

3D Detector Simulation with Synopsys TCAD



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- **Introduction**

- Past advances and future intentions
- The tool: Status and capabilities

- **Genic simulation principals**

- General Process Flow
- Optimization strategies
- Implantation models

- **Concrete cases**

- Test Diode example
- 2D IBL single pixel simulation
- Full 3D IBL single and multiple pixel geometries
- Edgeless Detectors Status

- **Dopant profile measurements**

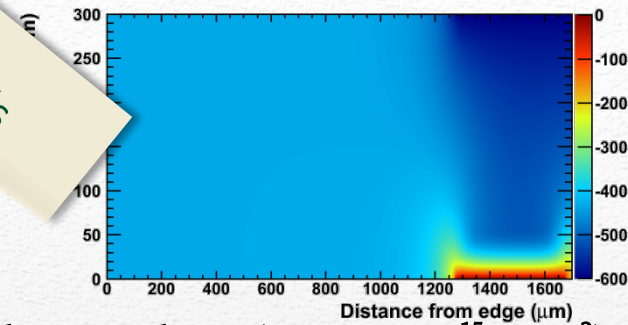
- **Conclusions and plans**



Outline

- Passing to 3D Simulations
- Migrating from SILVACO TCAD to Synopsys
- Both process simulation and irradiation model integration

Tools



IBL Voltage simulation (600V - $5 \times 10^{15} \text{ n}_{\text{eq}} \text{ cm}^{-2}$)

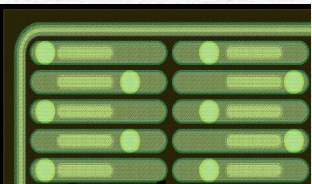
Intentions

Radiated IBL structures simulation

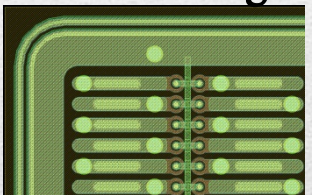
- Charge sharing and electrical field distributions
- Defects modeling and model testing

Validate Edgeless VTT geometry and radiation hardness

- Geometry and fabrication process flow simulation
- Detailed investigation of electrical field on detector edge
- Charge propagation in the substrate and boundary conditions effects
- Radiation hardness modeling and simulation



1 Guard Ring



Guard Ring + Bias Rail



No Guard Ring or Bias Rail

Introduction & Status

License

- One available license with minimum parallelization
- Three on-line license servers required
- Managed by LAL, accessible only via intranet
- No batch possibility at the moment (lxplus / ccage have no access to licenses)
- Multiple instances can be used, up to two per tool
- No multithreading support

- Portable Linux-based installation
- Out-of-the-box functionality
- No software dependencies
- Memory and CPU consuming

Status

*Technical support
can be an issue*

**Central Licensing management plus batch capabilities
essential**

Introduction & Status

- Create a fabrication process flow to simulate geometry
- Associate with corresponding mask directly from GDS files (usually provided)
- Introduce the required parameters (dose, energy, implantations)
- Set-up an appropriate meshing strategy for the desired application
- Set up required re-meshing along the process to speed up simulation
- Introduce variables and create multiple experiments
- Preview strictures and profiles, feed-in parameters to other tools



- I. No need for detailed geometry definition
- II. Graphical interphase for speed with command functionality
- III. Comprehensive simulation

- I. Detailed process flow never known
- II. Re-meshing mandatory in each geometry change
- III. Optimized for small scale devices and interface simulation between different materials

Generic Principals

1. The Mesh

- ✓ Define meshing strategy adapted to the specific geometry with finer cell size in transition regions
- ✓ Initial mesh valid until geometry change (first deposition, each), define re-meshing strategy before
- ✓ Avoid thick photosensitive layers since they are even meshed after stripping
- ✓ Usually simulate first few microns of substrate wafer and add full silicon thickness at the end
- ✓ In bilateral processes each flip causes geometry redefinition (no true bilateral integrated)

2. The model

- MC simulation or numerical solution to diffusion differential equations
- Number of particles to be simulated and extrapolate
- Physical model to be used



Optimising...

3. The refinements

- ❖ Implants energy and dose relative and absolute error
- ❖ Desired accuracy in concentration determination and profiles
- ❖ Grid refinements in transition regions (necessary to calculate solutions in dopants)
- ❖ Request multiprocessing

4. Implantation Model

- Analytic implantation: simple Gaussian/Pearson and dual Pearson functions, based on spatial distribution of ions described by moments depending on species, energy e.c.t. Numerical values given by tables
- Monte Carlo method atomistic simulation of ion implantation with Sentaurus MC, or Crystal-TRIM originated from the Transport of Ions in Matter (TRIM) code. Simulates ion implantation into single-crystalline materials or amorphous materials of arbitrary composition

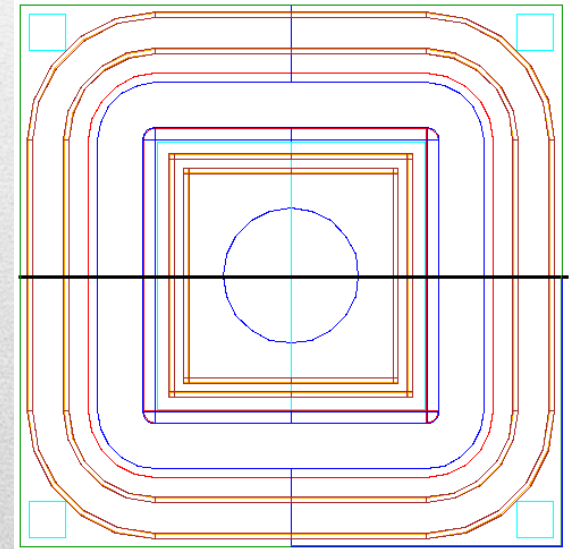
Optimizing....

