TCAD simulation I

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Overview

- **Introduction, needs for TCAD simulations**

- **Transport regimes and related equations**

- **Discretization techniques: meshing**

- **Discretization of semiconductor equations: Scharfetter-Gummel technique**

- **Examples**

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Introduction

Epitax growth *SiO$_2$ etch* *N^{++} implant* *P^{++} implant*

- TCAD (Technology Computer Aided Design) divides into three groups:
  - **Process simulation**, i.e. simulation of fabrication process steps (oxidation, implantation, diffusion…)
  - **Device simulation**, i.e. simulation of the thermal/electrical/optical behavior of electronic devices,(IV,CV, frequency response…)
  - **Device modeling**, i.e. creating compact behavioral models for devices for circuit simulation (SPICE, Cadence…)
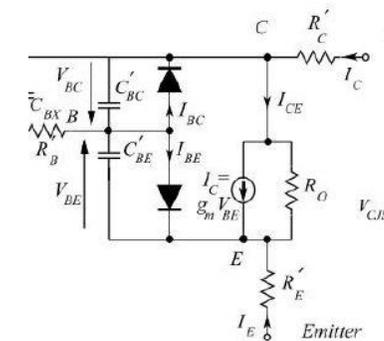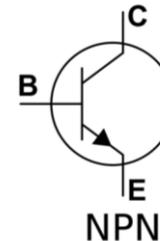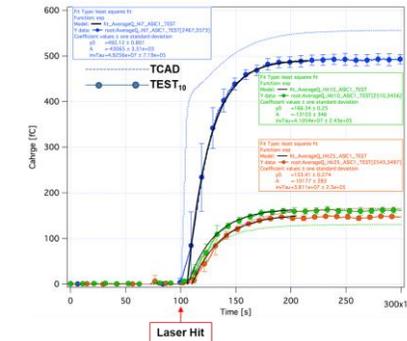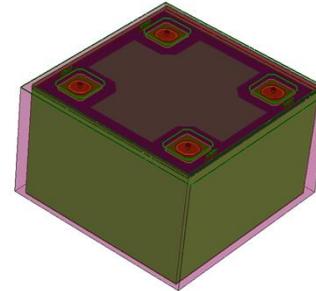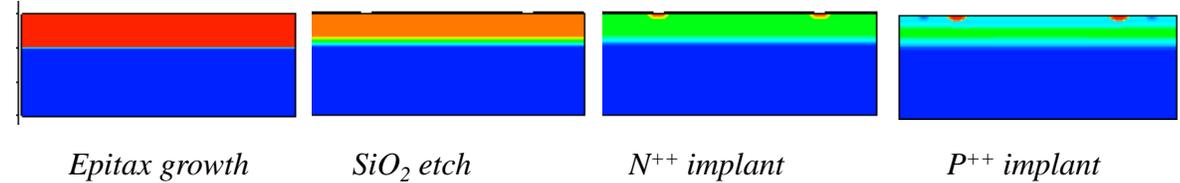
Introduction

- Reasons why TCAD simulations are needed:
  - Market demands cycle of design to production of 18 months or less. Typically 2-3 months required for wafer tape out implies short time for development
  - Reduce cost to run experiments on new devices and circuits
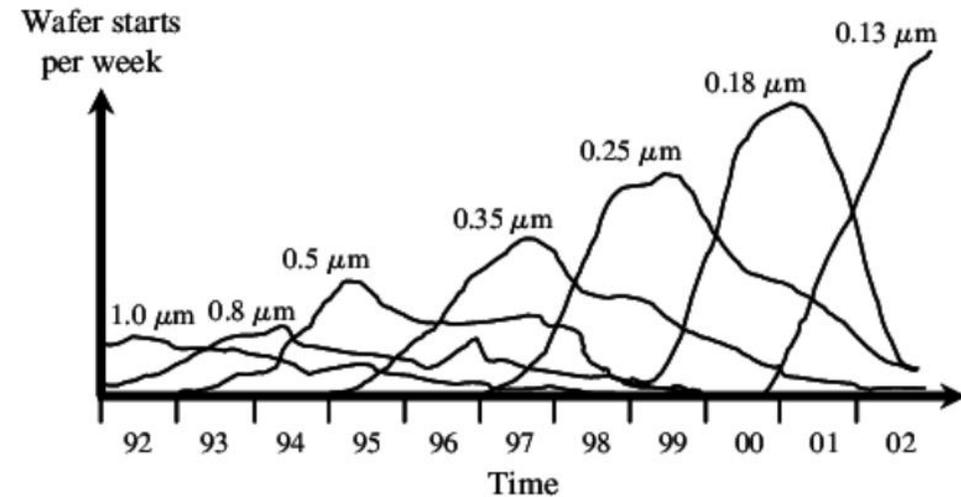
Shrinking product life cycles in semiconductor industry over time

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Introduction

- Main components of semiconductor device simulation include description of electronic structure, driving forces and transport phenomena

- The two kernels of semiconductor transport equations and fields that drive charge flow are coupled to each other and needs solving self-consistently
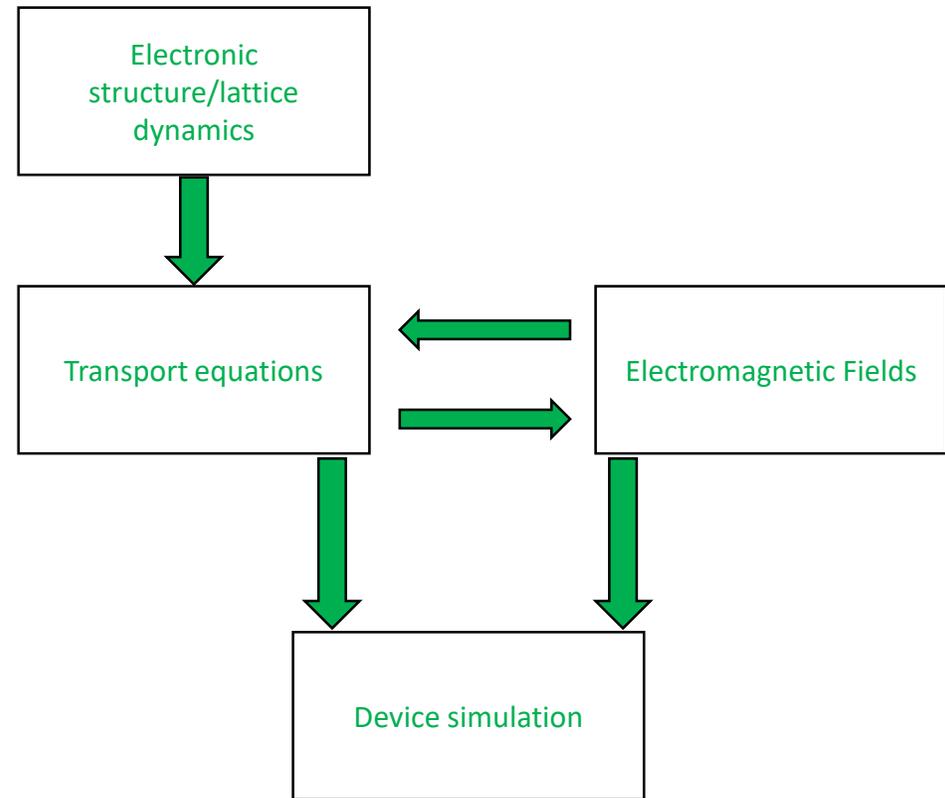
Transport regimes

