Computational Electronics

Introduction to Drift-Diffusion Model

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Hierarchy of Models

Representation of the physical structure or behavior of a device (or devices) by an abstract mathematical model which approximates this behavior. Such a model may either be a closed form expression (analytical model), or a system of simultaneous equations which are solved numerically.

Device Modeling - Modeling of the physical behavior of a semiconductor device. The term is often used in practice to mean the representation of a device in terms of a lumped parameter model used in higher level circuit simulation of complex integrated circuits. In the broader sense it includes both physical simulation and more abstract mathematical representations.

Device Simulation - Simulation of the device behavior by the approximate numerical solution of the (approximate) physical transport and field equations governing charge flow in the device, usually represented in a finite space (device domain).

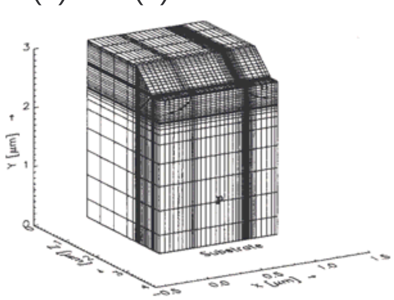
Goals of Device Modeling

Analysis - Simulating the behavior of a device (or circuits) with a physical model to understand the dependencies and limiting physical mechanisms in the device/circuit performance (e.g. effects of noise, limits on frequency/gain, trap effects, effects of geometry).

Design - Systematic use of a device/circuit model to achieve a desired functionality. For device design, and low level circuit design, the process is mainly an iterative, trial and error approach prior to actual physical implementation of a device or a circuit.

Physical Device Simulation

- There are 2 main components in physical device simulation:
  - (1) Charge motion due to driving forces and diffusion (transport)
  - (2) Fields due to charge distribution and motion (i.e current)
- Analytical solutions are only possible in 1D. Numerical solutions require discretization of (1) and (2) above onto a *mesh*, and solution of simultaneous algebraic equations
- (1) and (2) must be solved simultaneously (self-consistently)



Recessed MOSFET represented on 3D mesh over finite domain

Solution to the Field Equations

- In general, one needs to solve Maxwell's equations inside and outside the device:

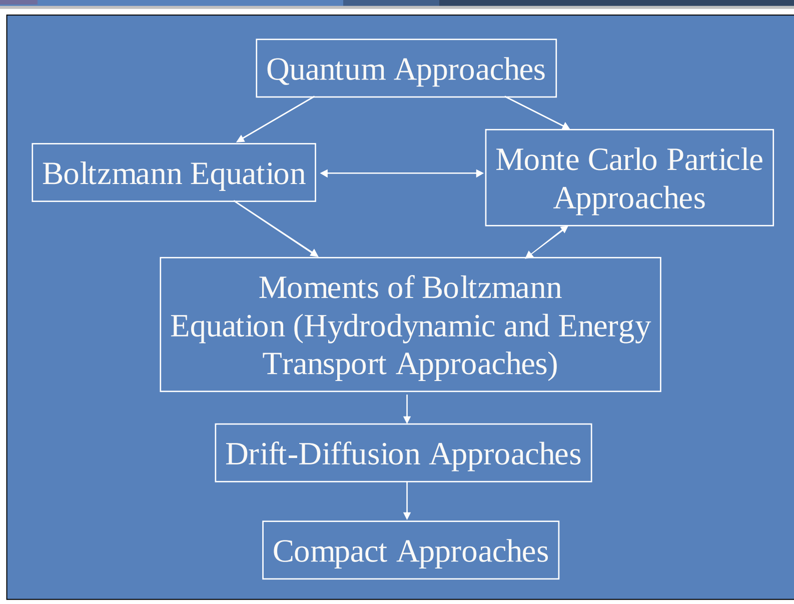
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla \cdot \mathbf{D} = \rho$$

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \qquad \nabla \cdot \mathbf{B} = 0$$

- Numerical techniques to solve include:
  - Time domain solutions (FDTD)
  - Frequency domain solutions (spectral techniques)
- At present, nearly all device simulation tools assume the quasi -static approximation, such that the electric field is obtained from Poisson's equation:

$$\nabla^2 V(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\varepsilon} \cdots\cdots\cdots \mathbf{E} = -\nabla V$$