- Simple geometry
- Known dopant profiles
- Large structure
- Experimental iv curves + compare with simulation

Pros: Simple geometry that allows model testing with simulated process flow
No Backside structure

Conns: Very large structure, enormous mesh with numerous cells which depletes available memory (in all platforms)

- Dimensions 3000 x 3000 μm
- No Nitride layer – p-spray

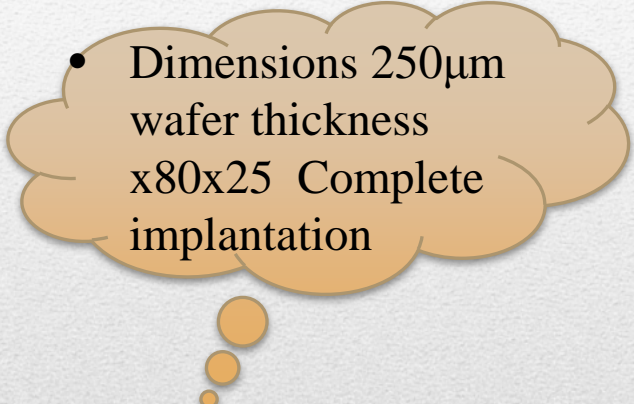


Concrete Cases: Test Diode

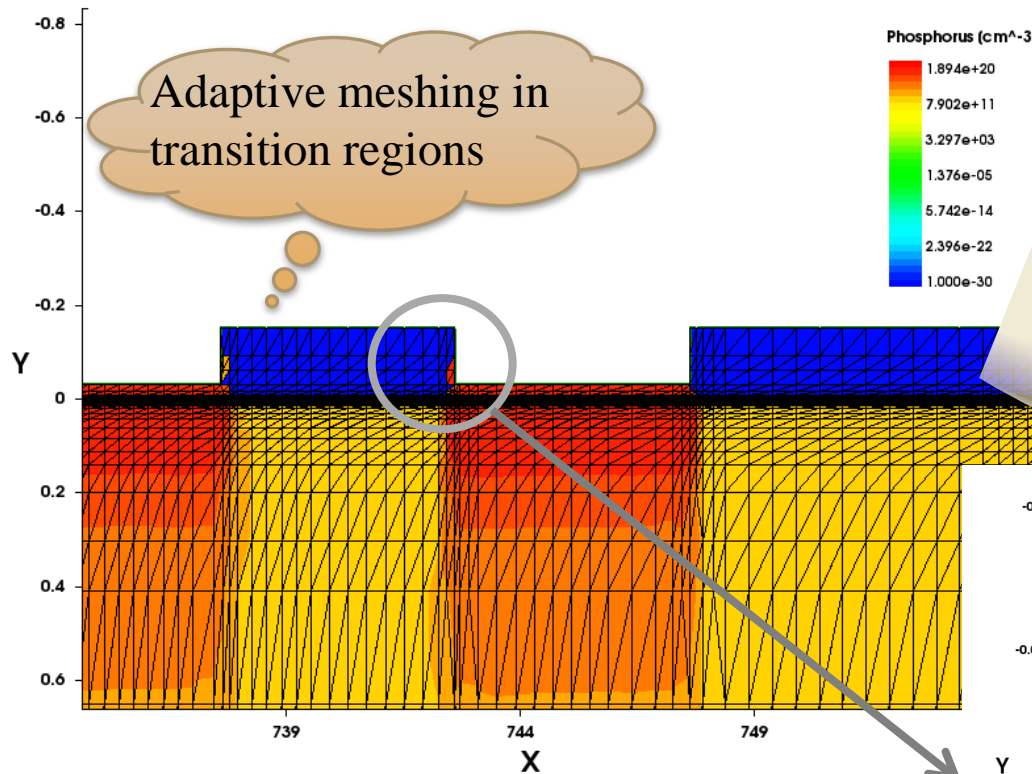
- Complete pixel geometry
- Have to start from basic parameters (dopant profiles not exactly known)
- Small structure
- Experimental iv curves to compare with simulation

Pros: Complicated geometry with multiple layers
Backside processing present
Have to do front and back side separately and merge results
Small size so limited number of grid cells

Conns: Aspects that are not yet completely understood in geometry file
24 hours for first implantation

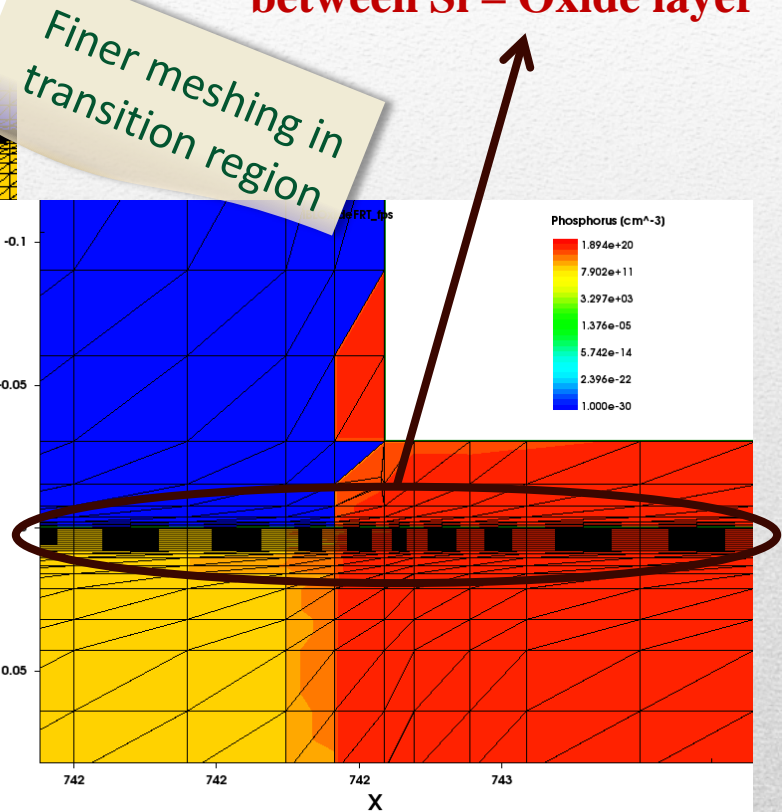
- 
- Dimensions 250 μ m wafer thickness x80x25 Complete implantation

