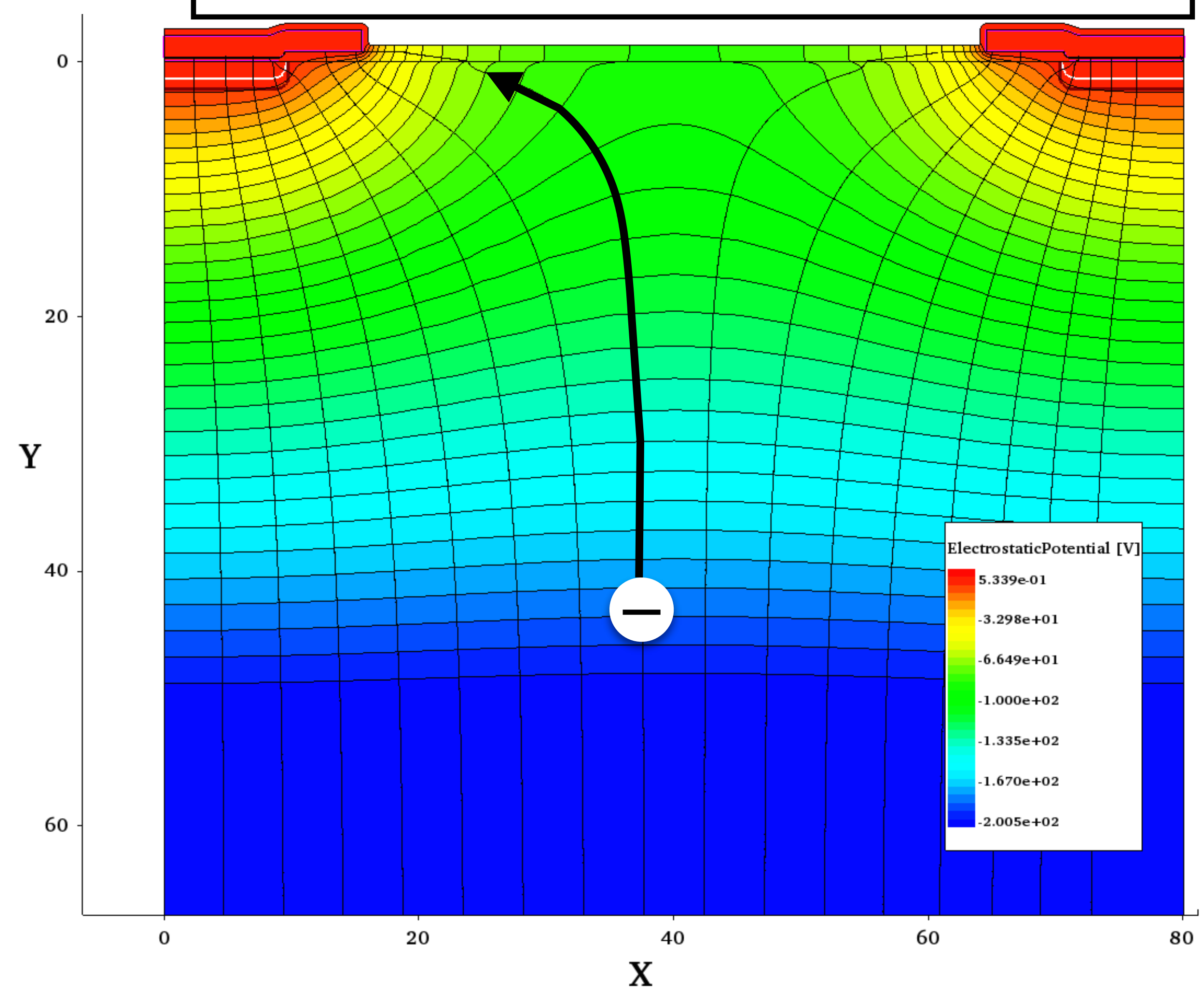
- AC coupled n^+-p sensor with p-spray ($N_{p\text{-}spray} = 5 \cdot 10^{11}$ cm^{-2})
- Neumann boundary conditions ($E_n = 0$)

- pitch 80 μm
- width 18 μm,
- thickness 200 μm
- $N_A = 3.4 \cdot 10^{12}$ cm^{-3}