- Usually only the quasi-static electric fields from the solution of Poisson's equation are necessary

- Transport regime in semiconductors depends on length scale

Modern Silicon technology already requires tools to describe transport in quantum regime [D. K. Ferry and S. M. Goodnick, Transport in Nanostructures, 1997]

	$L \ll l_{e-ph}$			$L \sim l_{e-ph}$	$L \gg l_{e-ph}$
	$L < \lambda$	$L < l_{e-e}$	$L \gg l_{e-e}$		
Transport regime	Quantum	Ballistic	Fluid	Fluid	Diffusive
Scattering	Rare	Rare	$e-e$ (Many), $e-ph$ (Few)		Many
Model:					
Drift-diffusion					
Hydrodynamic		Quantum hydrodynamic			
Monte Carlo					
Schrödinger equation Green's function					
Applications	Nanowires, superlattices	Ballistic transistor	Present time ICs	Present time ICs	Older ICs

L: device length
l_{e-e}: electron-electron scattering length
l_{e-ph}: electron-phonon scattering length
λ: electron wavelength

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Transport regimes

- Charge carrier dynamics in Si detectors usually does not require QM

- Semiclassical laws of motions apply

- Drift-diffusion equations are valid, provided the electron gas is in thermal equilibrium with lattice temperature ($T_n = T_L$)

$$R \sim \frac{h}{2\pi} \frac{\gamma v}{<I>} = 1.2\ [nm]\ Ionization\ radius\ for\ MIP\ in\ Si$$

$$n = \frac{dE}{dx} \rho \frac{L}{E_{th}} \frac{1}{\pi R^2 L} \sim 2 \cdot 10^{19}\ charge\ density\ within\ Ionization\ radius\ and$$

$$n^{-1/3} \sim 3.3[nm]$$

$$\lambda \leq \frac{h}{\sqrt{2meV_b}} \sim \begin{cases} 0.38\ [nm]@10\ V \\ 0.12\ [nm]@100\ V \end{cases} De\ Broglie\ wavelength\ of\ carriers$$

$$@\ full\ depletion$$

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Drift diffusion model

- The semiconductor equations derived form 1st moment of BTE are referred to as Drift Diffusion model

- The model consists of Poisson's equation, continuity and current density equations for electrons and holes

- They express charge and momentum conservation

- Their self-consistent solutions are obtained via discretization, using finite element methods FEM

$$\partial_t f + \mathbf{u} \cdot \nabla_\mathbf{r} f + \frac{\mathbf{F}}{\hbar} \cdot \nabla_\mathbf{k} f = C[f]$$

$$\text{div}\,(\varepsilon \cdot \text{grad}\,\psi) = q \cdot (n - p + N_A - N_D)$$

$$\text{div}\,\mathbf{J}_n - q \cdot \frac{\partial n}{dt} = q \cdot R$$

$$\text{div}\,\mathbf{J}_p + q \cdot \frac{\partial p}{dt} = -q \cdot R$$

$$\mathbf{J}_n = q \cdot n \cdot \mu_n \cdot \mathbf{E} + q \cdot D_n \cdot \text{grad}\,n$$

$$\mathbf{J}_p = q \cdot p \cdot \mu_p \cdot \mathbf{E} - q \cdot D_p \cdot \text{grad}\,p$$

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Discretization and meshing

- The device simulations process consists of two steps:

- The test volume is obtained through grid generation ('mesh generation')

- Solving the discretized differential equations using Finite-Boxes method (box integration method) . This method integrates PDEs over a test volume.

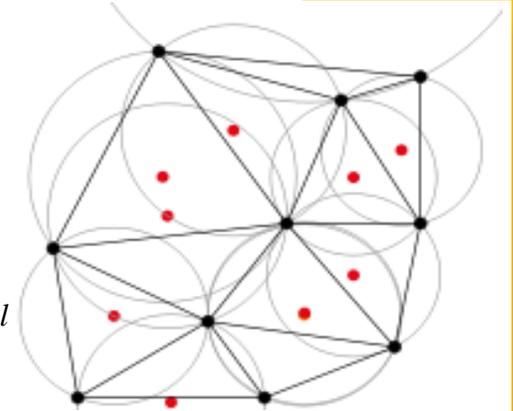UNIVERSITY OF OXFORD
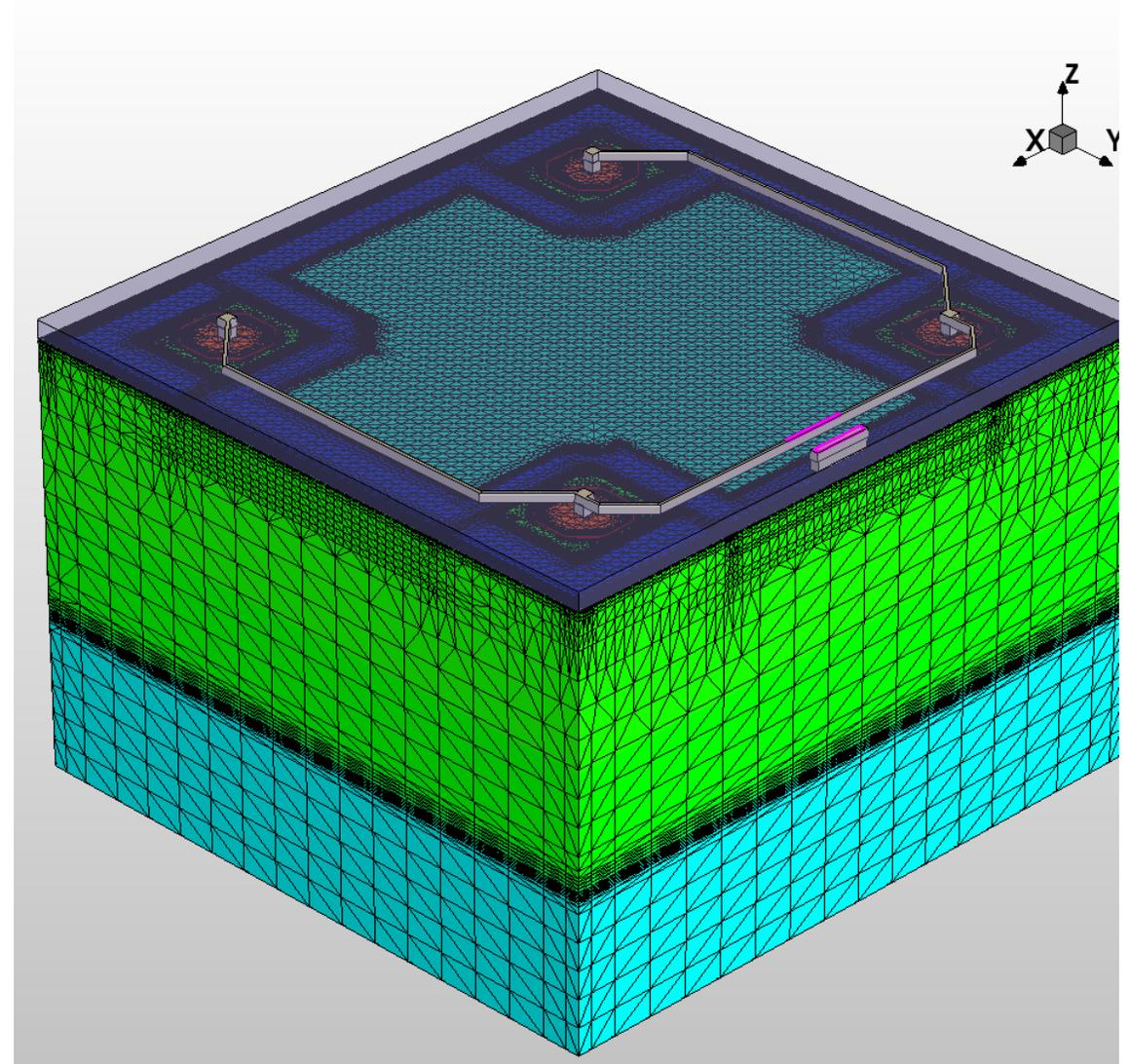
Discretization and meshing