Hierarchy of Semiconductor Simulation Models



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Drift-Diffusion Equations

- **Derivation of the Current Continuity Equations**
- **Derivation of the Electron Current Equation**
- **Validity of the Drift-Diffusion Model**
- **Physical Limitations of the DD Model**
- **Choice of Variables in the Drift-Diffusion Model**
- **Boundary Conditions**

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Derivation of the Current Continuity Equations

- Start from Maxwell's equations given in the previous slide:

$$\begin{cases} \nabla \times \mathbf{H} = \mathbf{J} + \dfrac{\partial \mathbf{D}}{\partial t}, & \nabla \times \mathbf{E} = -\dfrac{\partial \mathbf{B}}{\partial t} \\ \nabla \cdot \mathbf{D} = \rho, & \nabla \cdot \mathbf{B} = 0 \end{cases}$$

- Applying the divergence operator to the first equation leads to:

$$\nabla \cdot \mathbf{J} + \frac{\partial \rho}{\partial t} = 0$$

- Use: $\mathbf{J} = \mathbf{J}_n + \mathbf{J}_p$ and $\rho = e\left(p - n + N_D^+ - N_A^-\right)$

- Arrive at the following final results:

$$\begin{cases} \dfrac{\partial n}{\partial t} = \dfrac{1}{e}\nabla \cdot \mathbf{J}_n + U \\ \dfrac{\partial p}{\partial t} = -\dfrac{1}{e}\nabla \cdot \mathbf{J}_p - U \end{cases}$$

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Derivation of the Electron Current Equation

- Start from the steady-state Boltzmann transport equation (for 1D case) in the relaxation-time approximation

$$v\frac{\partial f}{\partial x}-\frac{eE}{m^*}\frac{\partial f}{\partial v}=-\frac{f-f_0}{\tau},\quad f_0(x,v)=n(x)\left(\frac{2\pi k_BT}{m^*}\right)^{-1/2}\exp\left(-\frac{m^*v^2}{2k_BT}\right)$$

- Multiply by the velocity *v* and integrate over *v*, to get:

$$\int v^2\frac{\partial f}{\partial x}dv-\frac{eE}{m^*}\int v\frac{\partial f}{\partial v}dv=-\frac{1}{\tau}\int vfdv$$

$$\frac{\partial}{\partial x}\left[n(x)\left\langle v^2\right\rangle\right]\qquad\frac{eE}{m^*}n(x)\qquad\qquad\frac{1}{e\tau}J_n(x)$$

- Final expression:

$$J_n(x)=en(x)\mu_nE+e\tau\left\langle v^2\right\rangle\frac{\partial n(x)}{\partial x}+e\tau n(x)\frac{\partial\left\langle v^2\right\rangle}{\partial x}$$

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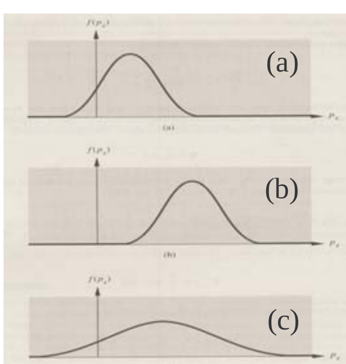
- Neglect the drift energy and use the Einstein relation for the consideration of the diffusion coefficient and mobility, to get:

$$J_n(x)=en(x)\mu_nE+eD_n\frac{\partial n}{\partial x}+e\underbrace{\frac{D_nn(x)}{T_e}}_{\textbf{Soret Coefficient}}\frac{\partial T_e}{\partial x}$$



(a) Low-field distribution function

(b) High-field distribution function when the kinetic energy gained appears mostly as drift energy

(c) High-field distribution function for conditions under which the kinetic energy gained from the field appears mostly as thermal energy

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Validity of the Drift-Diffusion Model

(a) Approximations made in its derivation

- Temporal variations occur in a time-scale much longer than the momentum relaxation time.
- The drift component of the kinetic energy was neglected, thus removing all thermal effects.
- Thermoelectric effects associated with the temperature gradients in the device are neglected, i.e.

$$\mathbf{J}_n(x) = en(x)\mu_n\mathbf{E} + eD_n\nabla n$$
$$\mathbf{J}_p(x) = ep(x)\mu_p\mathbf{E} - eD_p\nabla p$$

- The spatial variation of the external forces is neglected, which implies slowly varying fields.
- Parabolic energy band model was assumed, i.e. degenerate materials can not be treated properly.

