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
Introduction

- 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...)

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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

Introduction

- Main components of semiconductor device simulation include fabrication process, 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].

$L$: device length
$l_{e-e}$: electron-electron scattering length
$l_{e-ph}$: electron-phonon scattering length
$\lambda$: electron wavelength

Transport regimes

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

• Semiclassical laws of motions apply

• Drift-diffusion (DD) equations are often valid, i.e. provided the electron gas is in thermal equilibrium with lattice temperature (\(T_e = T_L\))

\[
R \sim \frac{\hbar v \gamma}{2\pi \langle l \rangle} \approx 3.5 \text{ [nm]} \text{ Ionization radius for MIP in Si}^*
\]

\[
n = \frac{dE}{dx} \frac{L}{\rho E_{th} \pi R^2 L} \sim 2.5 \cdot 10^{18} \text{ MIP charge density within Ionization radius}
\]

\[
\lambda \leq \frac{\hbar}{\sqrt{2meV_b}} \sim \begin{cases} 0.38 \text{ [nm]@10 V} \\ 0.12 \text{ [nm]@100 V} \end{cases} \text{ De Broglie wavelength of carriers} \quad \text{@ full depletion}
\]

Drift diffusion model

• The semiconductor equations derived from 0th and 1st moment of BTE are referred to as Drift-Diffusion* model

• The model consists of Poisson's equation and PDEs: the continuity and current density equations for electrons and holes

• They express charge and momentum conservation

• Their self-consistent solutions are obtained via discretisation, using finite element methods (FEM)

\[
\frac{\partial t f + \mathbf{u} \cdot \nabla f}{\hbar} + \nabla \cdot \mathbf{F} = C[f] \quad \text{BTE}
\]

\[
\nabla \cdot J_n - q \frac{\partial n}{\partial t} = qR \\
\nabla \cdot J_p + q \frac{\partial p}{\partial t} = -qR
\]

Continuity equations

\[
J_n = q\eta\mu_nE + qD_n\nabla n \\
J_p = q\rho\mu_pE - qD_p\nabla p
\]

Current density equations

\[
\nabla \cdot \varepsilon \nabla \phi = e(n - p - N_D + N_A)
\]

Poisson's equation

Discretization and meshing

- The device simulations process consists of two steps:

  1. The test volume is obtained through grid generation (‘mesh generation’)

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

• The meshing used in most FEM methods relies on Delaunay triangulations:

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

• The Delaunay triangulation of a discrete point set $\mathbf{P}$ in general corresponds to the dual graph of the Voronoi diagram for $\mathbf{P}$

  the set of all locations $\mathbf{x}$ closest to $P_i \in \mathbf{P}$ than to any other point of the grid

\[ T_{\text{D},k}(\mathcal{P}_{\text{D},k}) \iff \exists \mathbf{x} \in \Omega \land \\
|\mathbf{x} - \mathbf{x}_i| = |\mathbf{x} - \mathbf{x}_j| \land \forall \mathbf{P}_i, \mathbf{P}_j \in \mathcal{P}_{\text{D},k} \land \\
|\mathbf{x} - \mathbf{x}_i| < |\mathbf{x} - \mathbf{x}_k| \land \forall \mathbf{P}_k \in \mathcal{P}_{\text{D},k}, \mathbf{P}_j \not\in \mathcal{P}_{\text{D},k} \]

The Delaunay triangulation with all the circumcircles and their centres

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

\[ \Omega_i = \{ \mathbf{x} \mid |\mathbf{x} - \mathbf{x}_i| \leq |\mathbf{x} - \mathbf{x}_j| \land i \neq j, \mathbf{x} \in \Omega \} \]
Discretization and meshing

- Correct Delaunay triangulation* guarantees element-volume conservation, important in many problems (diffusion, charge generation, et cetera)
- Delaunay triangulation maximises the minimum angle of the triangle

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

\[ P_1 = V_1 + V_5 + V_6 \]
\[ P_3 = V_3 + V_5 + V_6 \]

