The Use of ISE-TCAD Package for Simulation

- General presentation of ISE-TCAD – not commercial!
- Simulation approach
- ISE-TCAD and MAPS - example
- ISE-TCAD picked up examples
- Conclusions

Grzegorz Deptuch

LEPSI-IReS Laboratoire d'Electronique et des Systèmes Instrumentaux – Institut de Recherches Subatomiques – Strasbourg, France

deptuch@lepsi.in2p3.fr

General presentation of ISE-TCAD

ISE-TCAD simulation package released by:

Integrated Systems Engineering

Development, Modeling, and Optimization of Microelectronic Processes, Devices, Circuits, and Systems

- software that covers whole spectrum of simulation aspects from fabrication processes of integrated circuits, semiconductor devices and circuits represented in abstract form (SPICE netlist), mixed systems (semiconductor + abstract), packaging (thermal, electromagnetic, etc.) to interaction with environmental factors (radiation), etc.

VIRTUAL FOUNDRY

+

PRODUCT DEVELOPMENT

Are there any advantages of using this software in instrumentation for high energy physics community ? Particularly: detector development, front-end circuits, radiation hardness analyses…

General presentation of ISE-TCAD

Main features:

- Calibrated process simulator *(interesting for developing new detector technologies),*
- Advanced solid state physics models included *(from standard drift-diffusion model to quantum electronics, nanoelectronics, tunneling and advanced transport models)*
- True 3D device simulator !!! Finite element method solver,
- Meshing engine for 2D and 3D for planar and nonplanar devices *(powerful but difficult to control and not always clearly documented),*
- Si, Ge, SiGe, GaAs, heterostructures, compound semiconductors, isolation materials… *(wide choice of materials),*
- Optoelectronics, interaction of light with material, interaction of radiation with material *(alpha particles, heavy ions, but no MIP model + statistics),*

Fantastic ! but…

- No Monte Carlo simulations *(transport, interaction of radiation with matters, modelling of radiation sources, etc.),*
- Hermeticity !!! weak influence of the user on the software, possibility of Tcl/Tk programming but difficult if not impossibly integration with existing tools…

e.g. Output files for 3-D simulations with >10 digit precision, tons of MB, no way to change if such precision is not needed, thus simulations slow and huge physical memories needed!

General presentation of ISE-TCAD

Software tools in the package:

Process Simulator	
DIOS	Current 1D/2D Si and SiGe Process Simulator
FLOOPS	Next Generation Process Simulator 1D/2D/3D
Device Simulator	
DESSIS	2D/3D, Si and heterodevices, general purpose
DESSIS-Laser	Semiconductor lasers
Structure Generation	
DEVISE	2D/3D graphical structure editor
MDRAW	2D graphical structure editor *(boundary and doping)*
PROLYT	Layout editor *(CIF, GDSII import)*
PROSIT	3D structure generator (masks and doping profiles)
DIP/GIP	3D interpolation tools *(from cross-sections to 3D structure)*
Meshing Generation	
MESH	2D/3D mesh generator
Compact Model Parameters Extraction	
ISExtract	Compact model parameters extractor (BSIM4)
Framework Tools	
GENESISe	Graphical front end, organization of simulation projects
LIGAMENT	Process simulation environment
OptimISE	Parametric and statistical analysis, and optimization
Tecplot-ISE	Advanced visualization, 1D/2D/3D
INSPECT	Plotting and data analysis, X-Y

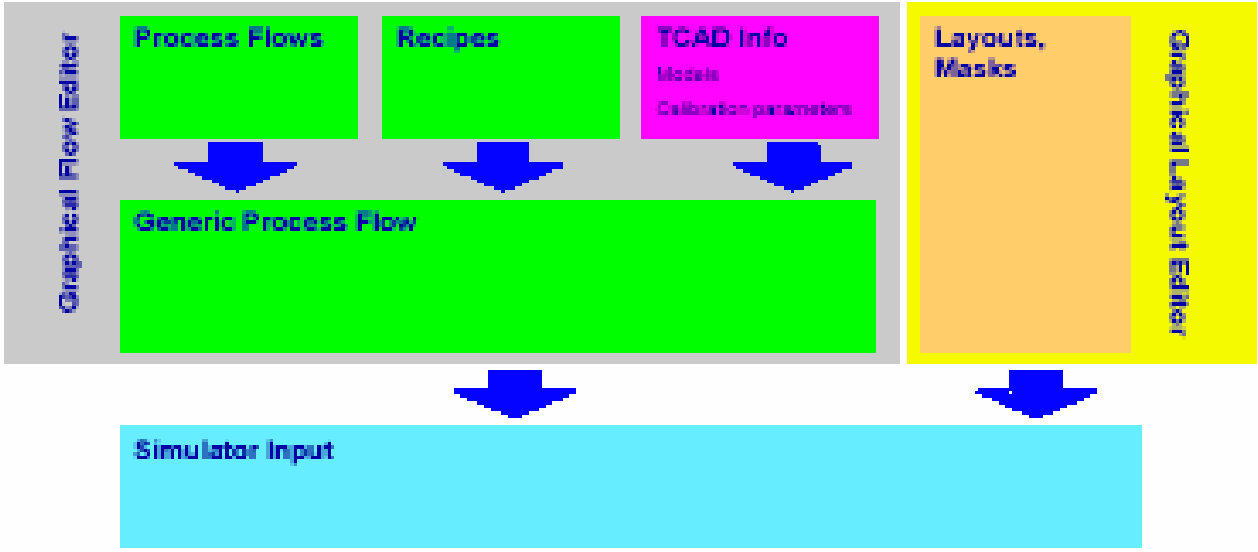
NO SCHEMATIC EDITOR !!!

ISE TCAD, see www.ise.com

Simulation approach

2 cases: 1: process simulation,

- **PROCESS SIMULATION - standard approach:** ***to create device structures through fabrication process simulations and passing to simulation of "virtual devices"*****,**



LIGAMENT - package serving interface for process simulation (DIOS, FLOOPS) that is, as much as possible, independent of the particular process simulator and the simulation dimension.

Inputs: a process flow, process libraries, layouts, and other TCAD-related information

Outputs: process simulator command files or other translation targets.

Simulation approach

1: process simulation,

c:/DB/ProcessTemplate/liq.cmd - Ligament Flow Editor 8.0

File Edit Preferences Help

Variables & Macros | Flow | Unfolded Flow

Names	Arg	Value	Arg	Value
Flow				
environment	title	0.18 NMOS	save	true
substrate	dopant	boron	concentration	0 /cm3
MOSLIB_gridding	L_gate	0.18 um	tensor	false
diffusion_defaults				
channel				
gate-oxidation				
poly-gate				
comment	text	poly gate		
deposit	material	poly	thickness	180 nm
pattern	layer	GATE	polarity	light_field
etch	material	poly	thickness	default
etch	material	oxide	thickness	default
etch	material	resist	thickness	default
poly-reoxidation				
anneal	time	40 sec	temperature	(700) (900) degC
anneal	time	20 min	temperature	900 degC
anneal	time	40 sec	temperature	(900) (700) degC
nldd-implant				
halo-implant	symmetry	true		
comment	text	halo implantation		
if	condition	$symmetry		
--MOSLIB_reflect				
endif				
implant	species	boron	dose	2.5e+012 /cm2
implant	species	boron	dose	2.5e+012 /cm2
implant	species	boron	dose	2.5e+012 /cm2
implant	species	boron	dose	2.5e+012 /cm2
if	condition	$symmetry		
--MOSLIB_unreflect				
endif				
RTA-halo-ldd				
nitride-spacer				
nplus-implant				
RTA_final				
MOSLIB_contacts	source	false	drain	true
MOSLIB_1D_cut	filename_root	channel_profile	position	0 nm

anneal(...)

Arg name	Arg type	Arg value	Arg unit
time	Time	20	min
temperature	Temperature	900	degC
pressure	Pressure	1	atm
nitrogen	Gas	1	l/min
hydrogen	Gas	0	l/min
oxygen	Gas	1	l/min
hcl	Gas	0	l/min
POCl3	Gas	0	l/min
steam_temperature	Temperature	0	degC
watersteam	Gas	0	l/min
pyrosteam	Gas	0	l/min
side	Side	both	
type	Type	default	

Generic	Process	Local: untitled	Lib: MOSlib.spr	Lib: thermalLib.s
comment	anneal	$ implant_pwell	MOSLIB_1D_cut	anneal_rec
insert	deposit	$ implant_nldd	MOSLIB_contacts	anneal_rec
load	epitaxy	$ implant_halo	MOSLIB_gridding	anneal_rec
save	etch	$ implant_nsd	MOSLIB_reflect	anneal_rec
if	implant	channel	MOSLIB_unreflect	
elif	pattern	diffusion_defaults		
else	pattern2d	full_device		
		gate-oxidation		
		halo-implant		
		nitride-spacer		
		nldd-implant		
		nplus-implant		
		poly-gate		
		poly-reoxidation		
		RTA-halo-ldd		
		RTA_final		

Mode: workspace: liq.wks

Simulation approach

1: process simulation,

poly-gate				
comment	text	poly gate		
deposit	material	poly	thickness	180 nm
pattern	layer	GATE	polarity	light_field
etch	material	poly	thickness	default
etch	material	oxide	thickness	default
etch	material	resist	thickness	default
poly-reoxidation				
anneal	time	40 sec	temperature	{700} {900} degC
anneal	time	20 min		
anneal	time	40 sec		

anneal (...)