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(b) Extension of the capabilities of the DD model

- Introduce field-dependent mobility $\mu(\mathbf{E})$ and diffusion coefficient $D(\mathbf{E})$ to empirically extend the range of validity of the DD Model.
- An extension to the model, to take into account the overshoot effect, has been accomplished in 1D by adding an extra term that depends on the spatial derivative of the electric field

$$J_n(x) = en(x)\left[\mu_n(E) + \mu_n(E)L(E)\frac{\partial E}{\partial x}\right] + eD_n(E)\frac{\partial n}{\partial x}$$

1. K.K. Thornber, IEEE Electron Device Lett., Vol. 3 p. 69, 1982.
2. E.C. Kan, U. Ravaioli, and T. Kerkhoven, Solid-State Electron., Vol. 34, 995 (1991).

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Physical Limitations of the DD Model (discretization)

- The complete DD Model is summarized below:

Current equations:
$$\mathbf{J}_n = en\mu_n\mathbf{E} + eD_n\nabla n$$
$$\mathbf{J}_p = ep\mu_p\mathbf{E} - eD_p\nabla p$$

Continuity equations:
$$\frac{\partial n}{\partial t} = \frac{1}{e}\nabla\cdot\mathbf{J}_n + U$$
$$\frac{\partial p}{\partial t} = -\frac{1}{e}\nabla\cdot\mathbf{J}_p - U$$

Poisson Equation:
$$\nabla^2 V = \frac{e}{\varepsilon}\left(n - p + N_D^+ - N_A^-\right)$$

- A numerical scheme that solves the continuity equation should:
  - (a) Conserve the number of particles in the device,
  - (b) Respect local positivity of the carrier density, and
  - (c) Respect monotonicity of the solution.

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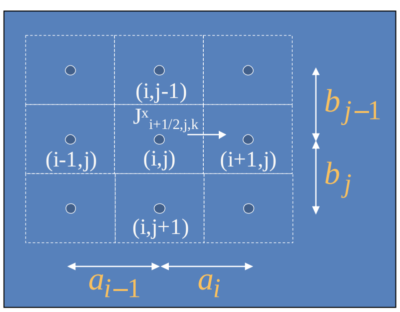
- Conservative schemes for the continuity equation are achieved with the following discretization scheme:



$$\frac{n_{i,j}^{k+1} - n_{i,j}^{k}}{\Delta t} = U_{i,j}^{k} + \frac{1}{e}\frac{J_{i+1/2,j}^{k} - J_{i-1/2,j}^{k}}{0.5(a_{i-1} + a_i)} + \frac{1}{e}\frac{J_{i,j+1/2}^{k} - J_{i,j-1/2}^{k}}{0.5(b_{j-1} + b_j)}$$

- Requirements:
  - (a) the mesh size must be smaller than the Debye length L_D
  - (b) Time step must be smaller than the dielectric relaxation time: $t_{dr} = \varepsilon/(eN\mu)$

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Choice of Variables in the Drift-Diffusion Model

- Natural variable formulation: (V, n, p)
- Quasi-Fermi level formulation: (V, ϕ_n, ϕ_p)

$$n = n_i \exp\left[\frac{e(V-\phi_n)}{k_B T}\right], \quad p = n_i \exp\left[\frac{e(\phi_p - V)}{k_B T}\right]$$

- Slotboom variables: (V, Φ_n, Φ_p)

$$\Phi_n = n_i \exp\left(-\frac{e\phi_n}{k_B T}\right) \rightarrow n = \Phi_n \exp\left(\frac{eV}{k_B T}\right)$$

$$\Phi_p = n_i \exp\left(\frac{e\phi_p}{k_B T}\right) \rightarrow p = \Phi_p \exp\left(-\frac{eV}{k_B T}\right)$$