- The meshing used in most finite elements methods (FEM) relies on Delaunay triangulations:

the interior of the circumsphere of each element contains no mesh vertices.

- The Delaunay triangulation of a discrete point set **P** in general corresponds to the dual graph of the Voronoi diagram for **P**
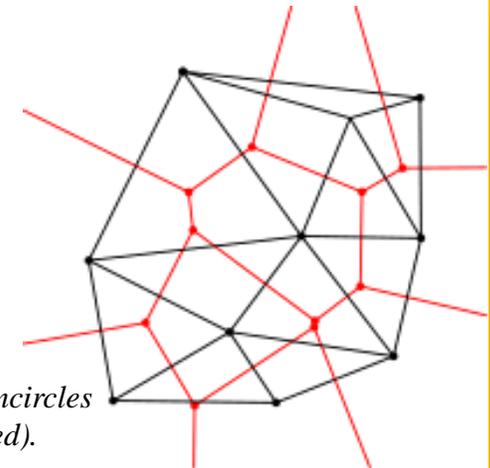
the set of all locations x closest to P_i than to any other point of the grid

The Delaunay triangulation with all the circumcircles and their centres

$$T_{D,k}(\mathcal{P}_{D,k}) \Longleftrightarrow \exists \mathbf{x}$$
$$\mathbf{x} \in \Omega \quad \wedge$$
$$|\mathbf{x} - \mathbf{x}_i| = |\mathbf{x} - \mathbf{x}_j| \; \forall \, P_i, P_j \in \mathcal{P}_{D,k} \quad \wedge$$
$$|\mathbf{x} - \mathbf{x}_i| < |\mathbf{x} - \mathbf{x}_k| \; \forall \, P_i \in \mathcal{P}_{D,k}, P_j \notin \mathcal{P}_{D,k}$$

Connecting the centres of the circumcircles produces the Voronoi diagram (in red).

$$\Omega_i = \{\mathbf{x} \mid |\mathbf{x} - \mathbf{x}_i| \leq |\mathbf{x} - \mathbf{x}_j| \; \forall \, i \neq j, \mathbf{x} \in \Omega\}$$

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Discretization and meshing

- Correct Delaunay triangulation guarantees element-volume conservation, important in many problems (diffusion, charge generation, et cetera)

- Delaunay triangulation maximizes the minimum angle.

Voronoi boxes do not overlap (each circumcircle does not include a point of another triangle). Each can be uniquely assigned to its corresponding grid points.

$$P_i = V_i$$

Voronoi boxes do overlap (each circumcircle does include a point of another triangle). Each cannot be uniquely assigned to its corresponding grid points. Wrong volumes calculated
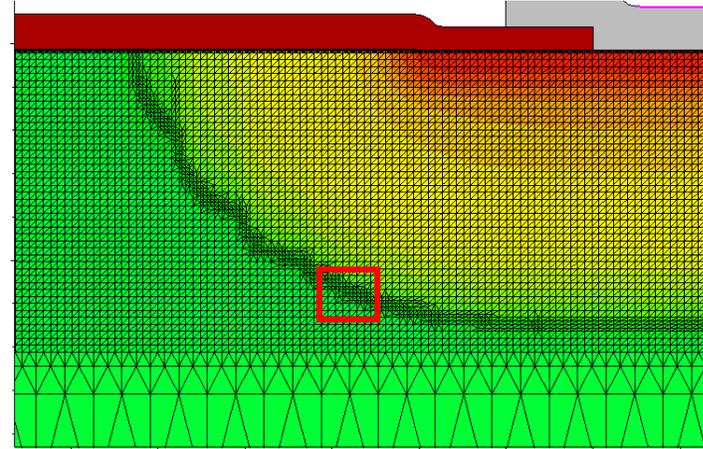
$$P_1 = V_1 + V_5 + V_6$$

$$P_3 = V_3 + V_5 + V_6$$

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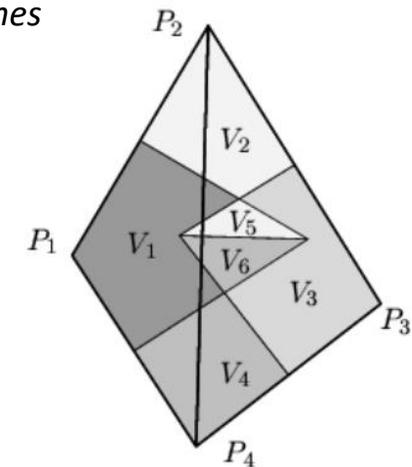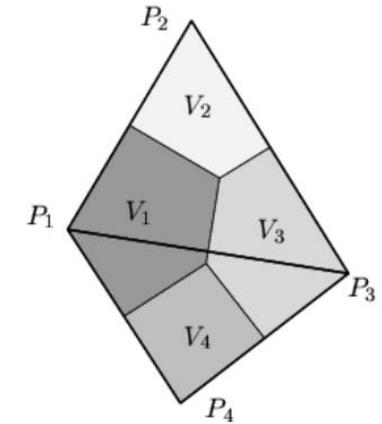
Discretization and meshing

- Discretization of equations imposes some constraints on spatial and temporal mesh size