Arg name	Arg type	Arg value	Arg unit
time	Time	20	min
temperature	Temperature	900	degC
pressure	Pressure	1	atm
nitrogen	Gas	1	l/min
hydrogen	Gas	0	l/min
oxygen	Gas	1	l/min
hcl	Gas	0	l/min
POCl3	Gas	0	l/min
am_temperature	Temperature	0	degC
watersteam	Gas	0	l/min
pyrosteam	Gas	0	l/min
side	Side	both	
type	Type	default	

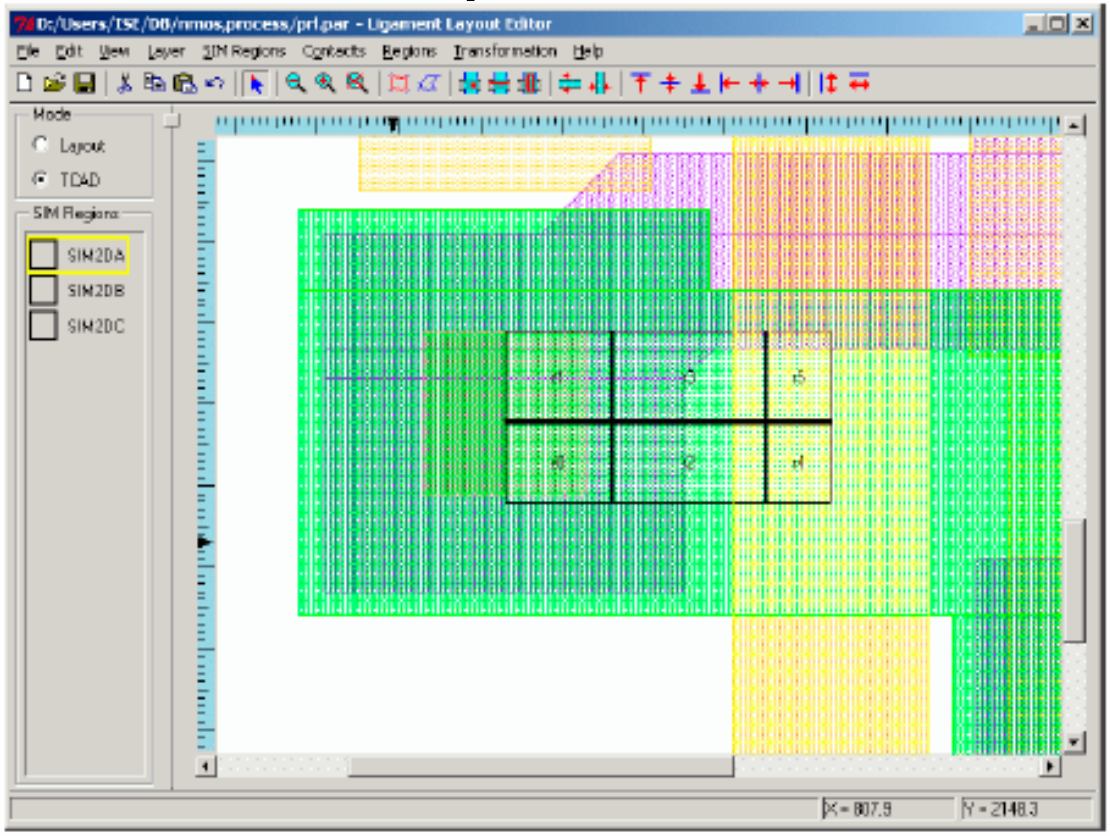
Full process flow – basic steps defined at physical level – parameterisation for mutli-variant process simulation *(DoE)*

Generic	Process	Local: untitled	Lib: MOSlib.spr	Lib: thermallib.s
comment	anneal	implant_pwell	MOSLIB_1D_cut	anneal_rec
insert	deposit	implant_nldd	MOSLIB_contacts	anneal_rec
load	epitaxy	implant_halo	MOSLIB_gridding	anneal_rec
save	etch	implant_nsd	MOSLIB_reflect	anneal_rec
if	implant	channel	MOSLIB_unreflect	
elif	pattern	diffusion_defaults		
else	pattern2d	full_device		
		gate-oxidation		
		halo-implant		
		nitride-spacer		
		nldd-implant		
		nplus-implant		
		poly-gate		
		poly-reoxidation		
		RTA-halo-ldd		
		RTA_final		

Process simulation *(DIOS, FLOOPS)* carried out basing on models of implantation, diffusion, etching, etc, 3D structure obtained or 2D cross-sections for interpolation *(DIP/GIP)*

Simulation approach

1: process simulation,



- Layout editor *(PROLYT)* CIF/GDSII import + export (←→ CADENCE),
- process simulation for selected areas of interest (1D, 2D +3D) → structure for (interpolation *DIP/GIP*) with contacts, meshing and electrical simulation !!!

Simulation approach

2 cases: 2: idealised geometries simulation,

- special circumstances: *process simulation is not needed; for conceptual studies or fast parametric analysis idealized device geometries directly created with analytic doping profiles* using device editor and then simulation.

  - *Device geometry is defined*

    a) from the mask layout and the process flow (PROSIT) – process emulation,

    b) by user drawing the geometry in 2D (MDRAW) or in 3D (DEVISE).

PROSIT

Information for geometry:

boundaries:

```
resolution 0.1 5 10
domain 13 -5 -1 15 2 15
```

materials/regions:

```
region Silicon Silicon
region Oxide  Oxide
region Nitride Nitride
region Resist Resist
region SubstContact Contact
region GateContact  Contact
region SourceContact Contact
region DrainContact Contact
```

procedures:

```
proc Contact {region mask} {
 deposit $region 1.0
 pattern $mask
 etch  $region 2.0
 strip  Resist
}
```

process flow:

```
side front
pattern pwell dark
implant pwell
strip  Resist
pattern nsource dark
implant source
strip  Resist
```

Information used by mesh generator:

doping:

```
doping substrate Boron  2e+15 Silicon
doping pwell   Boron  Gauss 0  1.5e17 0.0 3e16 0.5
doping source Arsenic Gauss 1.8 3.8e20 0.0 1e20 0.1
doping drain Arsenic Gauss 1.8 3.8e20 0.0 1e20 0.1
```

mesh refinement:

```
refine default 13. -5.  -9.0  100. 100. 100. 0.2 0.2  2.0 1.0
refine drain   13. -1.3 -0.2 13.6 0.1 0   0.05 0.05 0.2 0.1
refine source  13. -3.5 -0.2 13.6 -2. 0   0.05 0.05 0.2 0.1
refine channel 13. -2.3 -0.1 13.6 -1. 0   0.1 0.02 0.1 0.02
```

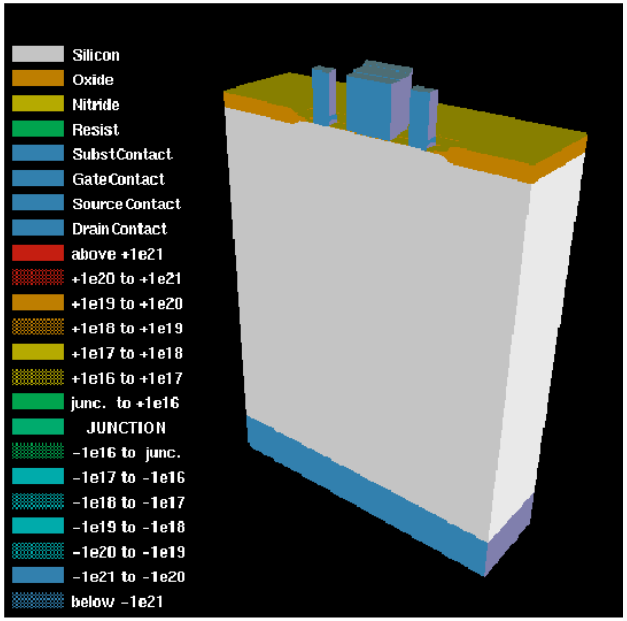
Analytically defined doping profiles are used

Simulation approach

2: idealised geometries simulation,

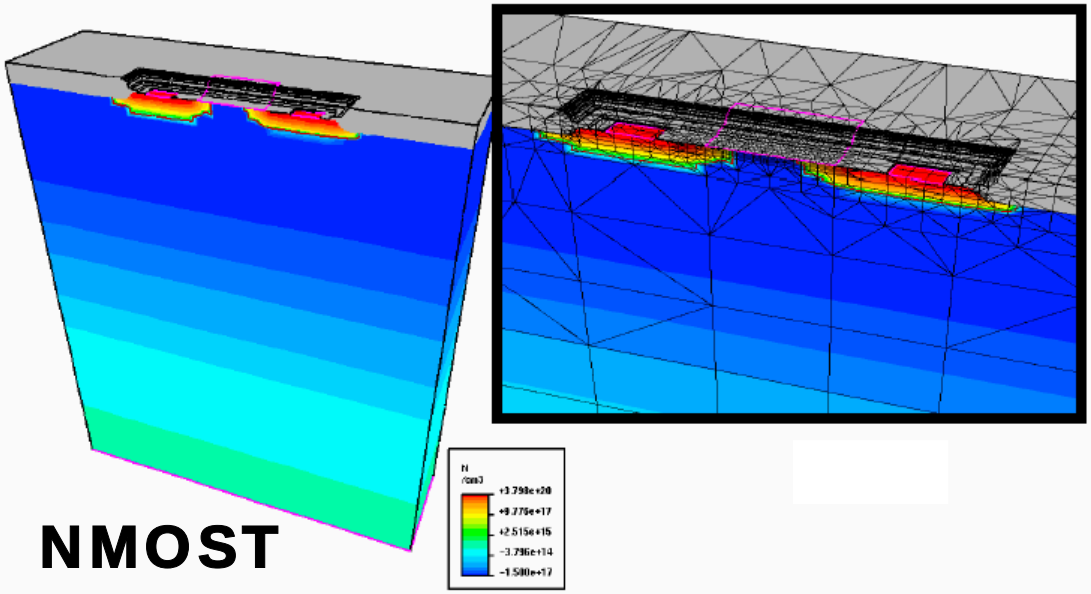
PROSIT

final device geometry:



MESH

geometry + doping + refinement → device model:



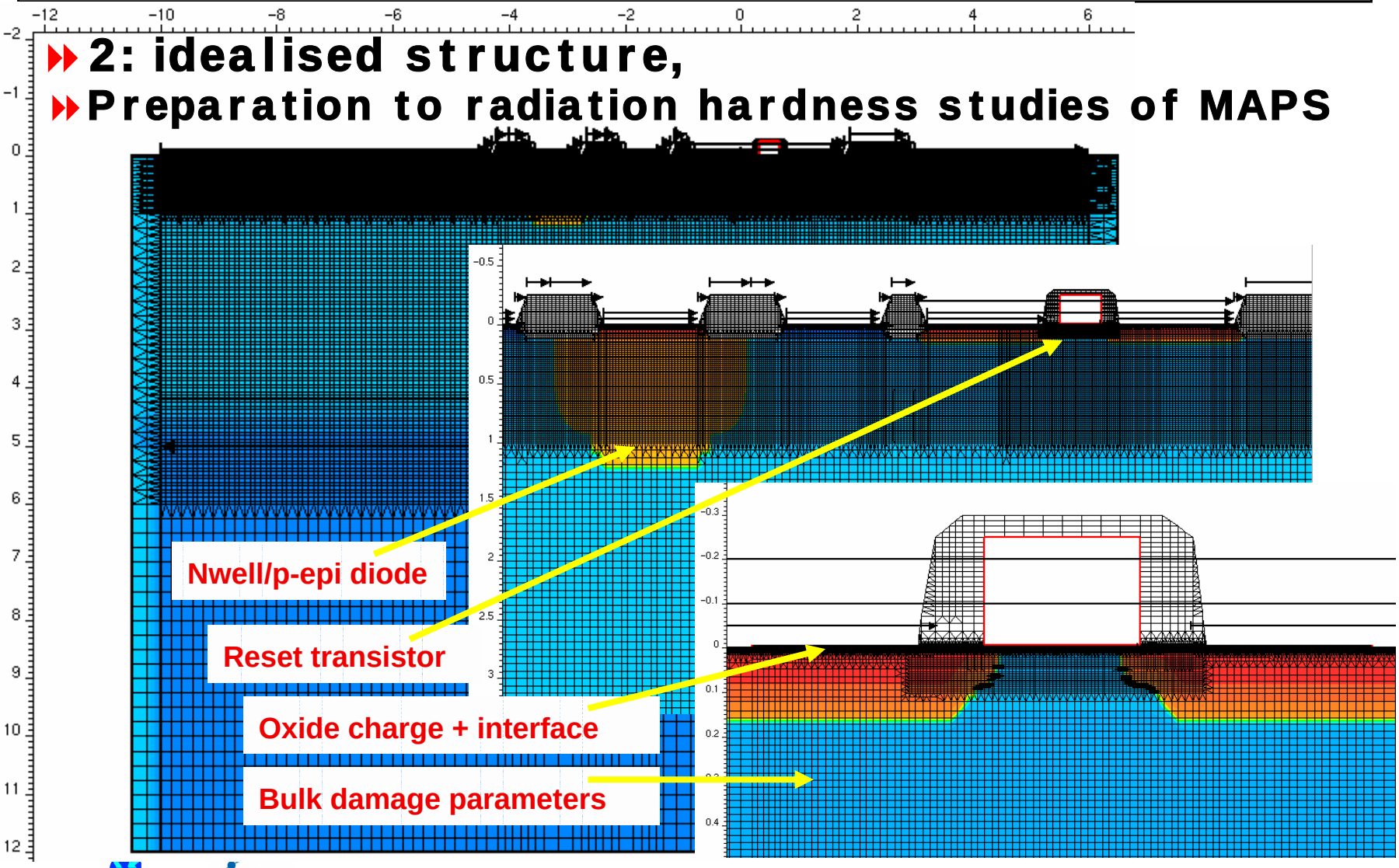
- mesh generation common step for both simulation approaches –

a) 2D geometry & doping can be obtained from DIOS, 3D needs interpolation (DIP) or FLOOPS (new),

b) PROSIT *(with process flow)*, MDRAW, DEVISE can be used for "hand" drawn geometries.

Simulation approach

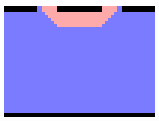
- 2: idealised structure,
- Preparation to radiation hardness studies of MAPS



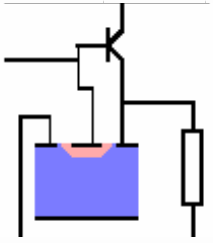
Simulation approach

DESSIS - solver,

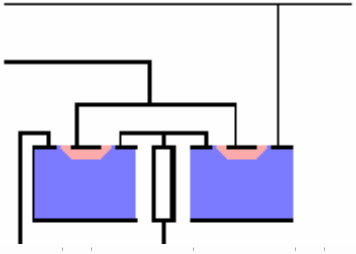
- electrical behavior - single semiconductor device in isolation or several physical devices combined in a circuit. Terminal currents, voltages and charges computed based on a set of physical device equations (carrier distribution + conduction mechanisms).



single device



single device + circuit



multiple devices + circuit

Device Physics 1D, 2D, 3D, and 2D cylindrical geometries Drift-diffusion Thermodynamic Hydrodynamic Monte Carlo Schrödinger solver Heterostructures Composition-dependent parameters Thermionic emission	**Mixed Mode** Electrothermal netlists Mixed dimension physical devices Device-specific physics Berkeley Spice circuit models Open compact model interface
Interface Physics Tunneling through insulators Hot carrier injection Interface traps Bulk Traps Ferroelectrics Optical generation Single Event Upset (SEU) (alpha particles and heavy ion)	**Analysis** AC DC Noise Transient

Simulation approach

DESSIS - solver,

```
File {
    ...
}
Electrode {
    ...
}
Thermode {
    ...
}
Physics {
    ...
}
```

```
Plot {
    ...
}
CurrentPlot {
    ...
}

Math {
    ...
}
```

```
Solve {
    ...
}
```

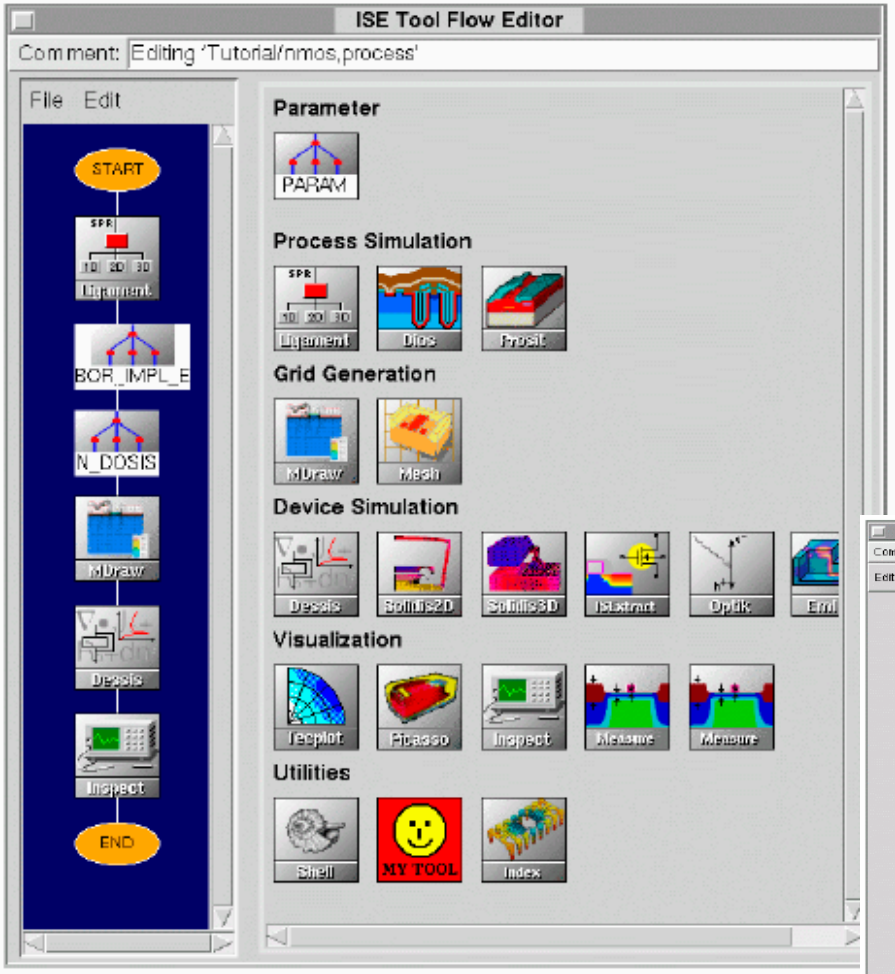
DESSIS command file structure

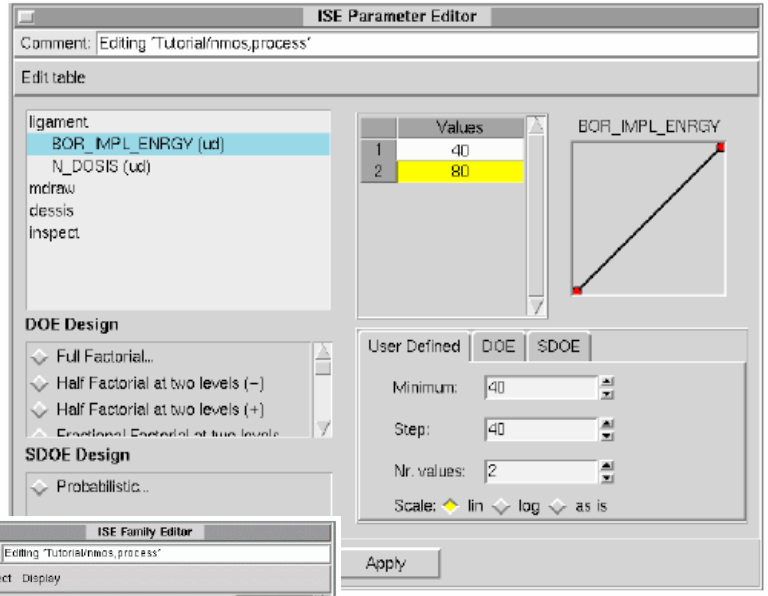
Physics section:

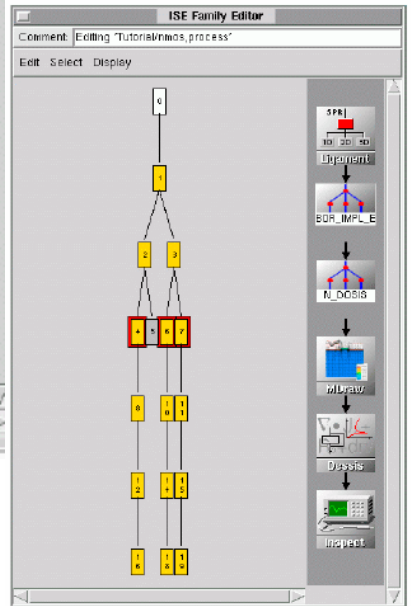
```
AreaFactor = <float>
Charge(<options>)= <float>
EffectiveIntrinsicDensity
(BandGapNarrowing (<models>)
Hydrodynamic
Hydrodynamic (<carrier>)
Mobility(<models>)
Recombination (<models>)
Temperature = <float>
Thermodynamic
Traps (<options>)
AlphaParticle (<options>)
Amorphous (<options>)
AnalyticTEP
Fermi
GateCurrent(<model>)
HeavyIon (<options>)
IncompleteIonization
MagneticField =
(<float>,<float>,<float>)
Noise (<options>)
OptBeam (<options>)
Piezo (<specifications>)
MoleFraction
[e|h]QCvanDort
RecGenHeat
Radiation (<options>)
Schroedinger
```

Simulation approach

GENESIS – simulation environment,





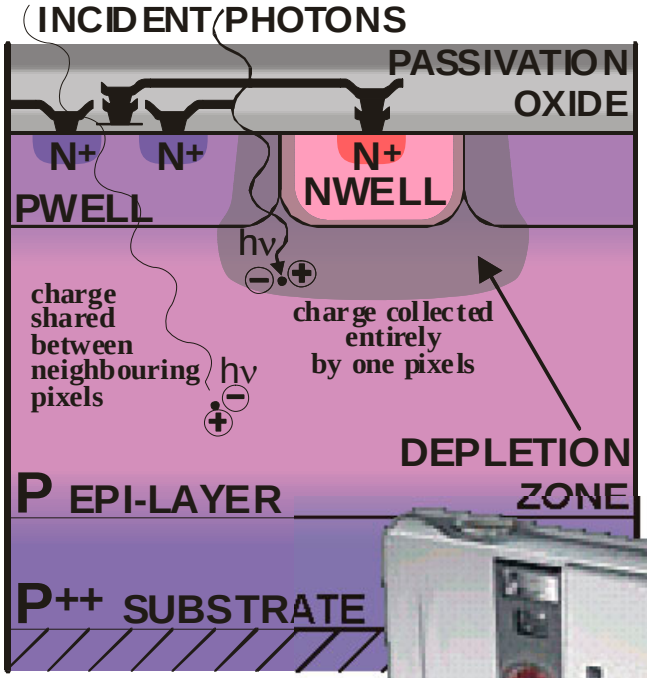


Simulation projects – tool flows + parameters

Design of experiment (DOE) for analyses with varied parameters, parallel execution on several machines, interface to visualisation, extraction and optimisation tools

ISE-TCAD and MAPS - example

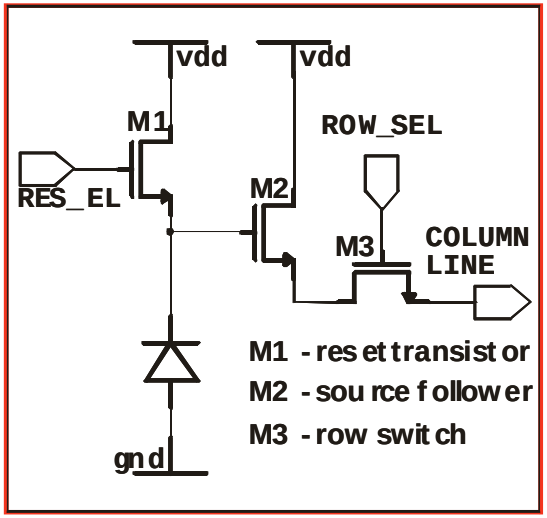
From digital photography



'warmest' colour = highest electric potential in the device

MIMOSA V 1×10^6 pixels micro-photograph

classical 3T pixel schematics

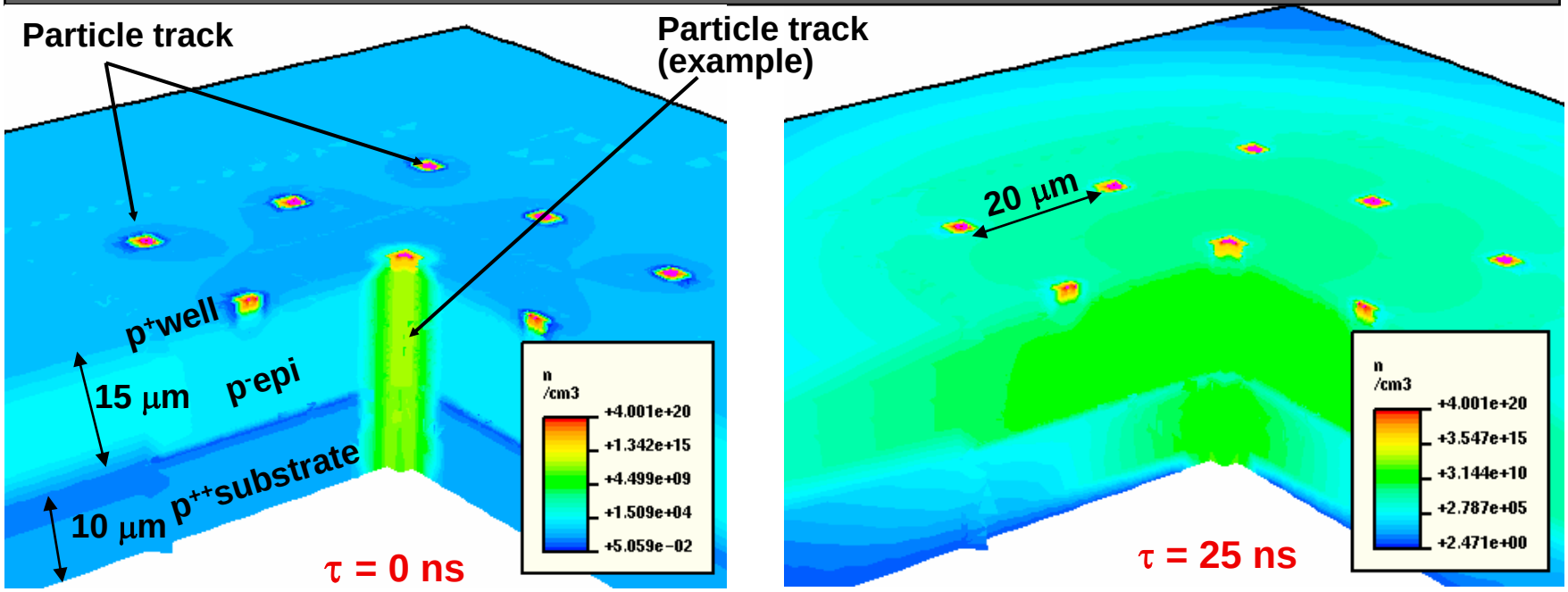


to charged particle detection

Monolithic Active Pixel Sensors (MAPS) advantages:

decoupled charge sensing and signal transfer (improved radiation tolerance, random access, etc.), small pitch (high tracking precision), low amount of material, fast readout, moderate price, SoC, etc.