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Normalization of Variables

<u>Standard way of scaling due to de Mari:</u>

Space:	Intrinsic L_D ($N=n_i$) Extrinsic L_D ($N=N_{max}$)	$L_D = \sqrt{\varepsilon k_B T/(e^2 N)}$
Potential:	Thermal voltage	$V_T = k_B T / e$
Carrier density:	Intrinsic density Extrinsic density	$N=n_i$ $N=N_{max}$
Diffusion Coeff:	D_0	$1cm^2/s$
Mobility	μ	$\mu = D_0 / V_T$
Recomb./Gen.	R	$R = D_0 N / L_D^2$
Time:	T	$T = L_D^2 / D_0$

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Boundary Conditions

From the aspect of device physics, one can distinguish between the following device boundaries:

(1) Contacts, which allow a current flow in and out of the device
- Ohmic contacts: purely <u>voltage</u> or purely <u>current controlled</u>
- Schottky contacts

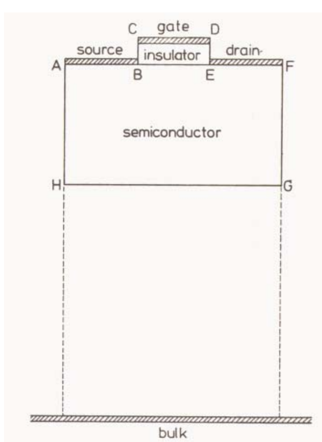
(2) Contacts where only voltages can be applied

(3) Interfaces, where current flow disappears

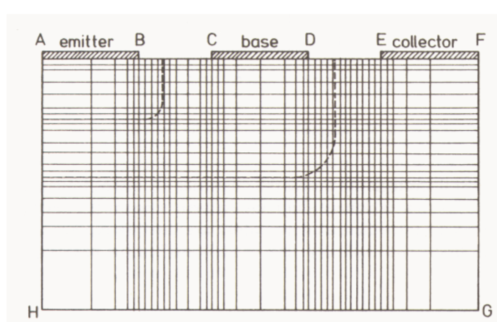
(4) Artificial boundaries, where neither electric field nor current flow exists

Boundary Conditions, Cont'd

Examples of different boundary conditions:



MOSFET



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Ohmic Contacts

(A) Boundary conditions for Ohmic contacts

Electrostatic potential:

- Voltage-controlled ohmic contact (Dirichlet boundary conditions):

$$V(t) = V_b + V_{applied}$$

n-type sc: $N_D >> N_A \rightarrow V_b = V_t \ln(N_D / n_i)$

p-type sc: $N_A >> N_D \rightarrow V_b = -V_t \ln(N_A / n_i)$

- Current-controlled contact (integral boundary condition):

$$\int_{D_0} (\mathbf{J}_n + \mathbf{J}_p) \cdot d\mathbf{A} - I(t) = 0, \quad V(t) = V_b + const.$$

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Ohmic Contacts, Cont'd

Electron and hole densities:

- The electron and hole densities are determined by assuming charge neutrality and thermal equilibrium

n-type sc: $n = \frac{1}{2}\left[\sqrt{N_D^2 + 4n_i^2} + N_D\right], \quad p = n_i^2 / n$

p-type sc: $p = \frac{1}{2}\left[\sqrt{N_A^2 + 4n_i^2} + N_A\right], \quad n = n_i^2 / p$

- Low temperatures:

$$N_D^+ = \frac{N_D}{1 + 2\exp\left(\frac{E_D - E_F}{k_B T}\right)}, \quad N_A^- = \frac{N_A}{1 + 4\exp\left(\frac{E_A - E_F}{k_B T}\right)}$$

Donor and acceptor energy levels for common semiconductors in Si [eV]

Arsenic	Phosphorus	Antimony	Boron
0.054	0.045	0.039	0.045

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Schottky Contacts

(B) Boundary conditions for the Schottky contacts

Electrostatic potential:

Dirichlet boundary condition: $V(t) = V_{schottky} + V_{applied}$

Material:	Aluminum	Platinum	Titanium
$V_{schottky}$ [V]	0.68	0.8	0.6
$v_{n,p}$ [cm/s]	5×10^6	5×10^6	5×10^6

