Quantum Device Simulation

Overview Of Atlas Quantum Features
Introduction

- Motivation for using Quantum models
- Overview of Atlas Quantum features
- Discussion of Quantum models
Motivation

- Reduction in device size -> coherence length of electrons
- Thin gate oxides -> Capacitor-Voltage shift, Cox, Vt
- Carrier distribution near interfaces and delta doping not accurately described by classical models
- Tunneling in heterojunctions and Schottky junctions
• Many technologies have developed with noticeable quantum effects
• MOS - electron distribution near thin gate oxides
• HEMT, HBT, heterojunction barrier diode etc.
• SOI structure with silicon films of few nm
• Quantum Well lasers, VCSELs, LEDs and photodetectors
• Five separate Quantum Models
  • 1 - Self-Consistent Schrodinger-Poisson Model
  • 2 - Quantum Moments Model
  • 3 - Bohm Quantum Potential
  • 4 - Hansch Quantum Correction Model
  • 5 - Van Dort Quantum Correction Model

• Three Thermionic Emission and Tunneling models
  • 1 - Heterojunction
  • 2 - Schottky contact
  • 3 - Direct gate oxide tunneling

• Quantum Well light emission models
Self-Consistent Schrodinger-Poisson Model

- One dimensional Schrodinger equation solved along y mesh
- Alternating Schrodinger and Poisson equations solved, i.e. decoupled but self-consistent
- Eigen-energies and eigenfunctions solved
- Fermi-Dirac statistics used
Self-Consistent Schrodinger-Poisson Model

- syntax:
  
  ```
  MODEL SCHRO
  OUTPUT EIGEN=N       // N is an integer
  METHOD CARRIERS=0    // no carrier continuity
  ```
Overview of Atlas Quantum Features

Self-Consistent Schrödinger-Poisson Model

Nn Isotype GaAs–AlGaAs Heterojunction
First Three Eigen-Energies

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Overview of Atlas Quantum Features
• Alternately, can solve non-self-consistent solution to include carrier continuity equations
• User control of quasi-Fermi level calculation
• Syntax:
  MODEL SCHRO POST.SCHRO ^FIXED.FERMI CALC.FERMI //
  Boolean parameters
  METHOD CARRIERS=2 // include carrier continuity
• Depending on the application, device and bias range, some combinations of FIXED.FERMI and CALC.FERMI may give unphysical results. Recommendation is to use FIXED.FERMI and CALC.FERMI both TRUE.
# Definition of Quasi-Fermi Parameters with Schrodinger / Poisson

## Table 1. Interpretations for post-processed Schrodinger solution.

<table>
<thead>
<tr>
<th>FIXED.FERMI</th>
<th>CALC.FERMI</th>
<th>Quasi-Fermi level Calculation method</th>
</tr>
</thead>
<tbody>
<tr>
<td>FALSE</td>
<td>FALSE</td>
<td>Quasi-Fermi level is calculated from the local electron density via drift-diffusion model</td>
</tr>
<tr>
<td>FALSE</td>
<td>TRUE</td>
<td>Quasi-Fermi level varies with Y position and is calculated to match the local classical and quantum mechanical charge concentration</td>
</tr>
<tr>
<td>TRUE</td>
<td>FALSE</td>
<td>Quasi-Fermi level is uniformly zero</td>
</tr>
<tr>
<td>TRUE</td>
<td>TRUE</td>
<td>Quasi-Fermi level is uniform across Y slice and is calculated to match the classical and quantum mechanical sheet charge.</td>
</tr>
</tbody>
</table>

(Table 3-53 of Atlas manual - clarification)
• Based on Wigner function equations of motion
• Used with 1 or 2 carrier solutions to obtain currents
• Quantum correction to the carrier statistics in current and energy flux equations
• Affects calculated values of carrier concentration near Si/SiO2 interfaces in MOS and heterointerfaces in HEMTs.
• Syntax:
  MODEL QUANTUM H . QUANTUM
  //electrons and holes, respectively
• Damping factor for convergence and tuning, QFACTOR, ramp to unity
• Quantum moments model also available in 3D
Quantum Moments Model