ISE-TCAD and MAPS – example



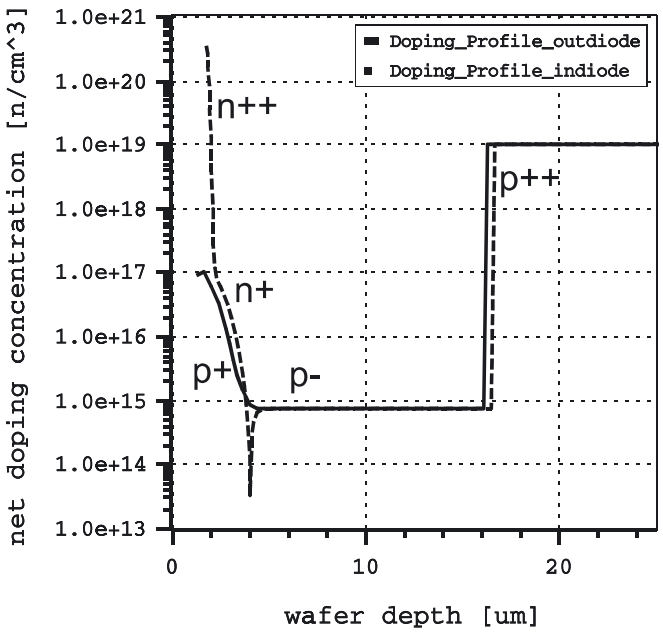
minority carrier concentration

mixed mode device and circuit simulator DESSIS-ISE from ISE-TCAD package

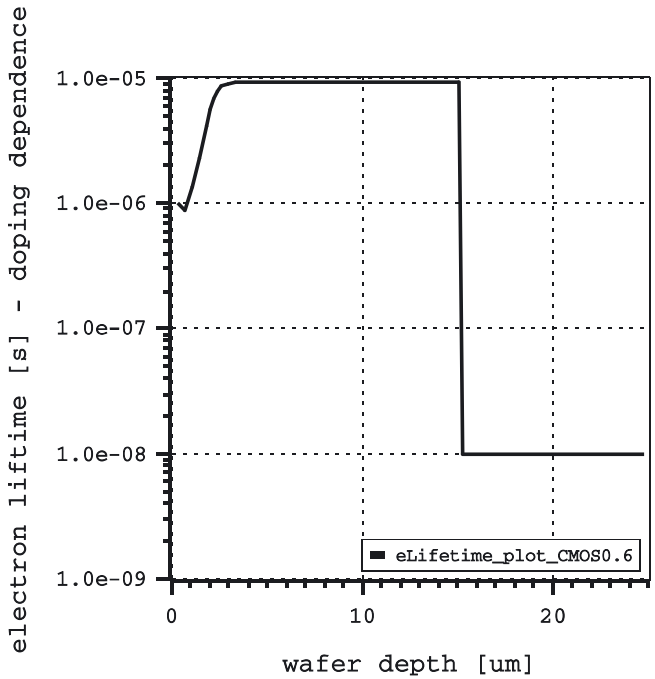
- ***Charge collection - relaxation process → equilibrium state (excess charge = ionising particle),***
- ***Device in 3-D, mesh with analytical description of doping profiles and boundary definition,***
- ***Different detector parameters investigated:***
  - ***thickness of the epitaxial layer and substrate,***
  - ***size of a pixel and collecting diodes,***
  - ***number of diodes per pixel.***

ISE-TCAD and MAPS - example

Simulation background:



doping profile



carrier lifetime from doping

$$\varepsilon_{si}\nabla^2\psi = -q\left(p - n + N_D^{+} - N_A^{+}\right)$$

$$\nabla\vec{J}_n = qR + q\frac{\partial n}{\partial t} \quad \text{and} \quad \nabla\vec{J}_p = qR + q\frac{\partial p}{\partial t}$$

$$\vec{J}_n = -nq\mu_n\nabla\varphi_n \quad \text{and} \quad \vec{J}_p = pq\mu_p\nabla\varphi_p$$

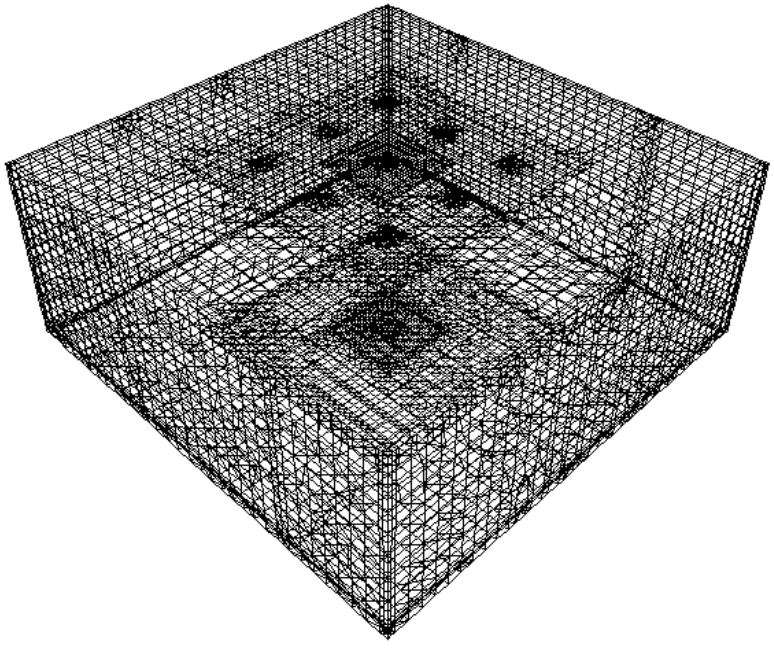
$$\tau_{dop}\left(N_i\right) = \tau_{\mathbf{min}} + \left(\tau_{\mathbf{max}} - \tau_{\mathbf{min}}\right)\left[1 + \left(\frac{N_i}{N_{ref,\tau}}\right)\right]^{-\gamma}$$

Set of Poisson equation and electrons and holes transport equations with

$$\mu_{dop}\left(N_D^{+} + N_A^{-}\right) \quad \tau_{dop}\left(N_D^{+} + N_A^{-}\right) \quad R^{SRH}$$

ISE-TCAD and MAPS - example

Simulation background:

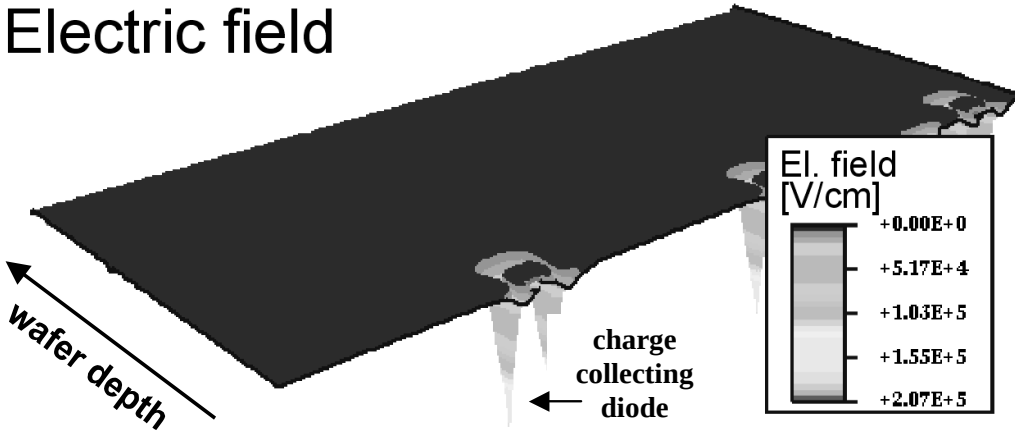


Mesh in 3-D
with adapted density

Big structures
in 3-D (?)