Potential at -600, $N_{ox} = 1 \cdot 10^{10}$ cm^{-2}



Potential at -600, $N_{ox} = 5 \cdot 10^{11}$ cm^{-2}



→ E-field in the silicon sensitive oxide charges

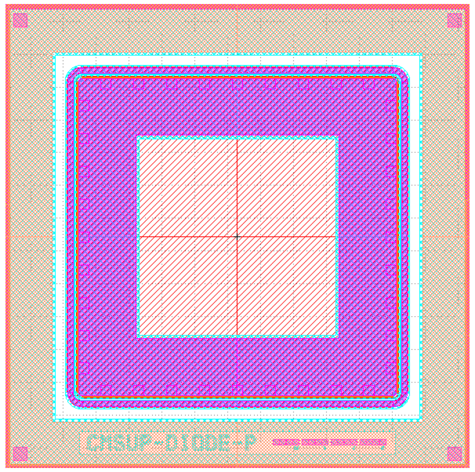
Examples of device simulations

Development of a bulk radiation damage model

DIODE MEASUREMENTS

Large and small diodes available from the CMS HPK campaign:

Diode 5mm x 5mm



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

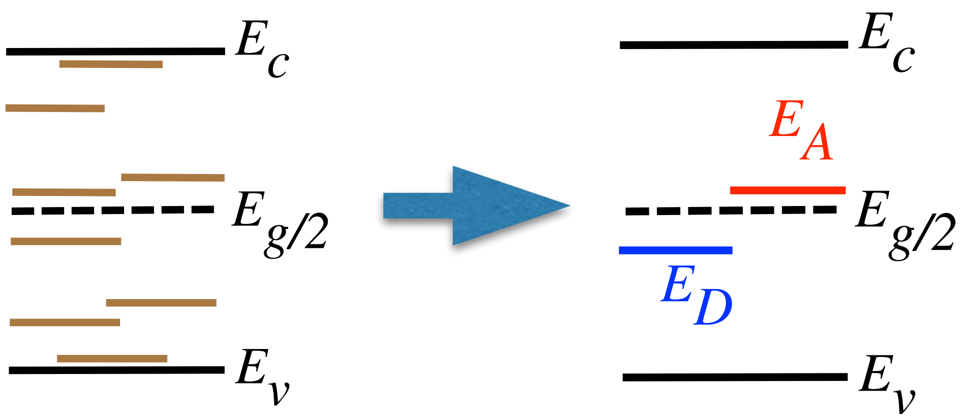
2. Irradiations
   - Protons **24 GeV/c**
     - Fluences: 0.3, 1, 1.5 , 2.4, 3 , 6, 7.75, $13 \cdot 10^{15}$ n_{eq}/cm^2

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

RADIATION DAMAGE MODELLING

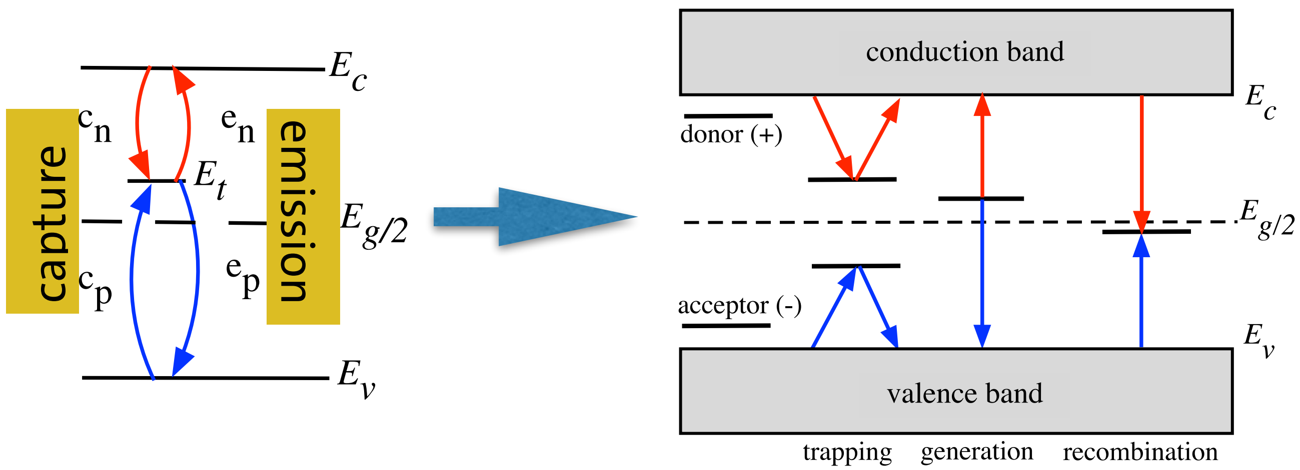
Radiation damage modelling:

- 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?)



Example: 2 trap model → 6 parameter

1. Energy levels: E_A , E_D **fixed**
2. Concentrations : N_A , N_D
3. Cross sections : σ^A_e , σ^A_h , σ^D_e , σ^D_h



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

with

$$f_D = \frac{v_h \sigma_h^D p + v_e \sigma_e^D n_i e^{E_D/kT}}{v_e \sigma_e^D (n + n_i e^{E_D/kT}) + v_h \sigma_h^D (p + n_i e^{-E_D/kT})}$$

$$f_A = \frac{v_e \sigma_e^A n + v_h \sigma_h^A n_i e^{-E_A/kT}}{v_e \sigma_e^A (n + n_i e^{E_A/kT}) + v_h \sigma_h^A (p + n_i e^{-E_A/kT})}$$

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

Trapping

$$\Gamma_h = v_h[\sigma_h^D N_D (1 - f_D) + \sigma_h^A N_A f_A]$$

$$\Gamma_e = v_e[\sigma_e^A N_A (1 - f_A) + \sigma_e^D N_D f_D]$$

PARAMETER TUNING

Attempts for the determination of new damage parameters:

- Simulate I-V, C-V and CCE with **infrared** for diodes for the fluences **3 , 6, 13•10[15]** n_{eq}/cm^2 and using the **optimiser of TCAD** for the determination of the free parameters i.e. minimise simultaneously for every fluence

$$F = \int_{-5V}^{-900V} (1 - \frac{I_{sim}}{I_{mes}})^2 \, dV + \int_{-5V}^{-600V} (1 - \frac{C_{sim}^{455Hz}}{C_{mes}^{455Hz}})^2 \, dV + \int_{-5V}^{-600V} (1 - \frac{C_{sim}^{1kHz}}{C_{mes}^{1kHz}})^2 \, dV$$
$$+ \int_{-200V}^{-1000V} (1 - \frac{CCEir_{sim}}{CEEir_{mes}})^2 \, dV$$

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 cylindrical coordinates at 5 voltages (CPU time: ≈50 min)

HPTM

Result of tuning: Hamburg Penta Trap Model (HPTM)