Discretization and meshing

- The discretisation of equations imposes some constraints on spatial and temporal mesh size.
- The mesh size should be smaller than the Debye length (i.e. the characteristic length for screening of field by charges) where charge variations in space have to be resolved.

\[ L_D = \sqrt{\frac{\varepsilon_s k_B T}{e^2 N}} \text{ Debye length} \]

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

• The 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

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

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

\[
\frac{\partial \Delta n}{\partial t} = -\frac{\Delta n(t = 0)}{t_{dr}}
\]

\[
\Delta n(\Delta t) = \Delta n(0) - \Delta t \frac{\Delta n(0)}{t_{dr}}
\]
Box integration method

- The discretisation of Poisson’s and continuity equations is done via Box Integration method.

- The LHS of equations is transformed via Gauss’ theorem and integrated over a Voronoi box $\Omega_k$ of point $P_k$.

\[
\nabla \cdot \varepsilon \nabla \varphi = e(n - p - N_D + N_A) \quad \equiv \int D \cdot dS = \int \rho dV
\]

\[
\nabla \cdot J_n - q \frac{\partial n}{\partial t} = q R
\]

\[
\nabla \cdot J_p + q \frac{\partial p}{\partial t} = -q R
\]
Box integration method

• Example of Poisson’s equation discretisation

• Assume that the electric potential is linearly varying over each elementary domain

\[ \nabla \cdot \varepsilon \nabla \varphi = e(n - p - N_D + N_A) \equiv \int D \cdot dS = \int \rho dV \]

\( i, j, k: \text{nodal indices} \)
\( L_i, L_j, L_k: \text{side vectors} \)
\( L_i, L_j, L_k: \text{magnitude side vectors} \)
\[ u := \frac{e}{k_B T} \varphi: \text{normalized potential} \]
Box integration method

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

- Flux of D vector associated to node k:

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

\[
\begin{align*}
&\frac{k_B T}{e} \varepsilon_s \frac{1}{L_i} (u_j - u_k) \\
&\frac{k_B T}{e} \varepsilon_s \frac{1}{L_j} (u_k - u_i) \\
&\frac{k_B T}{e} \varepsilon_s \frac{1}{L_k} (u_i - u_j) \\
&\frac{k_B T}{e} \varepsilon_s \left[ \frac{d_i}{L_i} (u_j - u_k) + \frac{d_j}{L_j} (u_i - u_k) \right]
\end{align*}
\]

 Flux of $D$
Box integration method

• Summing over all points $P_k$ of Voronoi boxes

• Same approach to discretise the **continuity equations** for electrons and holes

\[
\sum_k D_{ik} A_{ik} = \rho_k V_k \\
A_{ik}: \text{area of } K - Vbox \\
D_{ik}: \text{projection along grid line}
\]

\[
\sum_k J_{n,ik} A_{ik} = q (R_k + \frac{d}{dt} n_k) V_k
\]

\[
\sum_k J_{p,ik} A_{ik} = -q (R_k + \frac{d}{dt} p_k) V_k
\]
Scharfetter-Gummel discretisation

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

- Even so, this implies an exponential dependence of electron / hole density $n/p$ with position along grid’s edge

- Using previous discretization method would require very dense mesh: the Scharfetter-Gummel technique* includes such dependence, requiring less grid points


\[
\begin{align*}
J_n &= q n \mu_n E + q D_n \nabla n \\
J_p &= q p \mu_p E - q D_p \nabla p \\
\mu_n &= \frac{k_B T}{e} \mu_n \\
D_n &= \frac{k_B T}{e} \mu_n \\
J_n &:= q D_n [\nabla n - n \nabla u] \\
J_{nk} &:= q D_n \left[ \frac{dn}{dl_k} - n \frac{du}{dl_k} \right] \quad \text{projection along } L_k \sim \text{constant}
\end{align*}
\]
Scharfetter-Gummel discretisation

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

- Define the reduced current $j_{nk}$ and assume an average diffusion $D_{nk}$ along the edge

