

Network for Computational Nanotechnology (NCN)

Berkeley, Univ.of Illinois, Norfolk State, Northwestern, Purdue, UTEP



First-Time User Guide to MuGFET v1.1

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Introduction: What is MuGFET?

Nanoscale Multi-Gate Field Effect Transistor

Size of device decreases (Moore's Law) →number of gates increases for more efficient gate control









Introduction

MuGFET simulates quantum transport at the nanoscale, which is close to the atomistic dimension.

 \rightarrow Quantum transport simulation is necessary but is not the best choice for the following reasons:



Relatively long and large device

- Computationally very
 expensive
- Difficult to include all of the scattering processes







Introduction

The **Drift diffusion type simulator** works well enough to demonstrate characteristics of relatively long and large devices.

In What Ways?

- QM mechanics is not dominant if the lateral dimension of the transistor is larger than 10 nm.*
- •Physical insight can be provided, even if not strictly valid.
- •The subthreshold characteristic is still diffusion dominated.
- •The on-current can never be overestimated by the drift diffusion simulation.
- •The hot carrier transport can be taken care of by solving the energy balance equation.
- •The drift diffusion simulator is way faster than the quantum transport simulator.

*This statement is from a conversation with Prof. Vasileska at ASU







Introduction

*PROPHET: general partial differential solver developed at Bell Lab **PADRE: device simulator developed at Bell Lab



*https://www.nanohub.org/resource_files/tools/prophet/doc/guide.html **http://www.nanohub.org/resource_files/tools/padre/doc/index.html







Theory



*ECE612 Fall2008 lecture 8 note

- ε : dielectric constant
- V: potential
- n/p: electron/hole density
- q: elementary charge
- $J_{n/p}$: electron/hole current density

Self consistent calculation **Poisson equation** $\nabla \cdot (\varepsilon \nabla V) = q(n - p + N_A - N_D)$ Continuity equation $\frac{\partial n}{\partial t} = \frac{1}{a} \nabla \cdot \mathbf{J}_n + G(n, p) - R(n, p)$ $\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{J}_p + G(n, p) - R(n, p)$ $\mathbf{J}_n = -q\mu_n n\nabla V + qD_n \nabla n$ $\mathbf{J}_{p} = -q\mu_{p}p\nabla V - qD_{p}\nabla p$



- T: temperature
- G/R: generation/recombination rate
- μ_n, μ_n : electron/hole mobility
- D_n, D_p : electron/hole diffusion coefficient





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$$\nabla \cdot \mathbf{S}_{n,p} = -\mathbf{J}_{n,p} \cdot \nabla \psi - W_n - \frac{3k}{2} \frac{\partial}{\partial t} \left(\lambda_{n,p}^* n T_{n,p}^* \right)$$
$$\mathbf{J}_n = q D_{n,p} \nabla n - \mu_{n,p} n \nabla \psi + q n D_{n,p}^T \nabla T_{n,p}$$
$$\mathbf{S}_n = -K_{n,p} \nabla T_{n,p} - \left(\frac{\kappa \delta_{n,p}}{q} \right) \mathbf{J}_{n,p} T_{n,p}$$

 $\mathbf{S}_{n,p}$: energy flux density $D_{n,p}$: thermal diffusivity $W_{n,p}$: energy density loss rate $T_{n,p}$: carrier temperature $\mu_{n,p}$: electron mobility $K_{n,p}$: thermal conductivity

Drift Diffusion Model

 \rightarrow carrier velocity is saturated in the channel (where electric field is larger than critical value)

Reality

 \rightarrow Velocity overshoot: current gets higher

*https://www.nanohub.org/resource_files/2006/06/01581/int ro_dd_padre_word.pdf

Theory

Energy Balance Equation*







Outline of Interface

Device Type \rightarrow Structure \rightarrow Material \rightarrow Environment \rightarrow Simulator \rightarrow Simulate

Device Type + 2 Structure + 3 Material + 4 Environment + 5 Simulator + 6 Simulate
Examples: Double Gate p-FinFET - Gate length : 45 nm, Channel width : 30nm
Device Type
Class: FinFET
Spec
Dimension: 2D (Double Gate)
Gate Type: Metal
Gate
Source Channel Drain
Gate