- Mesh size should be smaller than Debye length (i.e. the characteristic length for screening of field by charges) where charge variations in space have to be resolved

$$L_D = \sqrt{\frac{\varepsilon_s k_B T}{e^2 N}} \; Debye \; length$$

$N = 10^{13} [cm^{-3}]: L_D \approx 1.3 \; [um] @ T = 300 \; [K]$
$N = 10^{17} [cm^{-3}]: L_D \approx 13 \; [nm] @ T = 300 \; [K]$
$N = 10^{19} [cm^{-3}]: L_D \approx 1.3 \; [nm] @ T = 300 \; [K]$

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Discretization and meshing

- Also temporal 'mesh' size should be smaller than the dielectric relaxation time t_{dr} (i.e. time it takes to charge fluctuations to decay under the field they produce)

- Time interval smaller than t_{dr} might give unrealistic transient results ('oscillations' in estimated transient currents)

$$\tau_{dr} \sim \frac{\varepsilon_s}{eN\mu} \; Dielectric \; relaxation \; time$$

$$N = 10^{13} [cm^{-3}], \mu_n \approx 1400 \left[[cm^{-3}V^{-1}s^{-1}] @T = 300 \, [K] : \tau_{dr} \approx 400 \, [ps] \right.$$

$$N = 10^{15} [cm^{-3}], \mu_n \approx 1350 \left[[cm^{-3}V^{-1}s^{-1}] @T = 300 \, [K] : \tau_{dr} \approx 4.8 \, [ps] \right.$$

$$\frac{\partial \Delta n}{\partial t} = \frac{\Delta n(t = 0)}{t_{dr}}$$

$$\Delta n \, (\Delta t) = \Delta n \, (0) - \Delta t \frac{\Delta n(0)}{t_{dr}}$$

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Box integration method

- Discretization of Poisson's and continuity equations is done via Box Integration method

$$\mathrm{div}\,(\varepsilon \cdot \mathrm{grad}\,\psi) = q \cdot (n - p + N_A - N_D) \quad \equiv \int D \cdot dS = \int \rho dV$$

- The LHS of equations is transformed via Gauss' theorem and integrated over a Voronoi box Ω_k of point P_k

$$\mathrm{div}\,\mathbf{J}_n - q \cdot \frac{\partial n}{\mathrm{d}t} = q \cdot R$$
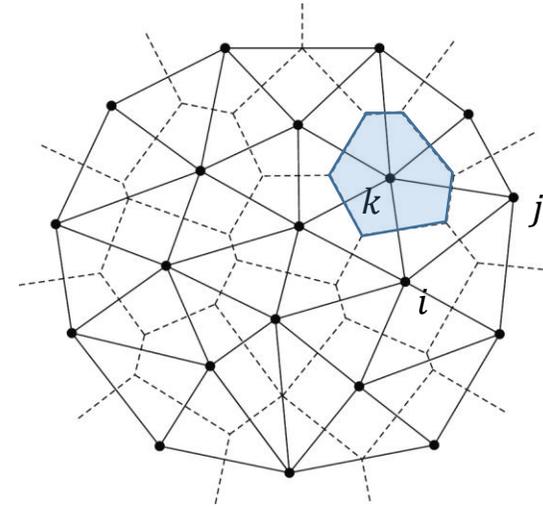
$$\mathrm{div}\,\mathbf{J}_p + q \cdot \frac{\partial p}{\mathrm{d}t} = -q \cdot R$$

Box integration method

- Example of Poisson's discretization

- Assume that the electric potential is linearly varying over each elementary domain
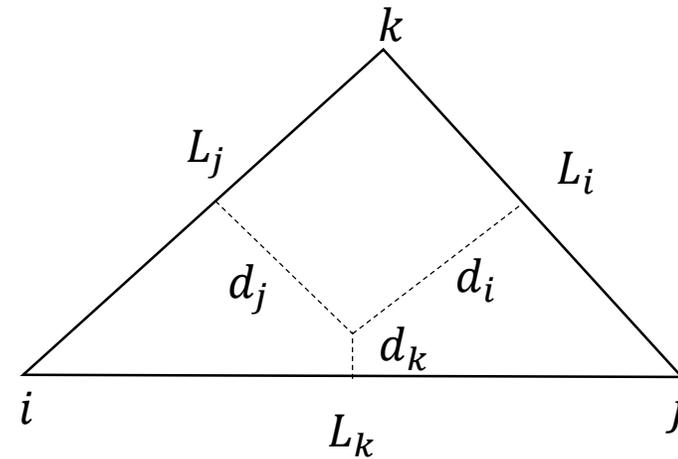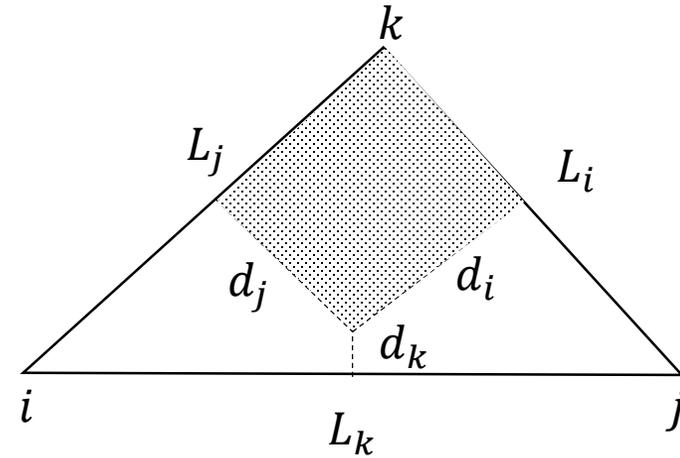
$i, j, k: nodal\ indices$

$\boldsymbol{L_i}, \boldsymbol{L_j}, \boldsymbol{L_k}: side\ vectors$

$L_i, L_j, L_k: magnitude\ side\ vectors$

$u := \dfrac{e}{k_B T} \varphi: normalized\ potential$

Box integration method

- Components of D vector along sides $L_{i,j,k}$

- Flux of D vector associated to node k:

- Discretization of RHS is obtained by multiplying the node value of charge by the area of the portion of the Voronoi box
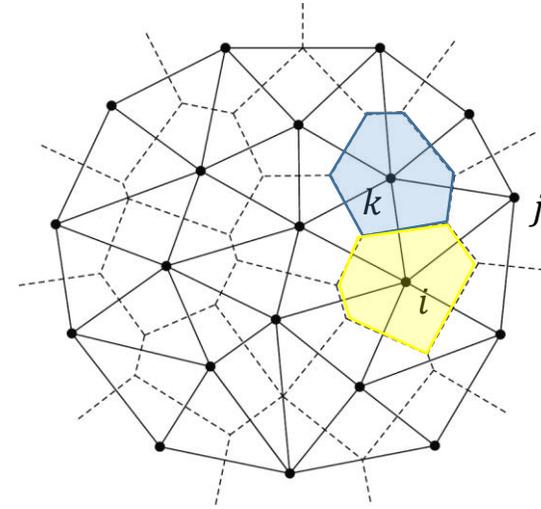

$$\frac{k_B T}{e} \varepsilon_s \frac{1}{L_i} (u_j - u_k)$$

$$\frac{k_B T}{e} \varepsilon_s \frac{1}{L_j} (u_k - u_i)$$

$$\frac{k_B T}{e} \varepsilon_s \frac{1}{L_k} (u_i - u_j)$$

$$\frac{k_B T}{e} \varepsilon_s [\frac{d_i}{L_i} (u_j - u_k) + \frac{d_j}{L_j} (u_i - u_k)] \quad Flux\ of\ D$$