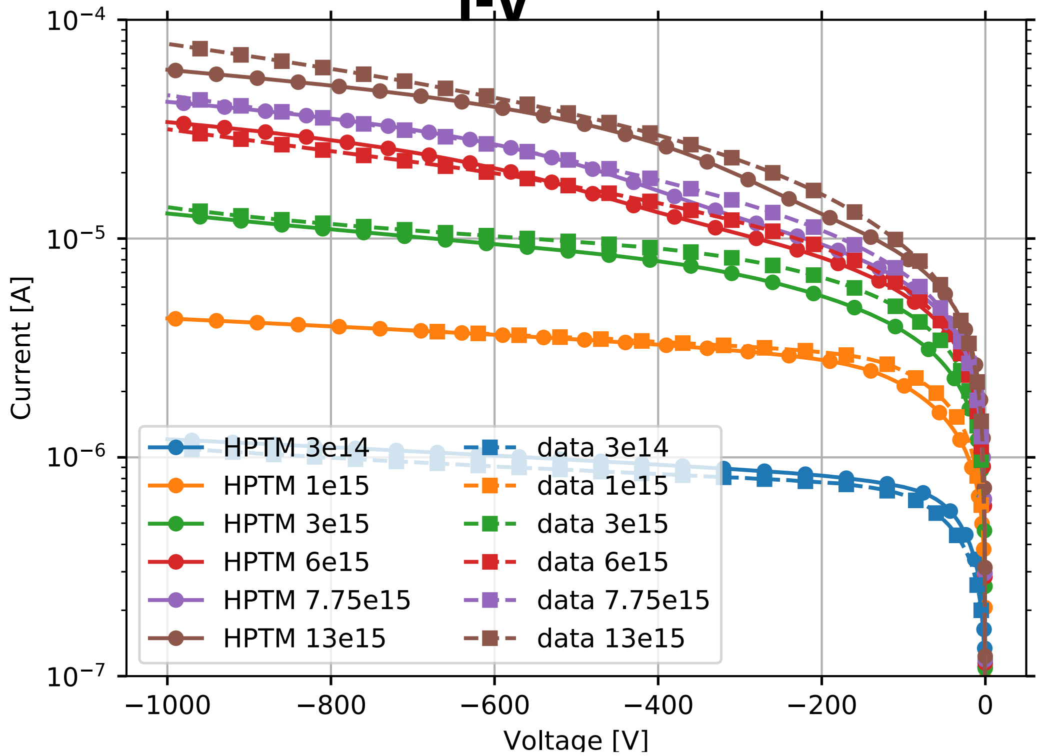
Defect	Type	Energy	g_{int} [cm^{-1}]	σ_e [cm^2]	σ_h [cm^2]
E30K	Donor	E_C-0.1 eV	0.0497	2.300E-14	2.920E-16
V_3	Acceptor	E_C-0.458 eV	0.6447	2.551E-14	1.511E-13
I_p	Acceptor	E_C-0.545 eV	0.4335	4.478E-15	6.709E-15
H220	Donor	E_V+0.48 eV	0.5978	4.166E-15	1.965E-16
C_iO_i	Donor	E_V+0.36 eV	0.3780	3.230E-17	2.036E-14

- Trap concentration of defects: **$N = g_{int} \cdot \Phi_{neq}$**
- Simulations for the optimisation have been performed at **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 : 11.7)
- Both cross section for the E30K and the electron cross section for the C_iO_i were fixed
  ➔ 12 free parameter
- Optimizsation done with the nonlinear simplex method