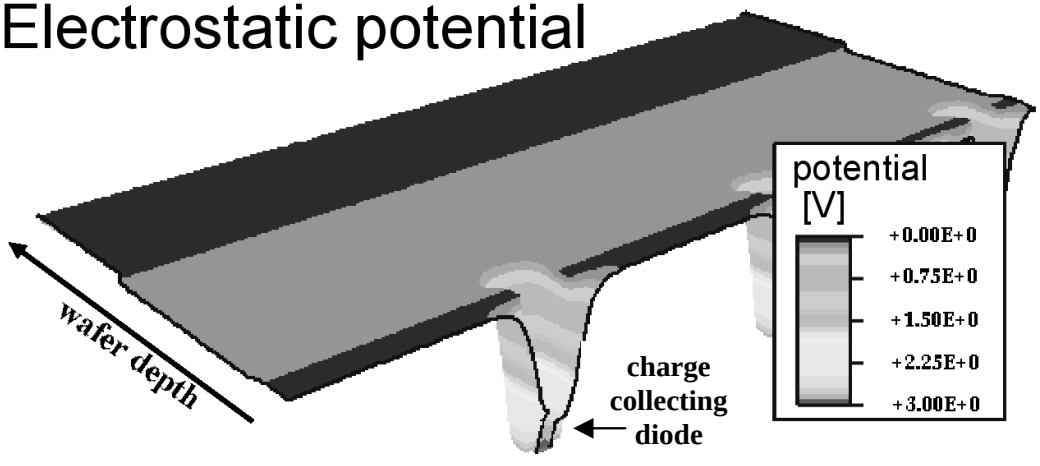
plane cross-section through diodes

Electric field



« TOSCA » solution for

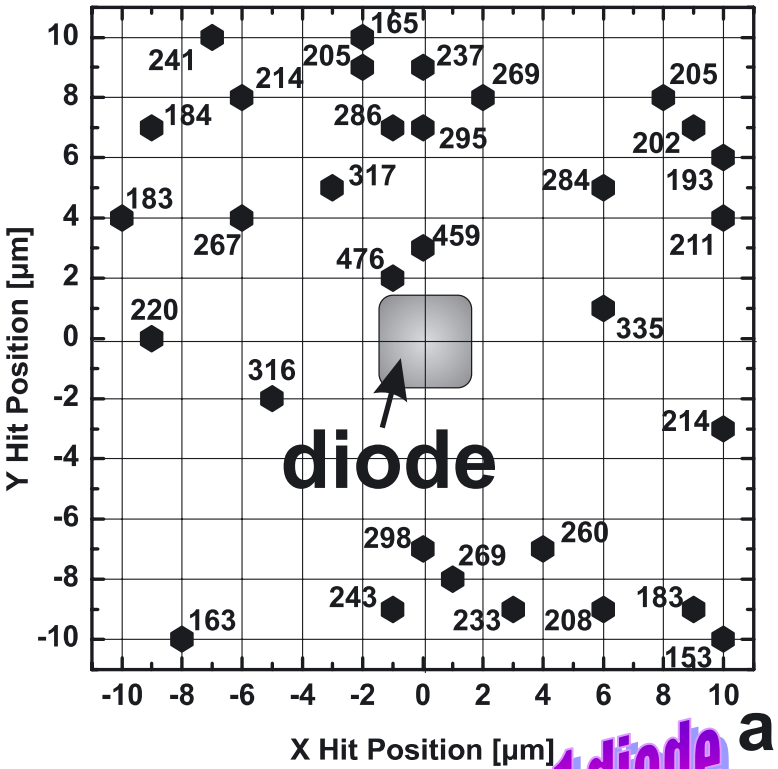
Electrostatic potential



ISE-TCAD and MAPS - example

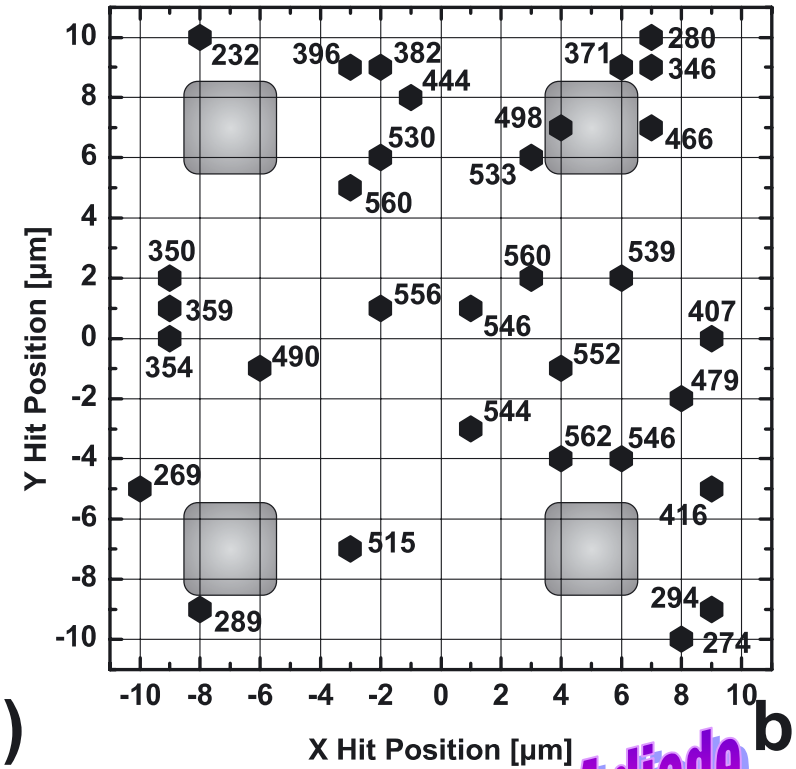
Charge collected as function of impact position:

- *Particle impact points chosen randomly within central pixel area ...*



a)

1 diode



b)

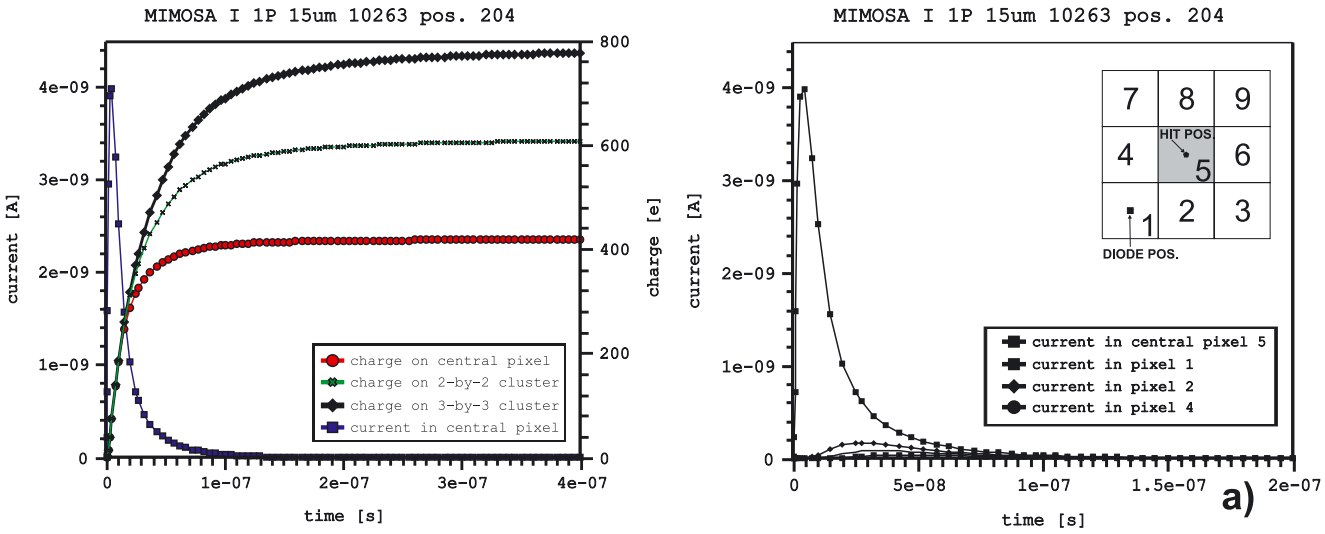
4 diode

More then 8 hours
Per single impact

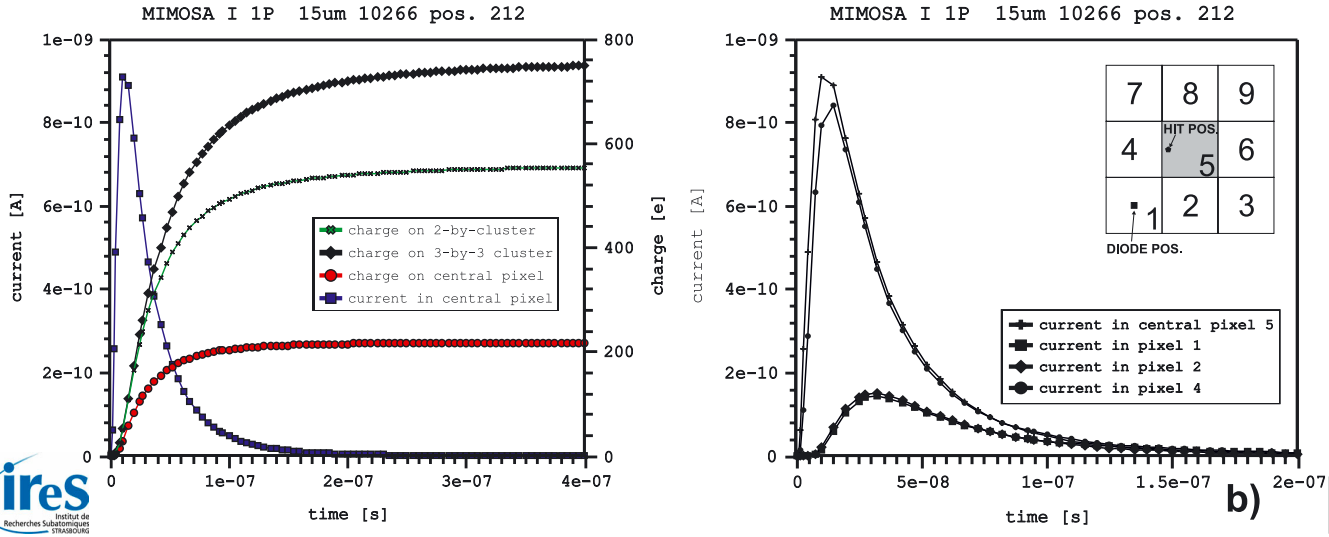
ISE-TCAD and MAPS - example

Transient simulations for charge collection:

1diode



Prototype with 15 µm epitaxial layer and 20 µm pitch

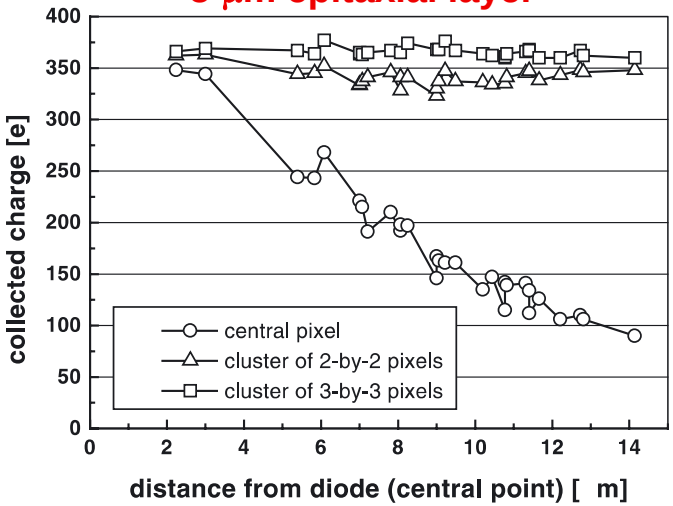


ISE-TCAD and MAPS - example

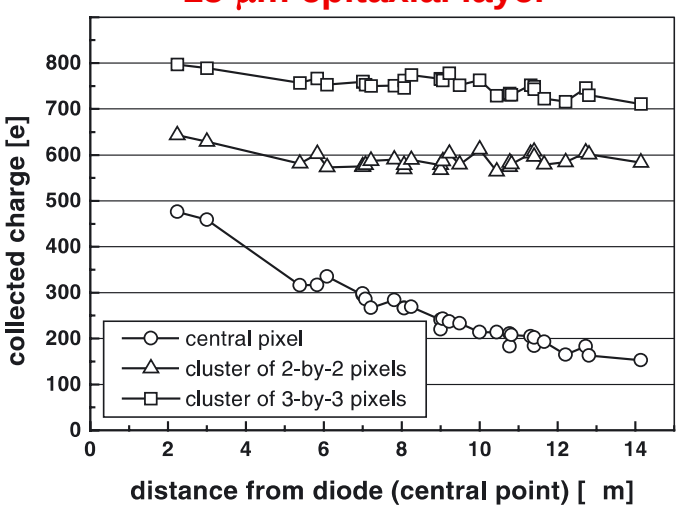
Charge collected as function of impact position:

1 diode

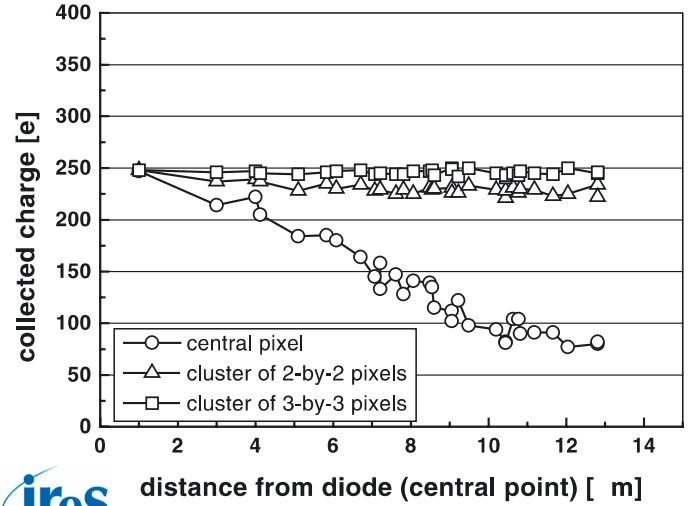
5 μm epitaxial layer



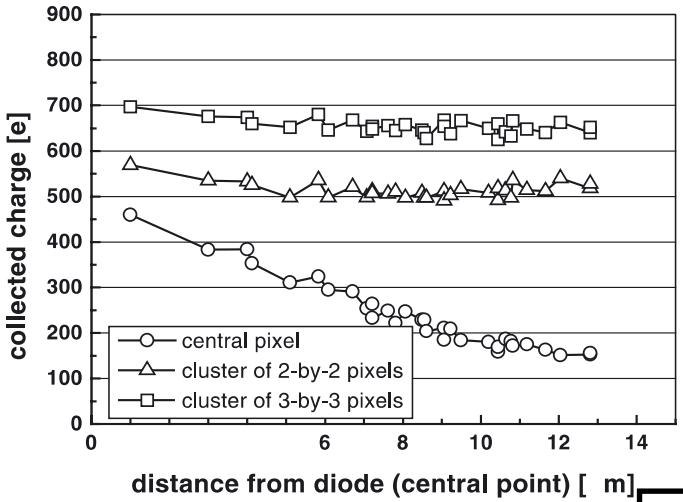
15 μm epitaxial layer



simulations supposing substrate thickness = 0 μm



370e⁻ ⇨ 250e⁻ (~32%)

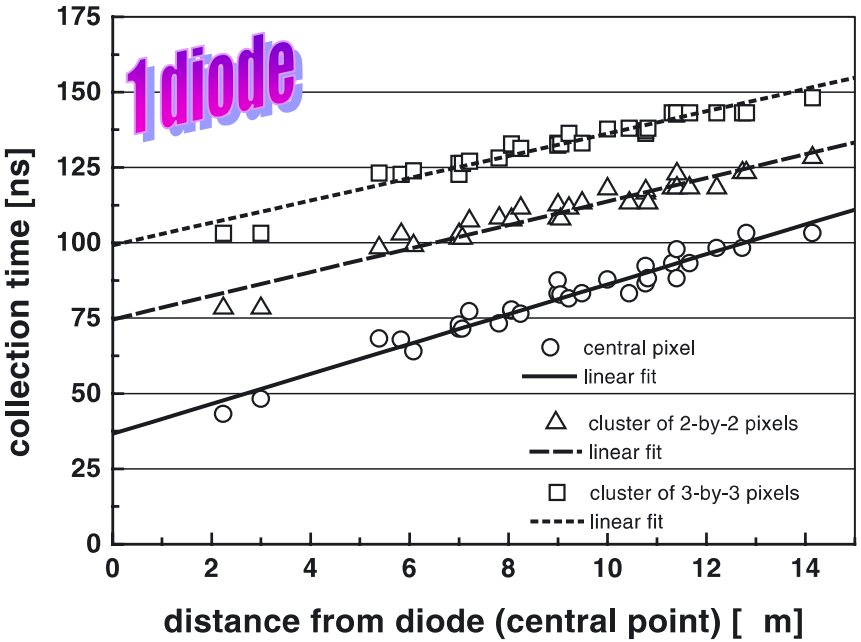


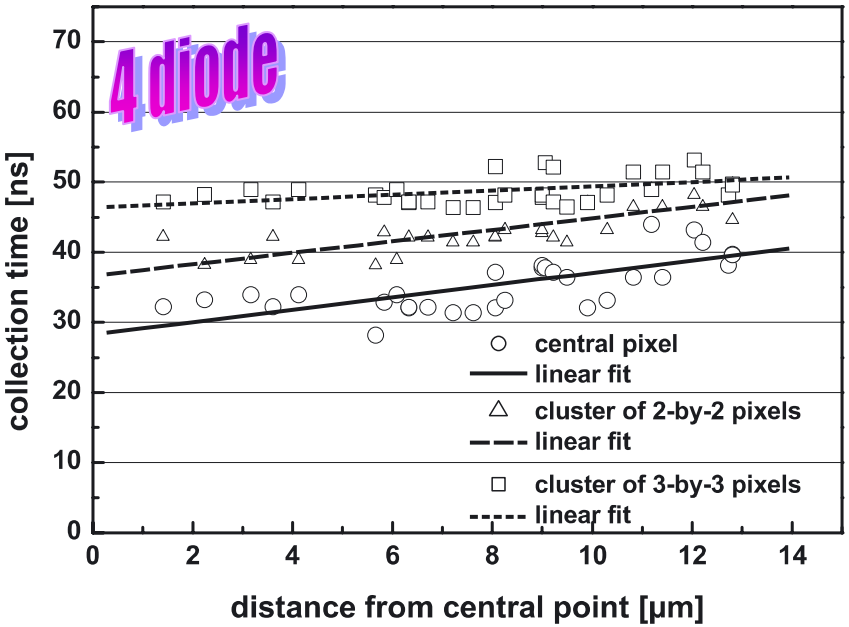
780e⁻ ⇨ 670e⁻ (~14%)

ISE-TCAD and MAPS -example

Estimation of charge collection time:

15 μm epitaxial layer + infinite substrate



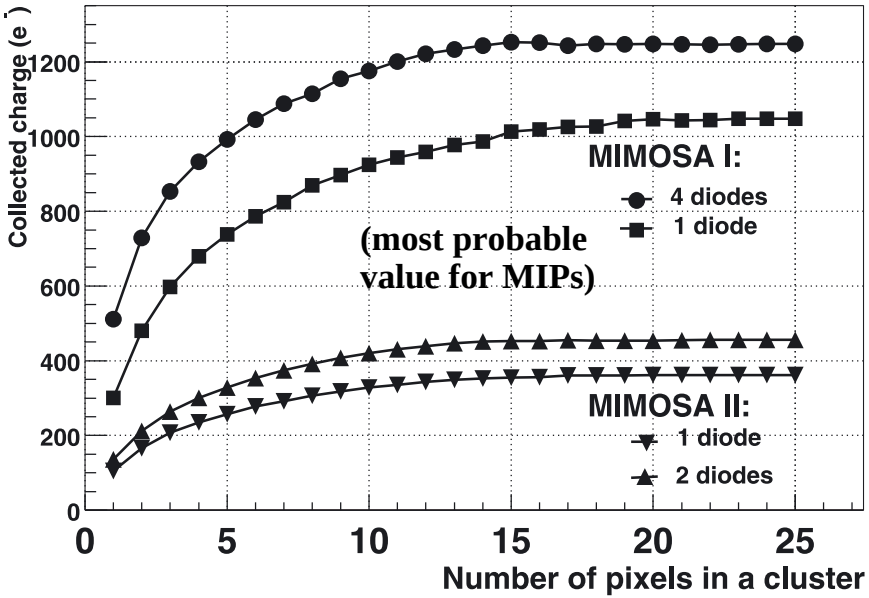


- **Important observations:**
- *charge collection time (90% of charge) <150ns,*
- *4-diode charge collection ~3 times faster,*
- *charge collection faster for thinner epitaxial layer.*