Concrete Cases: IBL 2D



Phosphorus profile

Transition region
between Si – Oxide layer

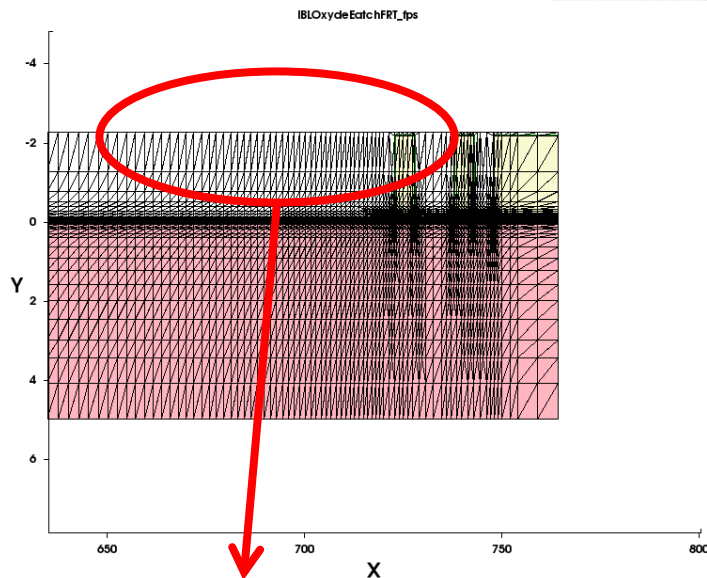
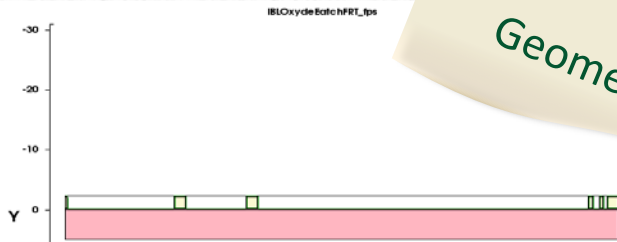


- *N profile in 2D IBL pixel simulation on the punch through side.*
- *Wafer is N with concentration of 10^{11} in the bulk. A thin 30nm Oxide layer remains.*

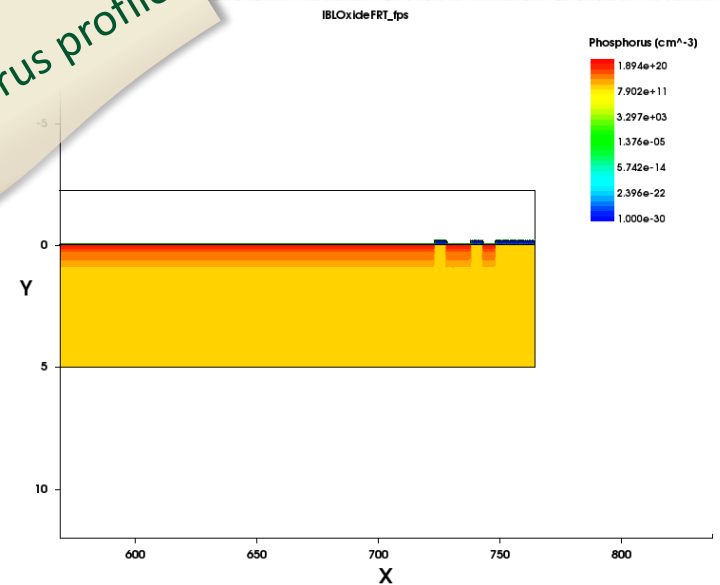
Concrete Cases: IBL 2D

Geometry

Phosphorus profile



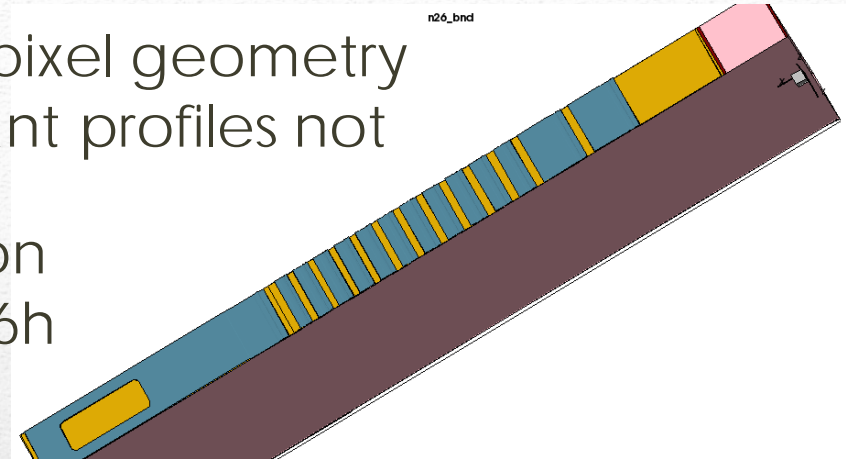
**Meshing of the
photosensitive region**