Box integration method

- Summing over all points P_k of Voronoi boxes

- Same approach to discretize continuity equations for electrons and holes

$$\sum_k D_{ik}A_{ik} = \rho_k V_k$$

$A_{ik}: area\ of\ K-Vbox$
$D_{ik}: projection\ along\ grid\ line$

$$\sum_k J_{n,ik}A_{ik} = e(R_k + \frac{d}{dt}n_k)V_k$$

$$\sum_k J_{p,ik}A_{ik} = e(R_k + \frac{d}{dt}p_k)V_k$$

Scharfetter-Gummel discretization

- In case of no strong generation-recombination current density varies little within each domain

- Still this implies an exponential dependence of electron / hole density with position along grid's edge

- Using previous discretization method would require very dense mesh: Scharfetter-Gummel technique includes such dependence, requiring less grid points [D. L. Scharfetter and H. K. Gummel, "Large-signal analysis of a silicon read diode oscillator," IEEE Trans. Electron Devices, vol. ED-16, pp. 64–77, Jan. 1969].
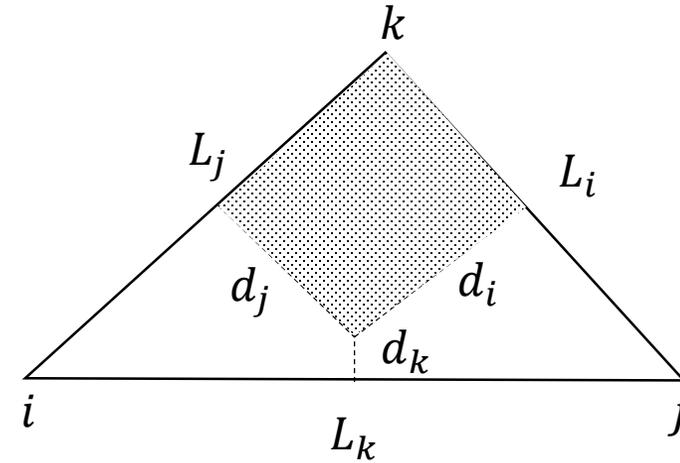
$$\mathbf{J}_n = q \cdot n \cdot \mu_n \cdot \mathbf{E} + q \cdot D_n \cdot \operatorname{grad} n$$

$$\mathbf{J}_p = q \cdot p \cdot \mu_p \cdot \mathbf{E} - q \cdot D_p \cdot \operatorname{grad} p$$
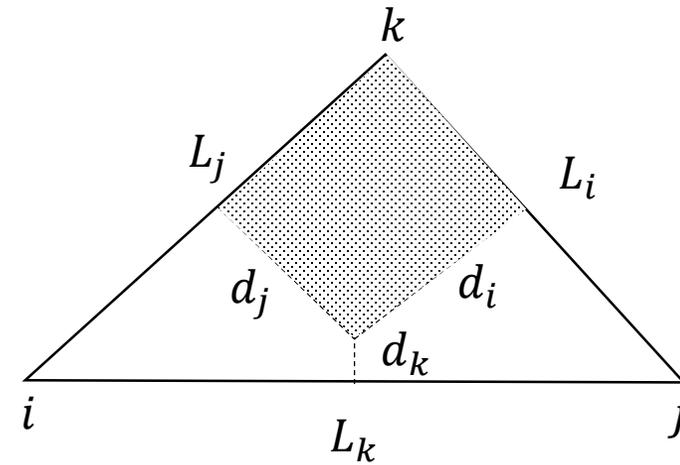
$$u := \frac{e}{k_B T} \varphi \qquad\qquad D_n := \frac{k_B T}{e} \mu_n$$

$$J_n := e D_n [\nabla n - n \nabla u] \qquad from\ J_n$$

$$J_{nk} := e D_n \left[\frac{dn}{dl_k} - n \frac{du}{dl_k} \right] \qquad projection\ along\ L_k \sim constant$$

Scharfetter-Gummel discretization

- Assume u varies linearly along the edge and current density $\simeq$ constant over the domain

- Define reduced current and assume and average diffusion along the edge
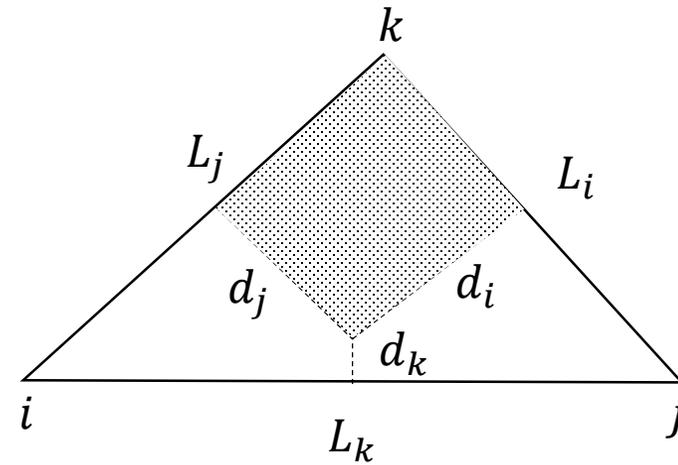
- Obtain first order equation in n along the edge

$$u = \frac{u_j - u_i}{L_k} l_k + u_i = a_k l_k + u_i$$

$$j_{nk} := \frac{J_{nk}}{eD_{nk}}, \qquad D_{nk} := <D_{ni}, D_{nj}>$$

$$j_{nk} = \frac{dn}{dl_k} - na_k$$

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Scharfetter-Gummel discretization

- Integrate from node i to node j, i.e. for $l_k = [0, L_k]$

- Obtain expression relating potential and carriers concentration

$$\int_0^{L_k} \exp(-a_k l_k)\, j_{nk} = \int_0^{L_k} \exp(-a_k l_k)\left(\frac{dn}{dl_k} - n a_k\right) d\, l_k$$

$$= \int_0^{L_k} \frac{d}{dl_k}(\exp(-a_k l_k)n\, dl_k$$

$$j_{nk} \frac{1}{a_k}(1 - \exp(-u_{ji})) = \exp(-u_{ji})n_j - n_i$$

$$j_{nk} = a_k\left(\frac{n_j}{\exp(u_{ji})-1} + \frac{n_i}{\exp(-u_{ji})-1}\right)$$

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Scharfetter-Gummel discretization