MuGFET	Device Type
Device Type + 2 Structure + 6 Material + 4 Environment	Class- FinFET or Nanowire
Examples: Double Gate p-FinFET - Gate length : 45 nm, Channel wit	Dimension
Device Type Class: FinFET Spec	Nitride Gate Oxide Si Oxide Si
Dimension: 2D (Double Gate)	Oxide Oxide
Gate	2D-Double Gate 3D-Triple Gate
	Nanowire- no dimension
Source Channel Drain	Gate Contact Wire Wire Source Extension
Structure >	 Gate type- metal or poly (polysilicon) (poly option is only valid in PADRE simulator)







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<u>F</u> ile
① Device Type → ② Structure → ③ Material → ④ Environment
Geometry-X Geometry-Y Geometry-Z Dopini
x Tox1 Wch Tox2
Diameter - Dch: 100nm
Oxide thickness - Tox: 2.5nm
Channel width - Wch: 30nm
Left wall oxide thickness - Tox1: 2.5nm
Right wall oxide thickness - Tox2: 2.5nm
< Device Type Material >
<pre></pre>

Device Structure

- Geometry-X: Lateral Direction
 - » Channel width
 - The width of silicon channel region
 - » Oxide thickness
 - Left wall
 - Right wall
 - X-direction is Radial Direction
 - » when you choose the nanowire

Note: The cross section should be large when compared to the electron wave length, so that the quantum effect will not appear to be using the Drift Diffusion Equation.





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File	
2 Structure + 6 Material + 4 Environment + 6)Simulator 🔸 (
Geometry-X Geometry-Y Geometry-Z	Dopin
$ \begin{array}{c} \end{array} \xrightarrow{Y} \leftarrow L_{s} \longrightarrow L_{g} \longrightarrow L_{d} - \\ \end{array} $	
Gate length - Lg: 45nm	
Source extension length - Ls: 50nm	
Drain extension length - Ld: 50nm	
Gate overlap to source - Os: 2nm	
Gate overlap to drain - Od: 2nm	
< Device Type	Material >

Device Structure

- Geometry-Y
 - » Lg: gate length
 - » Ls: source extension length
 - » Ld: drain extension length
 - Extension region has same width as the channel but is doped differently



*Y.K.Choi et. al. IEEE Electron Device Letters, 2002

» Os/Od: Gate overlap to source/drain







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2 Structure + 3 Material + 4 Environment + 5 Sim	ulator ++
Geometry-X Geometry-Y Geometry-Z	Dopini)
x y Gate Gate A y Gate Cate	-В
Channel height - Hch: 30nm	
Top oxide thickness - Top_ox: 2.5nm	
Substrate oxide thickness - Sub_ox: 50nm	
< Device Type	aterial >

Device Structure

Geometry-Z

- » Z directional geometry setting is only activated when you choose triple gate (3D) in device type
- » Hch: channel height
- » Top_ox: top oxide thickness
- » Sub_ox: substrate oxide thickness





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Rappture Interface - Doping

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<u>F</u> ile	
1 Device Type + 2 Structure + 3 Material + 4	Environment 🗕
Geometry-X Geometry-Y Geometry-Z	Doping
Gate	
Source Channel Drain	
Gate	
Source doping concentration: 1e+19/cm3	
Drain doping concentration: 1e+19/cm3	
Channel doping concentration: 1e+16/cm3	
Source doping type: P	•
Drain doping type: P	-
Channel doping type: N	•
Poly doping type: P	•
< Device Type	Material >

- Doping
 - ✓ Doping concentration in each section
 - ✓ Doping type in each section
- Gaussian Doping



- » Gaussian doping profile starts from the end of the source/drain extension region
- » Characteristic length is the length to which the doping drops by the factor exp(-1)





Material Property

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Rappture Interface - Environment





Simulator Options - PROPHET

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ure + 3 Material + 4 Environment + 5 Simulato	r 🔸 🙃 Simulat
Simulator: PROPHET	•
Options	
Only Equilibrium: 🔲 no	
Plot dimension: 1D(y)	-
Maximum number of Newton iteration: 1000	
Tolerance for Newton iteration: 1e-06	
Models	
Quantum corrections: 🔲 n	10
Lombardi's (Tansverse Field Dependent) Mobility: 🔲 n	10
< Environment	Simulate >