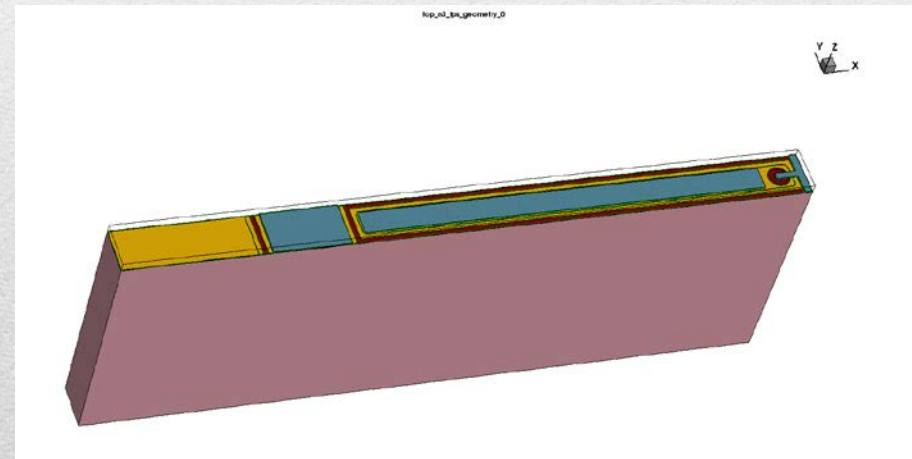
- *Images of the same region of the pixel in the punch through side.*
- *Dimension ration distorted to display surface structures*
- *All 250 μm of the wafer are simulated*
- *Photoresist is present in the upper left plot*

Concrete Cases: IBL 2D

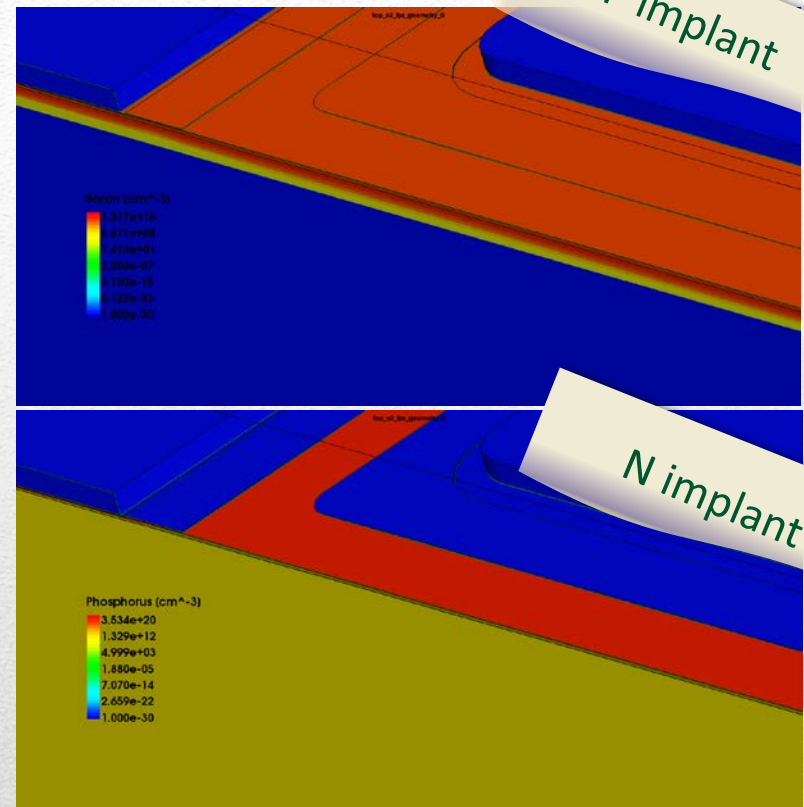
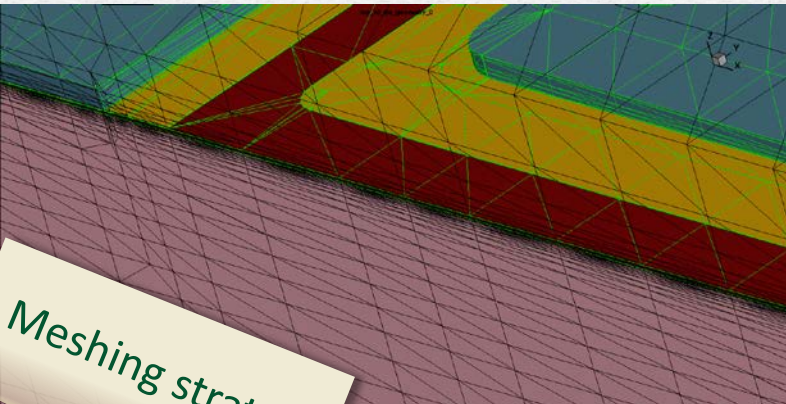
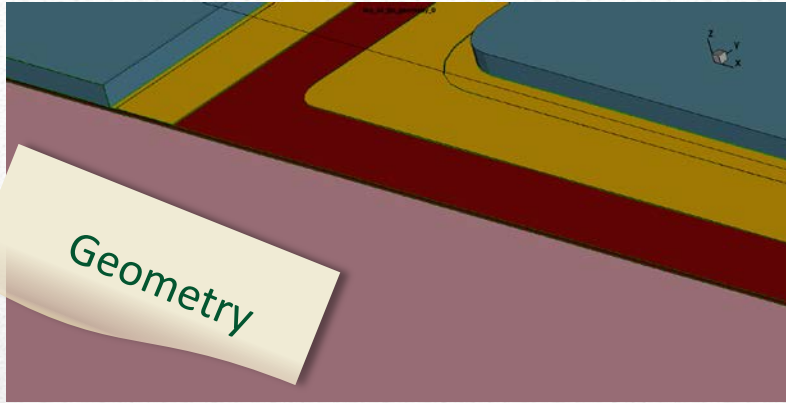
- Complete 3D double sided pixel geometry
- Use basic parameters (dopant profiles not exactly known)
- Full depth substrate simulation
- Time of full single pixel run ~ 6h
- Bilateral process flow