- Obtain the flux of current density relative to node k

- Scharfetter –Gummel discretization requires less fine mesh as the exponential dependence of carriers concentration is included in the discretization scheme

- It also depends on boundary values, i.e. 2D and 3D cases can be reduced to local 1D cases
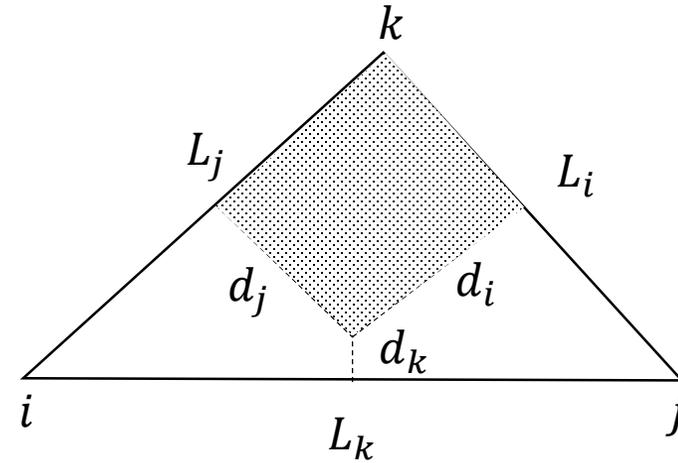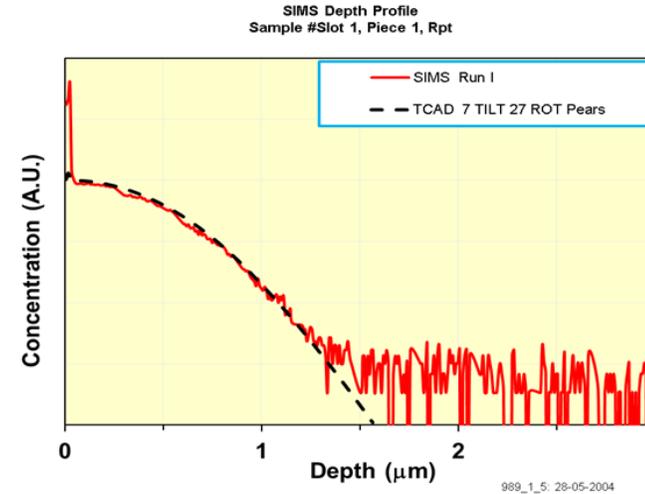

$$j_{nk} = \frac{1}{L_k}\left(\frac{u_{ji}n_j}{\exp(u_{ji})-1} - \frac{u_{ij}n_i}{\exp(u_{ij})-1}\right)$$

$$j_{nk} = \frac{1}{L_k}\left(B(u_{ji})n_j - B(u_{ij})n_i\right)$$ $\quad Bernoulli\ function\ B(x) = \frac{x}{\exp(x)-1}$

$$\nabla \cdot J_{nk}$$
$$= eD_{ni}\frac{d_i}{L_i}\left(B(u_{jk})n_j - B(u_{kj})n_k\right) + eD_{ni}\frac{d_j}{L_j}\left(B(u_{ik})n_i - B(u_{ki})n_k\right)$$

Simulation examples

- Examples from Synopsys TCAD (more on this from N. Owen lectures)

- Beside electrical simulation, process simulation is possible

- Most of the typical fabrication process steps can be simulated

Simulated process steps for LGAD fabrication

Simulation examples

SIMS and Pearson IV distribution − 31P

- High energy implants of ions can be simulated, either analytically or via MC

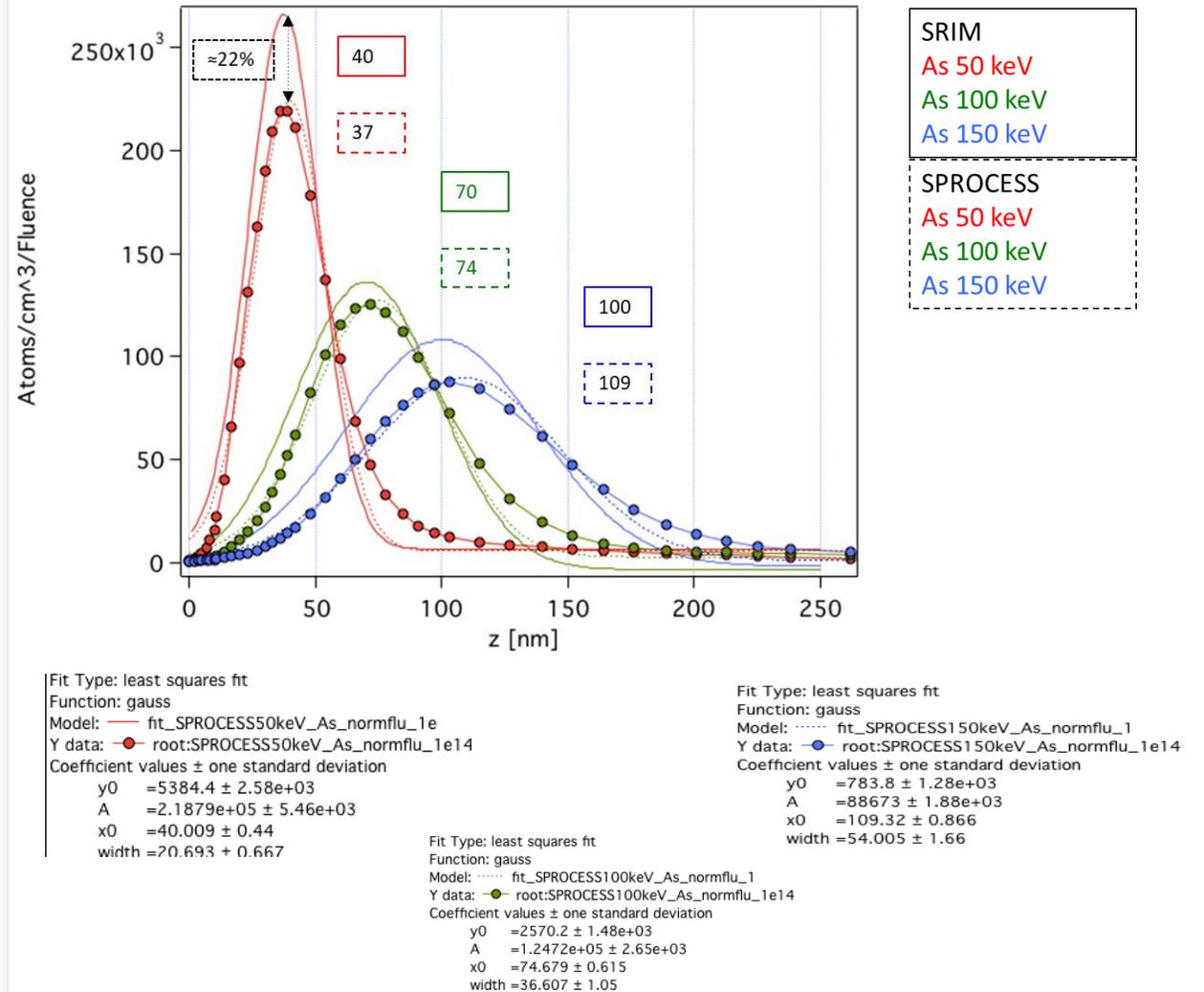- Creation of Frenkel defects following implantation can be obtained
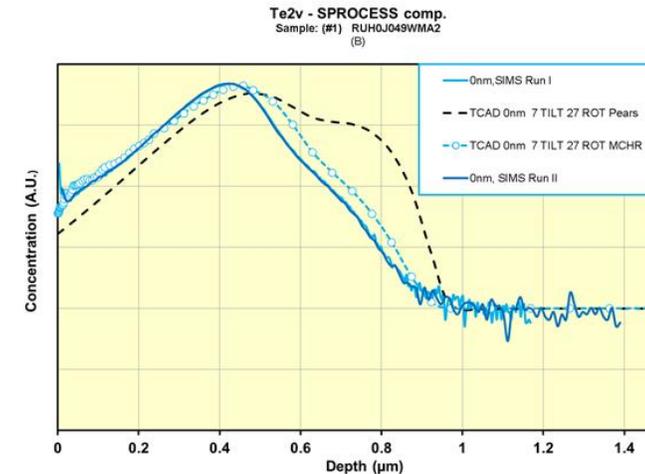
SIMS, Pearson IV distribution and MC run − 11B