ISE-TCAD and MAPS - example

Agreement with experiments

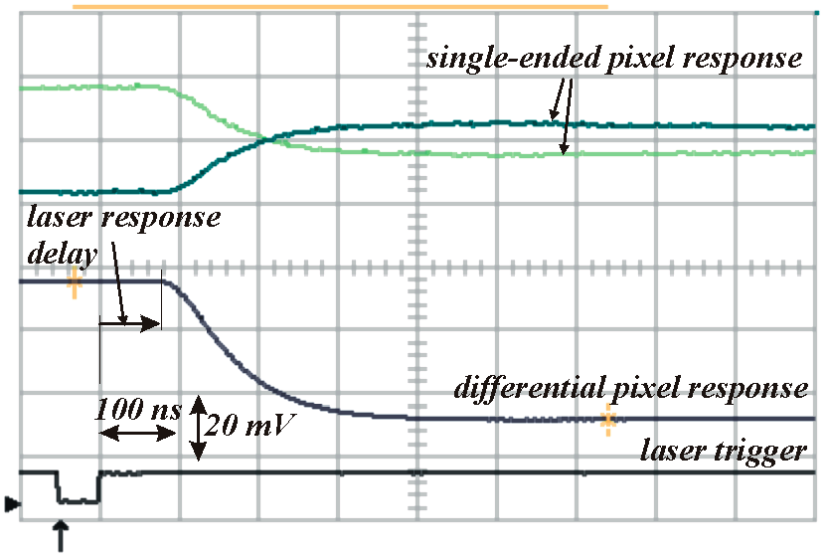
Collected charge



MIMOSA I – 14 µm epitaxial layer

MIMOSA II - <5 µm epitaxial layer

Collection time



Response convolved with readout chain; deconvolution ⇨ τ_{col}=100-150 ns

ISE-TCAD picked up example

Radiation hardness *(example)*

Alpha particle in digital circuit *(ISE-TCAD example)*

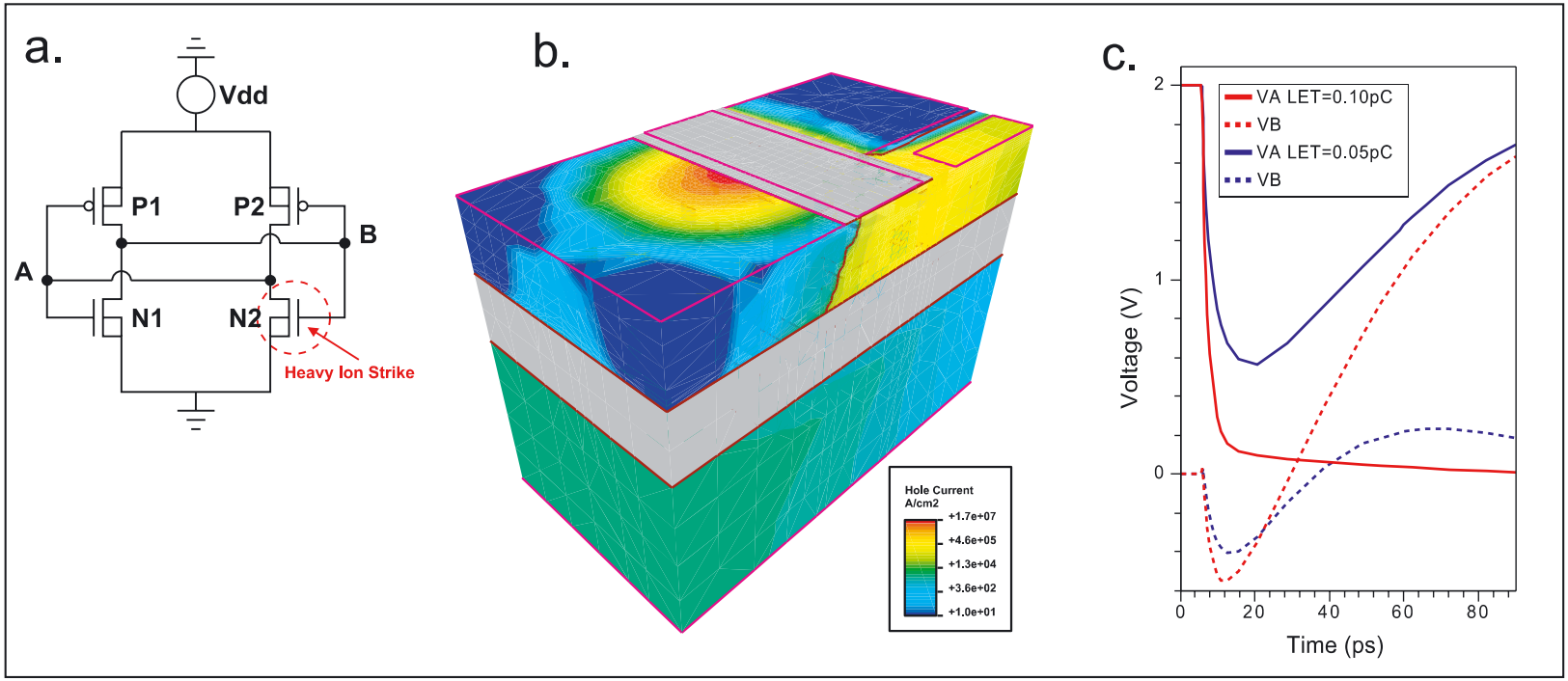


Figure 1 Simulated SEU of a SRAM cell.
(a) The SOI NMOS "N2" is simulated as a 3D physical device. The devices "P1", "P2", and "N1" are simulated as 2D physical devices, or alternatively as SPICE compact models.
(b) Hole current distribution in a body tied the SOI NMOS "N2" of a SRAM cell after a heavy ion strike.
(c) SEU switching dynamics of the SRAM cell after a heavy ion strike with an LET of 0.05pC (blue) and 0.10pC (red). The cell is able to recover from the low energy strike, while the high enery strike causes a soft error.

[1] ISE TCAD, see www.ise.com
[2] "SEU Response of an Entire SRAM Cell Simulated as one Contiguous Three Dimensional Device Domain." Ph. Roche, et. al. NSREC 98 proceeding and IEEE Trans. Nucl Sci. Vol45 pp2534- 2544

ISE-TCAD picked up example

Commercial CMOS Image Sensor - example

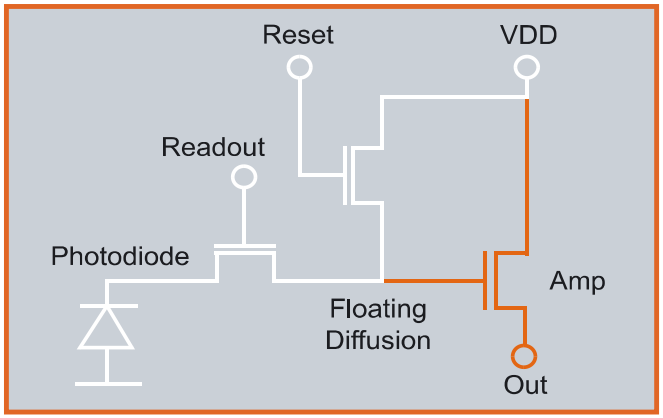


Figure 1: Circuit of CIS pixel; orange part was neglected in device simulation

optical – electrical interface

Simulation using OPTIK ISE and DESSIS ISE for electrical response, EMLAB ISE is used for estimation of optical crosstalk

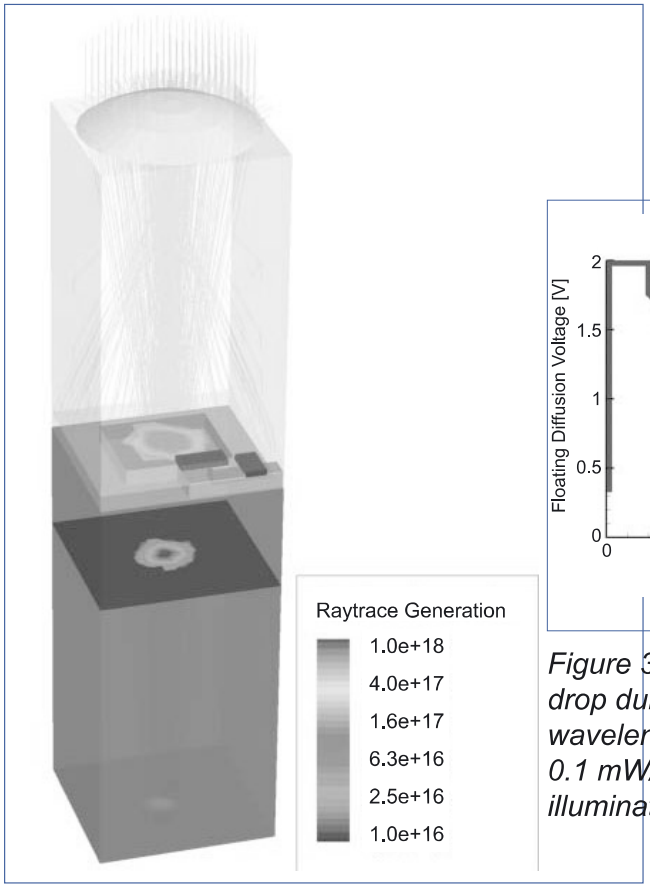


Figure 2: Carrier generation in a CIS pixel; light propagation through the lens onto the photodiode was simulated by 3D raytracing

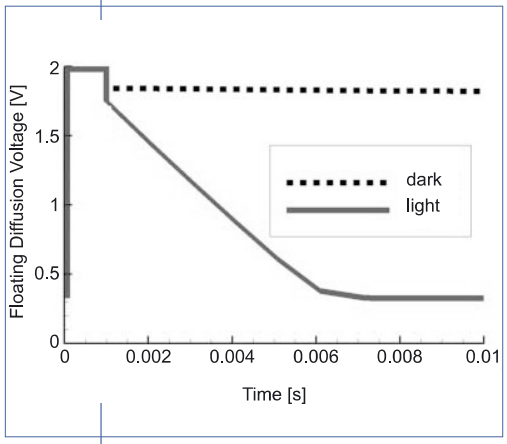


Figure 3: Floating diffusion voltage drop during illumination of pixel with a wavelength of 600 nm and a power of 0.1 mW/cm^2 compared with pixel not illuminated (dark)

Conclusions ...

- ISE-TCAD – advanced, extended, from process to device simulation environment.

- Continuously developed:
  1) ☺ New features and tools integrated, improvements,
  2) ☹ commercial licenses (v.8.0 LEPSI) 8.5, 9.0, 9.5 (10.0 announced) – cost ↗↗↗ ,
  3) ☹ high complexity, quite often "undocumented" behaviour → stacking the user → need of technical support → support barely available for scientific and educational institutes,
  4) ☹ non-standard environment – mixture of scripting languages, GUI → MsWindows,
  5) ☹ no directly implemented features for detector – but ☺ yes for commercial interest sensors,
  6) ☺ as close as possible to technology, ☹ not so useful... how to obtain data if no technology development institution?