- **Process flow with ~50 stages**
- **3 Pixel geometry also available**
- **Carried out with one energy and dose but several scenarios are available**

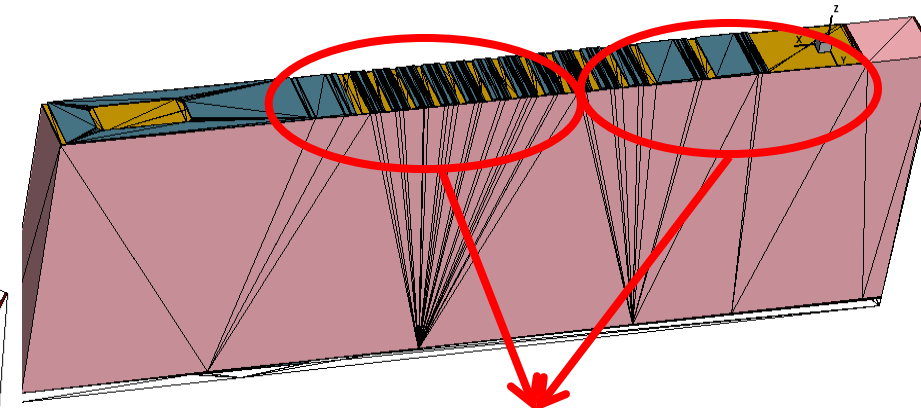
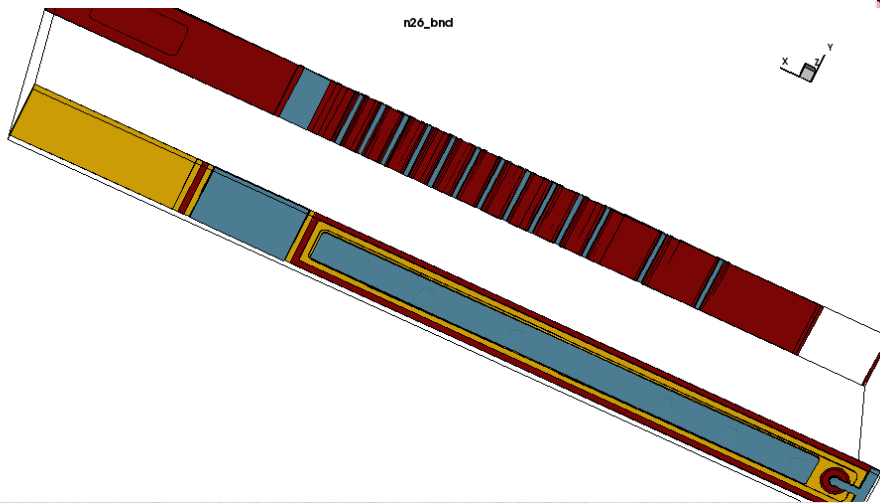
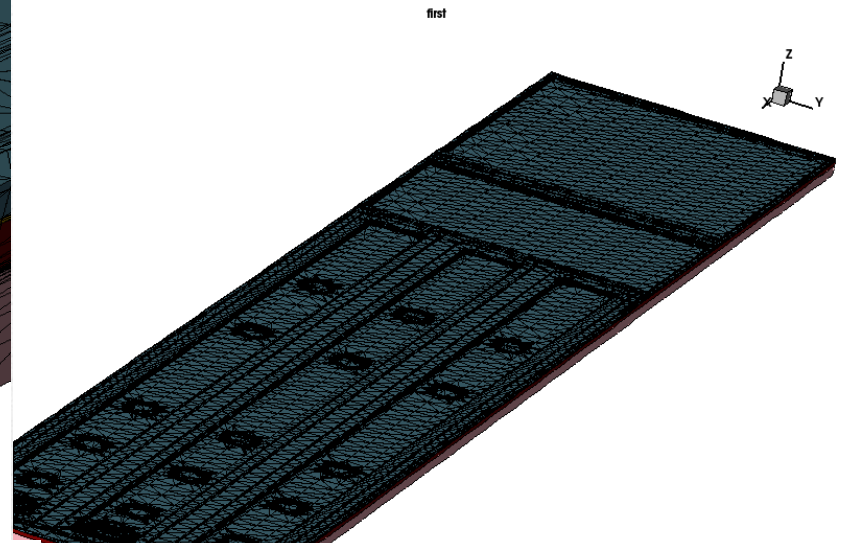
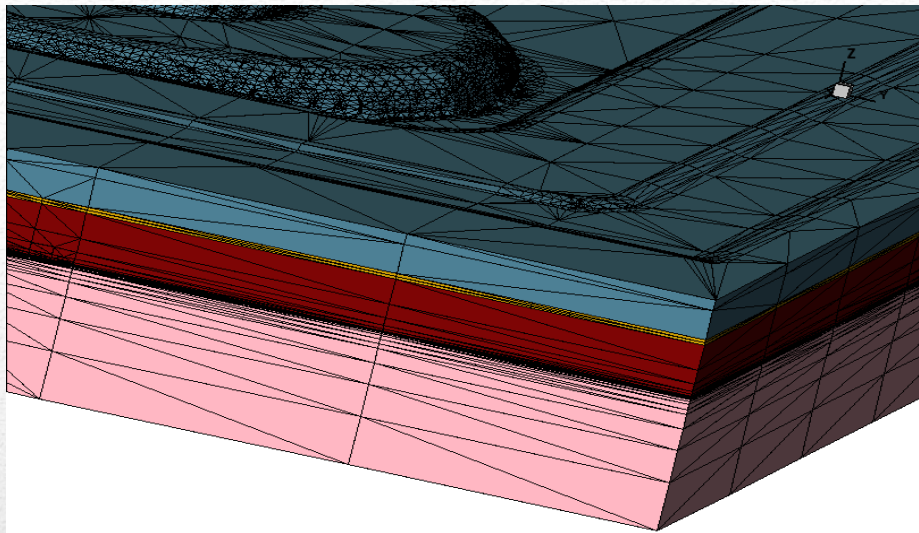