Current:

Neumann boundary conditions (thermionic-emission and diffusion theory):

$$\mathbf{J}_n \cdot \vec{\mathbf{n}} = -ev_n(n - n_0)$$
$$\mathbf{J}_p \cdot \vec{\mathbf{n}} = ev_p(p - p_0)$$

1. R. Hattori, J. Shirafuji, Jpn. J. Appl. Phys., Vol. 33, pp. 612-618, 1994.
2. J.R. Tucker, C. Wang, and P.S. Carney, Appl. Phys. Lett., Vol. 65, pp. 618-620, 1994.

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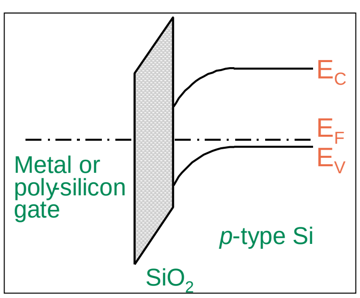
Gate Contact

(C) Gate contact (only voltage can be applied)

- Dirichlet boundary condition for the potential:



$$V(t) = \Phi_{MS} + V_{applied}$$

$$\Phi_{MS} = \frac{1}{e}\left[\chi_{sc} + (E_c - E_i)_{bulk}\right] - \Phi_M$$

- Values of the work-function for different gate materials:

Material:	n^+-poly	p^+-poly	Aluminum
Φ_{MS} [V]	0.55	-0.50	0.50

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Semiconductor/Oxide Interface

(D) Semiconductor/Oxide Interfaces

Electrostatic potential:

- The normal components of the dielectric displacement vector must satisfy the Gauss law in its differential form:

$$\varepsilon_{sc}\left.\frac{\partial V}{\partial \vec{\mathbf{n}}}\right|_{sc}-\varepsilon_{ox}\left.\frac{\partial V}{\partial \vec{\mathbf{n}}}\right|_{ox}=Q_{\mathrm{int}}$$

- For MOSFETs, simplified boundary condition would be:

$$\varepsilon_{sc}\left.\frac{\partial V}{\partial \vec{\mathbf{n}}}\right|_{sc}-\varepsilon_{ox}\frac{V_G-V}{t_{ox}}=Q_{\mathrm{int}}$$

Current:

- Neumann boundary conditions:

$$\begin{array}{lcl} \mathbf{J}_n\cdot\vec{\mathbf{n}}=-eR^{surf} & & \mathbf{J}_n\cdot\vec{\mathbf{n}}=0 \\ & \rightarrow & \\ \mathbf{J}_p\cdot\vec{\mathbf{n}}=eR^{surf} & & \mathbf{J}_p\cdot\vec{\mathbf{n}}=0 \end{array}$$

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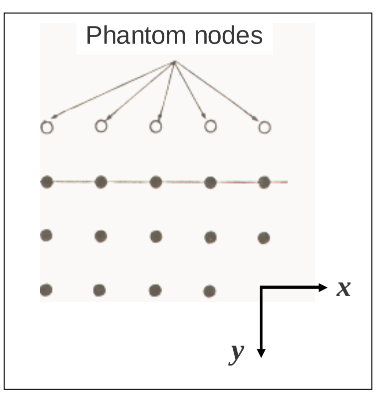
Artificial Boundaries

(E) Artificial boundaries

This type of boundary is not based on physical consideration. Therefore, it is called an artificial boundary. One applies Neumann boundary conditions for both the electrostatic potential and current, i.e.



$$\frac{\partial V}{\partial \vec{\mathbf{n}}}=0 \qquad \mathbf{J}_n\cdot\vec{\mathbf{n}}=0 \qquad \mathbf{J}_p\cdot\vec{\mathbf{n}}=0$$

$$\Rightarrow$$

$$\frac{V_{i,j+1}-V_{i,j-1}}{\Delta}=0 \qquad \frac{n_{i,j+1}-n_{i,j-1}}{\Delta}=0 \qquad \frac{p_{i,j+1}-p_{i,j-1}}{\Delta}=0$$