** Lombardi's mobility model : http://wwwtcad.stanford.edu/~prophet/user_ref/node8.html



Only Equilibrium

- » All of the bias steps will be ignored, if simply simulating the equilibrium condition.
- Plot dimension
 - » 1D(x): 1D plot across the channel
 - » 1D(y): 1D plot along the channel
 - » 2D: 2D plot
- Newton iteration parameters

(for convergence of the continuity equation and the Poisson equation)

- » Maximum number of iteration
- » Tolerance
- Models
 - » Quantum correction
 - » Lombardi's transverse field dependent mobility model**





Simulator Options - PADRE

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evice Type + (2) Structure + (3) Material + (4) Environment + (
Simulator: PADRE
Options
Grid preview: 🔲 no
Only equilibrium: 🔲 no
Plot dimension: 1D(y)
Maximum number of Newton iteration: 1000
Tolerance for Newton iteration: 1e-06
Models
Statistics: Fermi
Solve energy balance equation: 🔲 no
Bandgap narrowing: 🗹 yes
Concentration dependent mobility: 🖌 yes
Nonlinear drift velocity-field model: 🚽 yes
Vertical field dependent mobility: 🚽 yes
Carrier-carrier scattering: 🗹 yes
Impact ionization: 🗌 no

- Grid Preview
 - » The mesh structure can be seen before running the simulation.

*Models

- » Statistics: Fermi or Boltzmann
- » Energy balance equation
 - Includes the solve energy balance equation for the hot transport
- » Bandgap narrowing
- » Concentration dependent mobility
- » Nonlinear drift velocity field model
- » Vertical field dependent mobility model
- » Carrier carrier scattering model
- » Impact ionization

*http://www.nanohub.org/resource_files/tools/padre/doc/pad re-ref/models.html

*http://www.nanohub.org/resources/1514/







PADRE Option - energy balance equation

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File
avice Type + 2 Structure + 3 Material + 4 Environment + 3 Simulator + 6
Simulator: PADRE
Options
Grid preview: no
Only equilibrium: no
Plot dimension: 1D(y)
Maximum number of Newton iteration: 1000
Tolerance for Newton iteration: 1e-06
Models
Statistics: Fermi
Solve energy balance equation: 🗹 yes
Solve energy balance equation if you want to include hot carrier transport
Non Click to turn on/off
Vertical field dependent mobility: 🗹 yes
Carrier-carrier scattering: 🗹 yes
Impact ionization: 🔲 no

- When the energy balance equation is selected for solving, the continuity equation, Poisson equation, and energy balance equation are coupled to each other and solved independently.
- The equations do not easily converge, when the energy balance equation is selected.
- The bias steps should be small when solving energy the balance equation.
- Sometimes it is best not to choose a wide range of bias.
- A good strategy is to start from zero bias and increase it gradually.







Useful Plots for Device Design (input)

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<u>F</u> ile		
Device	e Structure 🔸 🕄 Bias and Temperature 🔸 🕘 Options 🔸 🕤 Simul	ate
Result:	Subthreshold Swing	
	Energy Band Diagram at equilibrium	
98 -	Doping, electron density, hole density at equilibrium	
	Net Charge Density at equilibrium	
	Electrostatic Potential at equilibrium	
G -	Electric Field at equilibrium	
/de	IV Characteristics (Id-Vg)	
> E. 07	Iransconductance	
0,,-		
N.	On-current	
- <u>פ</u>	Threshold Voltage	
оч.	Subthreshold Swing	
Jres	Drain Induced Barrier Lowering(DIBL)	
- 36 -	Energy Band Diagram at applied bias Vd=-0.05	
S	Doping, electron density, hole density at applied bias Vd=-0.05	
	Excess Carrier Density at applied bias Vd=-0.05	
-	Net Charge Density at applied bias Vd=-0.05	
	Electrostatic Potential at applied bias Vd=-0.05	
	Electric Field at applied bias Vd=-0.05	
	Energy Band Diagram at applied bias Vd=-1.05	
	Doping, electron density, hole density at applied bias Vd=-1.05	
1 resul	Excess Carrier Density at applied bias Vd=-1.05	ar
	Net Charge Density at applied blas Vd=-1.05	
. 01	Electrostatic Potential at applied bias Vd=-1.05	
vp	Lieutic Field at applied bias Yu=-1.00	
	Download	