Concrete Cases: IBL 3D



Detail of the p-Spray region between the pixels showing meshing, geometry and implants concentration

Concrete Cases: IBL 3D



Finer Meshing in the Guard Rings

Concrete Cases: IBL 3D

- Silicon Substrate
 - ❖ Type: n, Phosphorus doped
 - ❖ Orientation: 100
 - ❖ Resistivity 50000hm/cm³
 - ❖ Thickness: 250μm (actual depth for simulation 5μm)
- Oxide Layer
 - ❖ Isotropic deposition of 150nm
 - ❖ Anisotropic etching with a remaining 20nm layer
- Photoresist
 - ❖ 2μm isotropic deposition followed by strip etching after development
- n Implant
 - ❖ Phosphorus at 60keV, dose of 10¹⁵ particles/cm² with angle of - 90°

Default Parameters

➤ P Spray

- ❖ Boron at 100keV, dose of 10^{13} particles/cm² with angle of -90°

➤ Annealing

- ❖ 300 minutes at 900 C, pressure of 1atm (literature reference of 3 temperature zones and pressures in the order of 500torr)

➤ Metallization - Passivation

- ❖ Aluminum contacts formation from isotropic CVD deposit
- ❖ SiO₂ passivation layer for mechanical and electrical protection (no implication in simulation result)

Default Parameters

[illegible]


981

Unfolded Flow										
PP #header	title	IRI Complete	save	true	phosphorus	grid	true	debug	false	
envelope	material	Silicon	dopant			concentration	1e14 /cm3	resistivity	5000 ohm	
substrate	dios		sprocess	# Specify max	side			tsuprem4		
insert	dios		sprocess	patGet	Grid Ade	side		tsuprem4		
insert	text	Added process 1								
PP #header	dios		sprocess	# Remeshing str.	side			tsuprem4		
deposit	material	Oxide	thickness	150 nm	dopant		default	concentration	/cm3	
pattern	layer	FRITIMPLANT	polarity	dark_field	thickness		0.1 um	side	front	
etch	material	Oxide	thickness	120 nm	etch_type		anisotropic	overetch	0	
save	baseName	IRI Oxide&etch	format	plot	dios			sprocess		
implant	species	boron	dose	@PDOS@ /cm	energy	@PENERGY@	tilt	0 deg	0	
etch	material	Photoresist	thickness	default	etch_type		strip	overetch	0	
save	baseName	IRI Oxide&FRT	format	dump	dios			sprocess		
deposit	material	Nitride	thickness	50 nm	dopant		default	concentration	/cm3	
pattern	layer	FRITNITRIDE&FRT	polarity	dark_field	thickness		0.1 um	side	front	
etch	material	Nitride	thickness	default	etch_type		anisotropic	overetch	0	
save	baseName	IRI NITRIDE&FRT	format	plot	dios			sprocess		
implant	species	boron	dose	@PSPRAYDOS@	energy	@PSPRAYENERGY@	tilt	0 deg	0	
etch	material	Photoresist	thickness	default	etch_type		strip	overetch	0	
save	baseName	IRI NITRIDE&FRT	format	dump	dios			sprocess		
anneal	time	300 min	temperature	900 degC	pressure	1 atm		0 V/min		
pattern	layer	FRTOXIDE&FRT	polarity	dark_field	thickness		0.1 um	side	front	
etch	material	Oxide	thickness	default	etch_type		anisotropic	overetch	0	
etch	material	Photoresist	thickness	default	etch_type		strip	overetch	0	
save	baseName	IRI Contact&FRT	format	dump	dios			sprocess		
deposit	material	Aluminum	thickness	50 nm	dopant		default	concentration	/cm3	
pattern	layer	FRMETAL	polarity	light_field	thickness		0.1 um	side	front	
etch	material	Aluminum	thickness	default	etch_type		anisotropic	overetch	0	
etch	material	Photoresist	thickness	default	etch_type		strip	overetch	0	
save	baseName	IRI Metal&FRT	format	plot	dios			sprocess		
deposit	material	SiO2	thickness	50 nm	dopant		default	concentration	/cm3	
pattern	layer	FRTPASSIVAT&FRT	polarity	dark_field	thickness		0.1 um	side	front	
etch	material	SiO2	thickness	default	etch_type		anisotropic	overetch	0	
etch	material	Photoresist	thickness	default	etch_type		strip	overetch	0	
save	baseName	IRI Complete&FRT	format	plot	dios			sprocess		
insert	dios		sprocess	side			transform flip	tsuprem4		
insert	dios		sprocess	# Remeshing str.	side			tsuprem4		
deposit	material	Oxide	thickness	150 nm	dopant		default	concentration	/cm3	
pattern	layer	BCKIMPLANT	polarity	dark_field	thickness		0.1 um	side	front	
etch	material	Oxide	thickness	120 nm	etch_type		anisotropic	overetch	0	
save	baseName	IRI Oxide&Etch	format	plot	dios			sprocess		
implant	species	boron	dose	@PDOS@ /cm	energy	@PENERGY@	tilt	0 deg	0	
etch	material	Photoresist	thickness	default	etch_type		strip	overetch	0	
save	baseName	IRI Oxide&BCK	format	dump	dios			sprocess		
deposit	material	Nitride	thickness	50 nm	dopant		default	concentration	/cm3	
pattern	layer	BCKNITRIDE&FRT	polarity	dark_field	thickness		0.1 um	side	front	
etch	material	Nitride	thickness	default	etch_type		anisotropic	overetch	0	
etch	material	Photoresist	thickness	default	etch_type		strip	overetch	0	
save	baseName	IRI NITRIDE&BCK	format	plot	dios			sprocess		
pattern	layer	BCKOXIDE&FRT	polarity	dark_field	thickness		0.1 um	side	front	
etch	material	Oxide	thickness	default	etch_type		anisotropic	overetch	0	
save	baseName	IRI Contact&BCK	format	plot	dios			sprocess		
deposit	material	Aluminum	thickness	50 nm	dopant		default	concentration	/cm3	
pattern	layer	BCKMETAL	polarity	light_field	thickness		0.1 um	side	front	
etch	material	Aluminum	thickness	default	etch_type		anisotropic	overetch	0	
etch	material	Photoresist	thickness	default	etch_type		strip	overetch	0	
save	baseName	IRI Metal&BCK	format	dump	dios			sprocess		
deposit	material	SiO2	thickness	50 nm	dopant		default	concentration	/cm3	
pattern	layer	BCKPASSIVAT&FRT	polarity	dark_field	thickness		0.1 um	side	front	
etch	material	SiO2	thickness	default	etch_type		anisotropic	overetch	0	
etch	material	Photoresist	thickness	default	etch_type		strip	overetch	0	
save	baseName	IRI Complete&FRT	format	dump	dios			sprocess		