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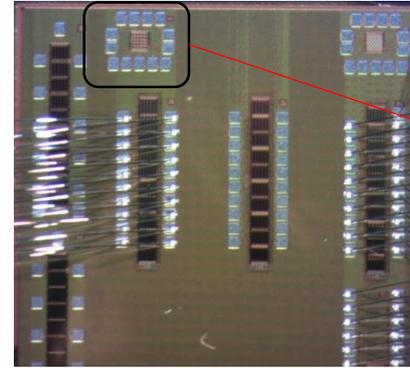# Simulation examples

- At least with As, MC (SRIM) and SPROCESS predictions on doping seem to agree within ≈ 20%

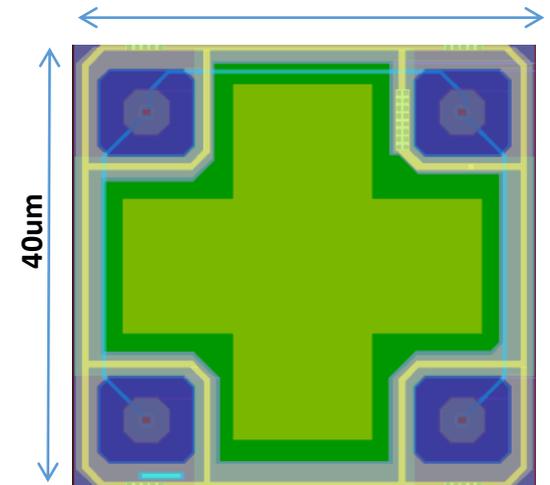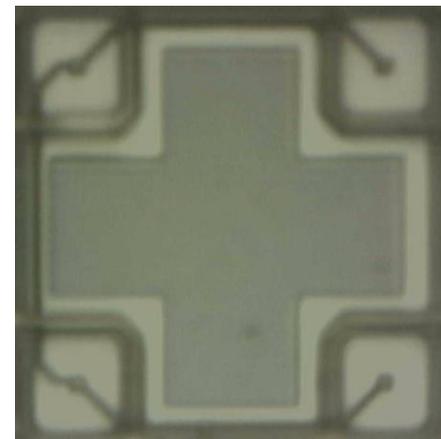- Note: SRIM assumes amorphous Si, <100> used for SPROCESS

Simulation examples

- Electrical simulation of a CMOS sensors (OVERMOS)

- A TCAD model of fabrication process of OVERMOS has been developed to investigate and predict the performances of the sensor
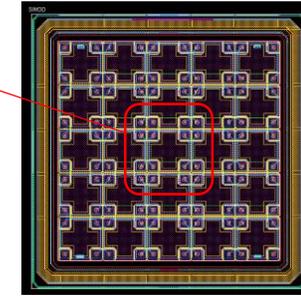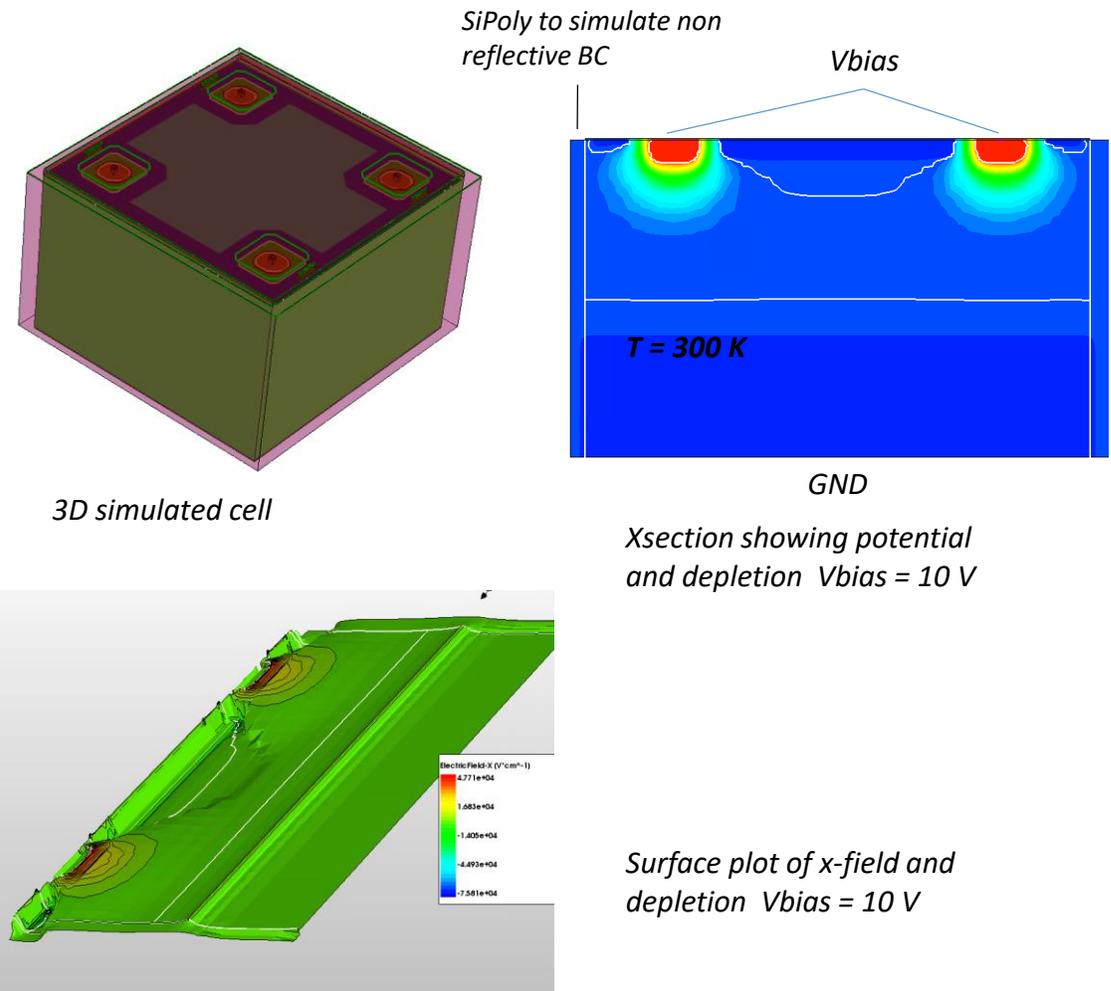