- IV characteristics
- Threshold voltage
- Subthreshold swing
- Transconductance
- Drain induced barrier lowering(DIBL)
- On/off current and its ratio
- Doping, electron, hole density
- Electrostatic potential
- Energy band diagram*
- Net charge density*
- Electric field*

*These plots are supported only in PADRE







Plots









3D plots are available but appear more slowly





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0 0

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What if You Just Hit "Simulate" ?

Aaterial + 4 Environment + 5 Simulator - 6 Simulate
ength : 45 m, Channel width : 30nm ength : 45 nm, Channel width : 30nm ength : 60 nm, Channel width : 40nm : 30nm, Diameter : 10nm - hot carrier : 30nm, Diameter : 10nm - no hot carrier Retrieving database to plot the result without simulation
Gate
<pre>he input parameters in your inputdeck is same as one of the example Device type: Double Gate p-FinFET Device Dimension: 30 nm (channel width), 45 nm(gate length) , 2.5 nm(oxide thickness) Doping : Source (p type 1.0e+19), Channel (n type 1.0e+16), Drain (p type 1.0e+19) Temperature : 300 K Bias : Vg from 0.5 to -1.5 with -0.1 step size (21 bias points) Vd from -0.05 to -1.05 with -1.0 step size (2 bias points) IV plot : Id-Vg Simulator : PADRE</pre>







Example p-finFET Lg=45nm, Wch=30nm, tox=2.5nm*



- The primitive finFET structure
- Gaussian doping using raised source and drain, dopants diffused to the source and drain extension region



• Ls and Ld(source/drain extension length) is same as spacer width.



*Sub 50-nm finFET: PMOS - Huang, et al., IEDM,1999









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Effect of Gaussian Doping Profile





Channel Formation - Quantum Correction



In reality, because of the quantum effect, the carriers flow at a distance from the surface \rightarrow threshold voltage changes







Drain Current Normalization

Normalization of Id (finFET)

» Normalization to the fin height

- ✓ This is the same as the conventional normalization, as based on the width of the channel (PADRE and PROPHET).
- » Normalization to the fin height *2
 - ✓ Multiply 2, due to the channel formation in both of the side walls.
- Comparison with experiment
 - » Divide 2 to the PADRE and PROPHET result, if the experimental result uses normalization to the fin height *2.

- Normalization of Id (nanowireFET)
 - » The drain current is sometimes normalized to the diameter in experiment.
 - » The drain current in PADRE and PROPHET is not normalized.
- Comparison with experiment
 - » Divide by the diameter to the PADRE and PROPHET results.
 - » Change the units to A/ μ m or μ A/ μ m











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*Experiment result from Y.K.Choi et. al. IEEE Electron Device Letters, 2002





Example - Nanowire



* Experiment -Sung DaeSuk, et al., IEDM 2005, pp 717-720, Dec 2005 **Nanowire - quantum ballistic transport simulation tool for nanowire structure - available in nanoHUB.org







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Summary

- The drift-diffusion simulator MuGFET using PROPHET and PADRE is upgraded to v1.1
- I have included the energy balance equation option to demonstrate the hot carrier effect on transport.
- The input interface has been upgraded for user's convenience.
- ✤ So that the Gaussian doping profile will be more realistic, I have upgraded it.







Final Thoughts

Possible Future Work Being Considered:

- » 3D visualization (open DX)
- » Refinement of 3D simulation
- » Process simulation using PROPHET to feed in the result to PADRE →realistic doping and geometry
- » AC response in PADRE
- » Quantum correction is already implemented
 →density gradient model in PROPHET
 →balance equation model into PROPHET?
- » Parallelization \rightarrow new code?
- » Modified drift diffusion model