30 steps with 5 macros, no back processing

55 separated steps, various variables and 8 macros

Process Flow Complexity

- 
- To Do, Effort on
the way
- GDS Files have been provided
 - Not complete understuding of the fabrication process
 - Scribe cleaning passivation poses simulation problem
 - Several efforts are in the way
 - Contacts in the near future with the industry (hoping to get input and details)

Edgeless Detectors

- Support a central licensing management which would allow multiple instances and parallelization
- Compare simulation results with experimental measurement in dopant profiles, charge shearing
- Simulate irradiated detectors and describe their behavior in the effort for radiation hardness
- Explore alternative geometries for bias rail / bias dot / guard ring structures

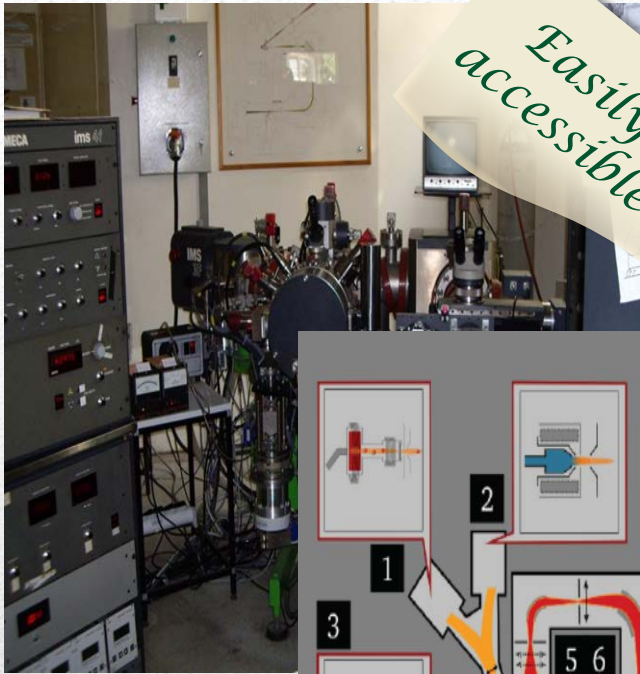
✓ Goal to simulate edgeless detectors
✓ likelihood approach for doping profiles to define correct parameters

Conclusions and plans

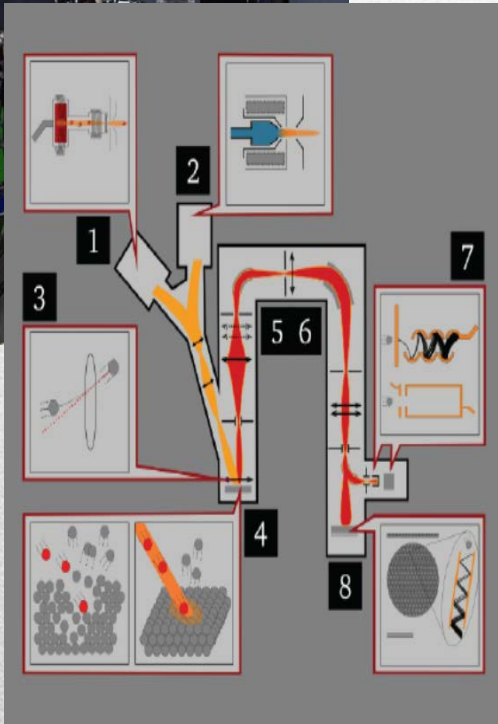


Backup

Easily
accessible



SIMS system
@ CNRS-
Meudon
(Cameca IMS
4F)