- Obtain first order equation in $n$ along the edge

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

\[ j_{nk} = \frac{J_{nk}}{qD_{nk}}, \quad D_{nk} = \langle D_{ni}, D_{nj} \rangle \]

\[ j_{nk} = \frac{dn}{dl_k} - na_k \]
Scharfetter-Gummel discretisation

- Integrate from node $i$ to node $j$, i.e. for $l_k = [0, L_k]$
- Obtain expression relating potential and carriers concentration

\[
\int_0^{L_k} \exp(-a_k l_k) j_{nk} = \int_0^{L_k} \exp(-a_k l_k) \left( \frac{dn}{dl_k} - n_{a_k} \right) dl_k
\]

\[
= \int_0^{L_k} \frac{d}{dl_k} \left( \exp(-a_k l_k)n \right) dl_k
\]

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

\[
j_{nk} = a_k \left( \frac{n_j}{\exp(u_{ji})-1} + \frac{n_i}{\exp(-u_{ji})-1} \right)
\]
Scharfetter-Gummel discretisation

- Obtain the flux of current density relative to node k

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

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

\[
\nabla \cdot J_{nk} = \frac{qD_{ni}}{L_i} \left( B(u_{jk})n_j - B(u_{kj})n_k \right) + \frac{qD_{ni}}{L_j} \left( B(u_{ik})n_i - B(u_{ki})n_k \right)
\]

BERNOULLI FUNCTION

\[
B(x) = \frac{x}{\exp(x) - 1}
\]

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

\[
j_{nk} = \frac{1}{L_k} (B(u_{ji})n_j - B(u_{ij})n_i)
\]
Simulation examples

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

- Beside electrical simulation, process simulation is possible

- Most of the typical steps of fabrication process can be simulated
Simulation examples

• Fabrication process and Electrical performances simulation of a Low Gain Avalanche Detector (LGAD) sensor

• The simulation of the fabrication included photolithography, etching, implantation, diffusion, metal deposition

• The electrical simulations included charge collection and gain due to impact ionisation w.r.t to a PIN diode

Simulation examples

- High energy implants of ions were simulated, both analytically or through Monte Carlo

- Results compared with Secondary Ion Mass Spectrometry (SIMS): Accuracy ≈ 10% or better
A note on ion implantation:

- At least with As, MC (SRIM) and SPROCESS predictions on doping seem to agree within ≈ 20%
- SPROCESS assumes amorphous Si, <100> used for SPROCESS
Simulation examples

- Internal field configuration vs. bias and temperature
- DC and AC characteristics can be obtained from the simulated model
Simulation examples

- Charge collection is simulated using laser light and MIP injection

- Spatial-temporal meshing different for Light and MIP injection

Device meshing for an optical charge injection in the PIN diode. The same meshing resolution was used for LGAD devices. Values in µm.

Device meshing for MIP charge injection. A meshing resolution of up to 0.3 nm was used in the radial direction along the MIP track. Values in µm.
Simulation examples

- The gain of the LGAD is defined as the ratio of collected charge w.r.t. the charge collected by a PIN diode, under the same biasing condition.
- The gain depends on the bias voltage applied, as this affects the impact ionisation, leading to charge multiplication.
- Different impact ionisation models predict different gain.

The transient current from optical charge injection in a PIN diode (line) and an LGAD (line with markers) at different percentage of breakdown voltage $V_{bd}$. The simulation uses the Okuto impact ionisation model with default values and $T = 21 \, ^\circ\text{C}$.

The simulation results of gain normalized to the percentage of $V_{bd}$ using MIP and IR charge injection for an LGAD.
Simulation examples

- The TCAD simulations using the Okuto-Crowell model* for impact ionisation match the measured LGAD gain up to values of the bias voltage of approximately 80% of the breakdown.

- Additional corrections to the modelling are needed to improve the accuracy of prediction.

- Due to the exponential dependence of impact ionisation on field / doping / parameters the task of LGAD modelling presents interesting challenges.

Thank you

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- 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