Comparison of Classical and Quantum Moments Model
Electron Concentration with Depth, Zero Bias

Overview Of Atlas Quantum Features
Quantum Moments Model

Comparison of Classical and Quantum Moments Model
Drain Current as a function of Drain Bias
Quantum Moments Model
Bohm Quantum Potential (BQP)

• 1 and 2 carrier solutions
• Syntax:
  Model BQP.N BQP.P
• Works with hydrodynamic energy balance models
• 3D
• Better convergence than Quantum Moments Model
• Better calibrated to Schrodinger-Poisson
BQP Calibration to Schrodinger-Poisson

QUANTUM Examples
BQP Calibration for NMOS Capacitor

- Gate Quasi-Static C-V (F/A/uM)

- Schrodinger-Poisson
- Parameter guess 1
- Parameter guess 2
- Calibrated Parameters

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BQP Comparison with Classical

Quasi-static C-V curves for an NMOS Capacitor
BQP vs. Semi-Classical

Accumulation
Depo
tion
Inversion

BQP
Semi-classical
Gate Quasi-Static C-V (F(Am))

Gate Voltage (V)

-3 -2 -1 0 1 2 3

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Quantum Effects in Optical Models

- Schrödinger solutions for bound state energies
- Bound state energies used in gain, spontaneous recombination and absorption models to predict allowed transitions
Quantum Well Optical Emission Models

Overview Of Atlas Quantum Features
3D Heterostructure Simulation

GaAs-AlGaAs HEMT with 'polysilicon' T-gate
Structure Created using DevEdit3D
• Calculates confinement near gate oxide in MOSFET
• Correction factor modifies density of states
• Syntax: MODEL HANSCH

• Intended for quantum confinement near Si/SiO2 interfaces
• Confinement modeled by broadening of the bandgap near interface
• Syntax: `MODEL N.DORT`

Some Quantum Effects are included as physical models in Blaze:

- Thermionic-field emission boundary condition based on the WKB approximation
- Thermionic emission and thermionic-field emission (tunneling) across heterointerfaces
- Isotype and p-n junctions
- Uniform and graded composition fraction
- Syntax: `INTERFACE THERMIIONIC X.MIN X.MAN Y.MIN Y.MAX` // for thermionic emission model
- Syntax: `INTERFACE THERMIIONIC TUNNEL X.MIN X.MAN Y.MIN Y.MAX` // for both thermionic emission and tunneling
- Syntax: `INTERFACE` statement directly after MESH, REGION and ELECTRODE statements, and before statements MODEL and MATERIAL

Thermionic Emission and Tunneling models I: Heterojunction

Calculated Conduction Band Profiles
n GaAs / N AlGaAs diode, Bias of -0.1 V

Conduction Band Energy (V)

ND = 1e15
ND = 1e16
ND = 5e16

GaAs  AlGaAs

0  0.1  0.2  0.3  0.4  0.5  0.6  0.7  0.8  0.9  1
0  0.1  0.2  0.3  0.4  0.5  0.6  0.7  0.8  0.9  1

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Thermionic Emission and Tunneling models I: Heterojunction

Calculated I–V characteristics for Two N-type Dopings
Tunnel and Thermionic Emission Currents

- Anode Current (A)

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Thermionic Emission and Tunneling Models II: Schottky Contact

- Atlas: Blaze
- Metal - semiconductor junction
- Models tunneling and thermionic emission at Schottky contacts
- Surface recombination enabled
- Syntax: CONTACTS E.TUNNEL
• Quantum models required for thin material layers (gate oxides, HEMTs, etc.)

• Atlas provides variety of quantum models
  • Schrodinger-Poisson - solver for eigenstates
  • Quantum Moments gives carrier concentration and current
  • Specialized MOS correction models

• Some tunneling/emission effects modeled through separate models in Blaze