Photograph of OVERMOS test structure and simulated cell

40um

40um

*Photograph of OVERMOS cell and .gds layout*

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Simulation examples

- Internal field configuration vs. bias and temperature

- DC and AC characteristics can be obtained from the simulated model

3D simulated cell

SiPoly to simulate non reflective BC

Vbias

T = 300 K

GND

Xsection showing potential and depletion Vbias = 10 V

Surface plot of x-field and depletion Vbias = 10 V

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Simulation examples

- Charge collection is simulated using laser light injection and compared with test results

- Laser beam is 5 x 5 um2 around 4.5 ns pulse width, 1064 nm wavelength, $\sim 10\ pJ$

- These values are introduced in the simulator
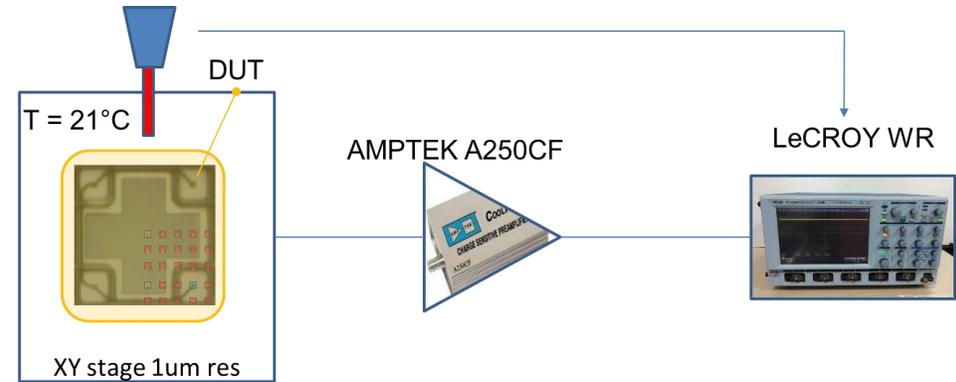
Test setup for charge collection measurement
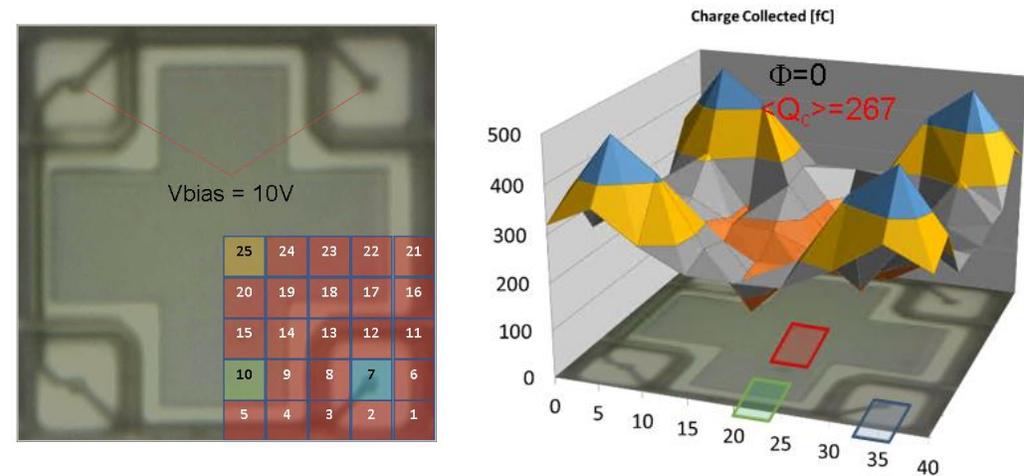
Charge is injected via laser at three different locations on cell. Results are mirrored to obtain a map of collected charge vs. position

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Simulation examples

- Effects of SiO2 reflection and attenuation of IR light can be implemented

- Quantum yield of optical generation, polarization, tilting, pulse width et cetera can all be included in the simulation

- TCAD simulations of non-irradiated OVERMOS reproduce experimental results, both in DC and in CC, with maximum discrepancy of the order of ~20%
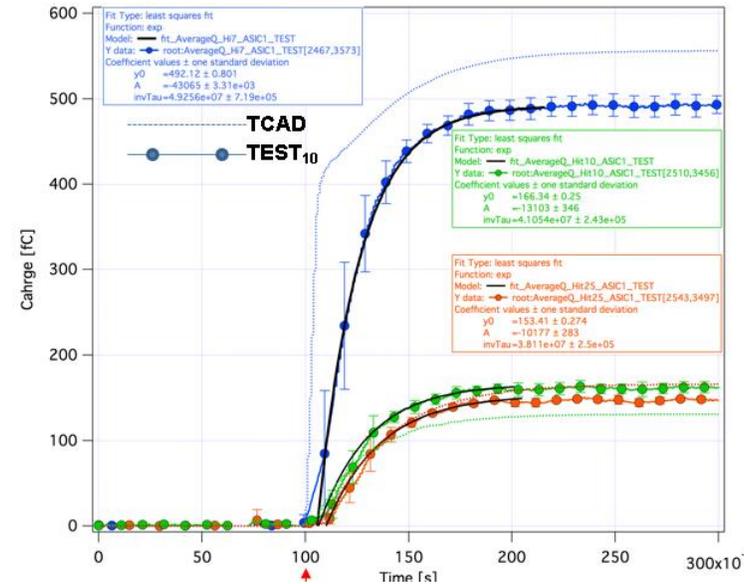
Transient of charge collection measurement and simulation

Q_{coll}	Test	TCAD	Δ%
\<Qh7\>	492	556	-13
\<Qh10\>	166	131	21
\<Qh25\>	153	166	-8.4

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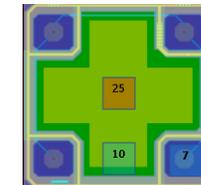
Thank you

giulio.villani@stfc.ac.uk

- Introduction to simulation
- Needs and transport regimes
- Meshing and discretization. Intro to DD model discretization. SG method
- Some examples of TCAD simulations: process and electrical device simulations, charge collection