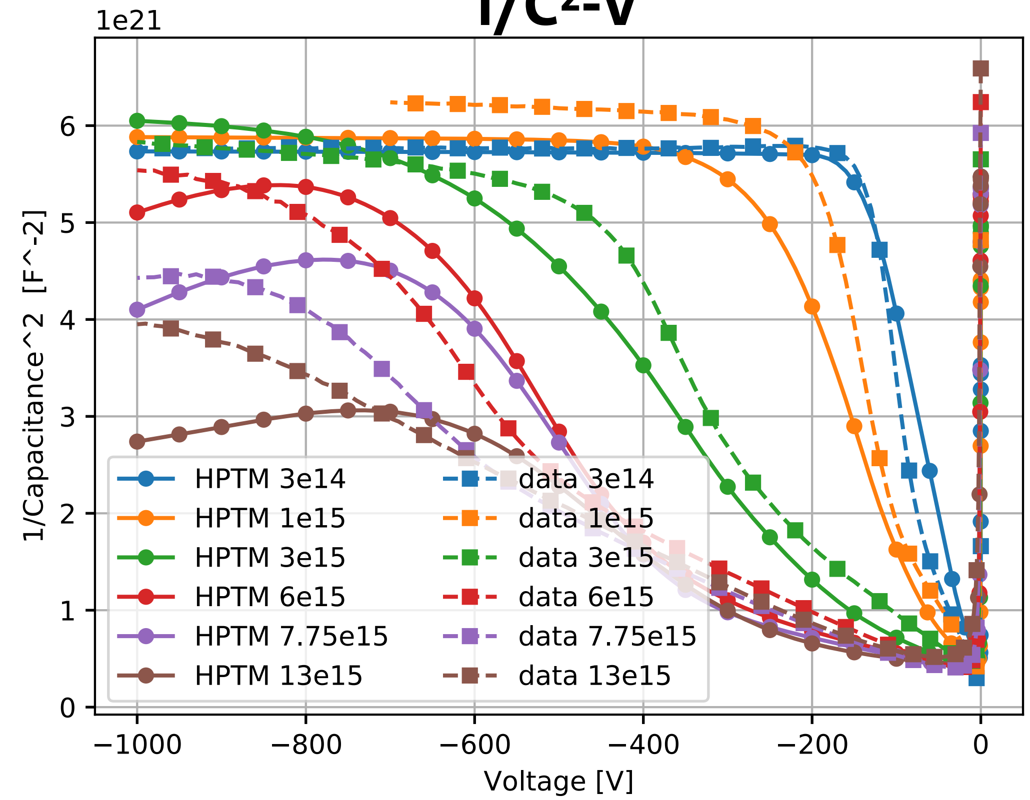
COMPARISON SIM. TO MEASUREMENTS

I-V, C-V and CCE-V for fluences from 0.3 - 13•10^{15} n_{eq}/cm^2 and T = -20 °C

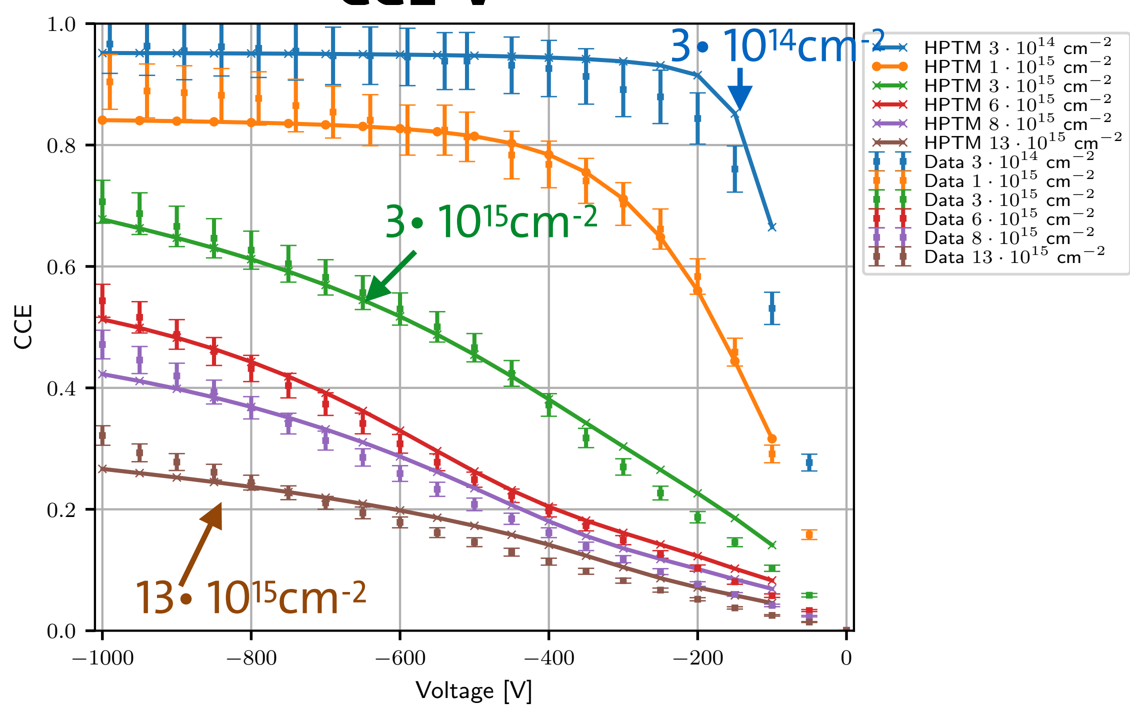
I-V



1/C²-V



CCE-V



- The simulation for 0.3 and 1•10^{15} n_{eq}/cm^2 are extrapolations and the 7.75•10^{15} n_{eq}/cm^2 is an interpolation
- The I-V, C-V simulations agrees with the measurements within 20% for all fluences
- CCE-V simulations for high voltages agrees with the measurements within 20% for all fluences

SUMMARY

- For ≈ 20 years, Synopsys Sentaurus TCAD has been a valuable tool for the HEP community in the sensor development
- It allows detailed process and device simulation in 1D, 2D and 3D
- TCAD simulations are important and helpful in
  - The design and optimisation of sensors
  - Understand and interpretation of measurements
  - Development of radiation damage models

Thank you for your attention!!!