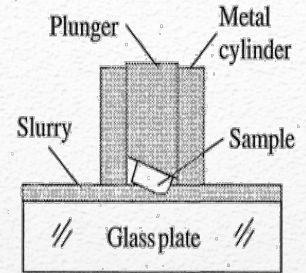
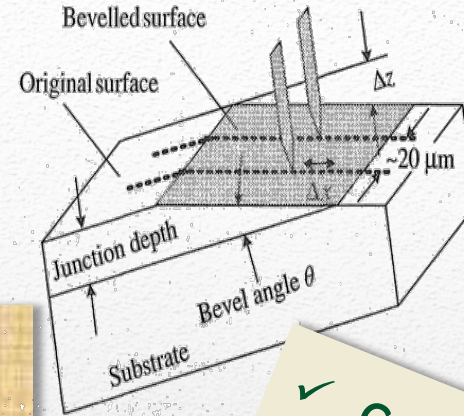
- Analytical technique to characterize the impurities in the surface and near surface ($\sim 30\mu\text{m}$) region
- Relies on sputtering of a primary energetic ion beam (0.5-20 keV) on sample surface and analysis of produced ionized secondary particles by mass spectrometry
- Good detection sensitivity for many elements: it can detect dopant densities as low as 10^{14} cm^{-3}
- Allows multielement detection, has a depth resolution of 1 to 5 nm and can give a lateral surface characterization on a scale of several microns
- Destructive method, since the act of the removing material by sputtering leaves a crater in a sample
- It determines the total dopant density profile

Dopants profiles – SIMS

Analytical technique to characterize the majority carrier and active dopant concentration profiles in semiconductor structures

Procedure

1. Pair of specially conditioned point contact probes which are stepped across the bevel surface of the semiconductor sample
2. Resistance between two probes is measured at each step
3. Resulting data computer processed into detailed carrier concentration and resistivity profiles from which dopant concentration profiles can be deduced



- ✓ Costly Technic carried out by Evans Analytical Group
- ✓ No full control of used parameters
- ✓ Development of in-house alternatives

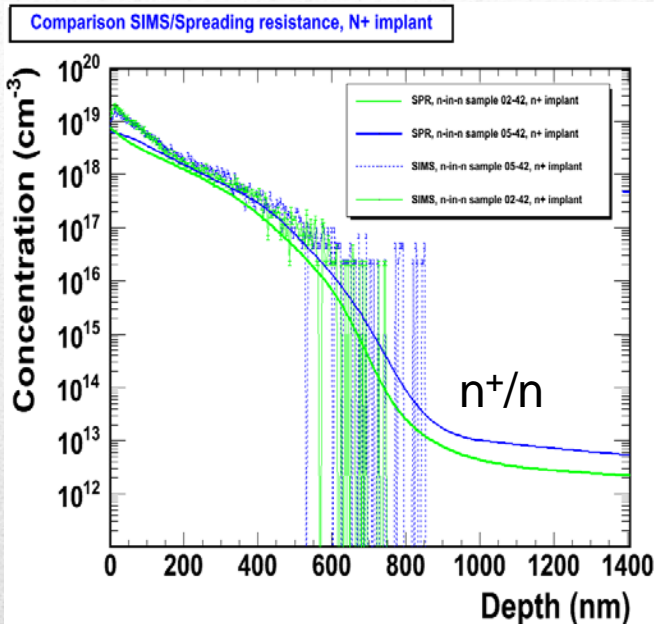
Dopants profiles — SRP

Pros: Very high dynamic range ($10^{12} - 10^{21} \text{ cm}^{-3}$)

Capable of profiling very shallow junctions (nm regime)

Conns: Destructive method

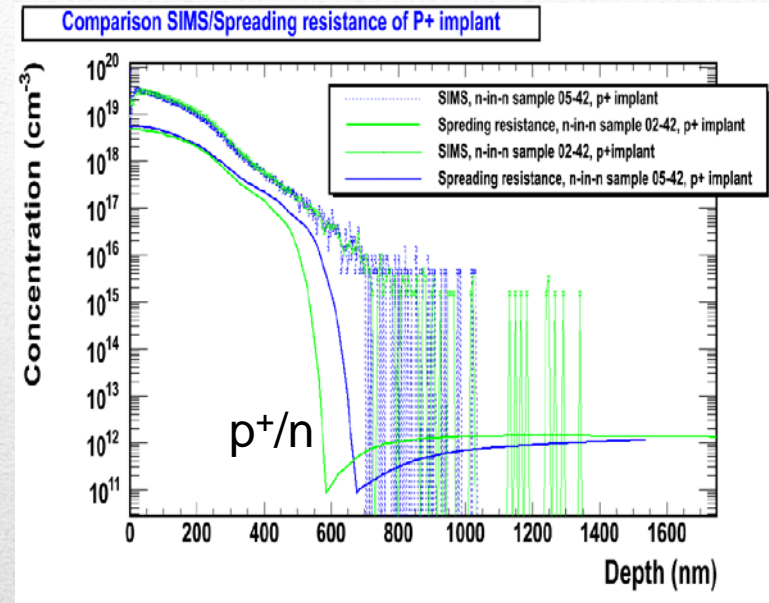
Dopants profiles



N+ implant characteristics

SIMS peak conc. $N_n \sim 1 \times 10^{19} \text{ cm}^{-3}$

SRP peak conc. $N_n \sim 8 \times 10^{18} \text{ cm}^{-3}$



P+ implant characteristics

SIMS peak conc. $N_p \sim 3 \times 10^{19} \text{ cm}^{-3}$

SRP peak conc. $N_p \sim 5 \times 10^{18} \text{ cm}^{-3}$

Measurements on n-on -n wafers
Good overall SIMS SRP agreement

Not all implanted dopant atoms are integrated in lattice positions, not all electrically active