Modeling Quantum and Coulomb Effects in Nanoscale Devices

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Ph.D. Dissertation Defense

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Talk Outline

- Abstract and the Simulated Devices
- Models Developed and Used
  1. Transport: MC Device Simulator and The Event-Biasing Techniques
  2. Quantum Effects: The Effective potentials
  3. Coulomb Effects: The MD Routines
- Device Simulation Results
- Conclusions …
Nanostructures Research Group

Major Journal Publications

Nanostructures Research Group

Models Developed and Used

- **Short-Range Interactions and Discrete/Unintentional Dopants**
  - Corrected Coulomb Approach
  - P^3M Algorithm
  - Fast Multipole Method (FMM)

- **Quantum Mechanical Size-quantization Effects**
  - Ferry’s Effective Potential Method
  - Quantum Field Approach

- **Long-range Interactions (3D Poisson Equation Solver)**

- **Boltzmann Transport Equations**
  - Particle-Based Monte Carlo Transport Kernel

- **Statistical Enhancement:**
  - Event Biasing Scheme

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Simulated Device Structures

A. Quantum Mechanical Narrow Channel Effect
B. Coulomb Effects


Quantum Effects: Quantum Field Approach

Statistical Enhancement: Event Biasing Scheme
In principle, the effective role of the potential can be written in terms of the non-local density as:

\[
\bar{V} = \int dr V(r) \sum_i n_i(r)
\]

\[
\sim \int dr V(r) \sum_i \int dr' \exp \left( -\frac{|r - r'|^2}{\alpha^2} \right) \delta(r' - r_i)
\]

\[
\sim \sum_i \int dr \delta(r - r_i) \int dr' V(r') \exp \left( -\frac{|r - r'|^2}{\alpha^2} \right)
\]

\[
\sim \sum_i \int dr \delta(r - r_i) V_{\text{eff}}(r)
\]

where the summation over \(i\) is a summation over the carriers themselves. The finite size of the electron has been replaced by smoothing of the real potential.

In three dimensions:

\[
V_{\text{eff}}(x, y, z) = \frac{1}{(2\pi)^{3/2} a_x a_y a_z} \iiint V(x', y', z') \exp \left( -\frac{(x-x')^2}{2a_x^2} - \frac{(y-y')^2}{2a_y^2} - \frac{(z-z')^2}{2a_z^2} \right) dx' dy' dz'
\]

(QM2) Quantum Field Approach

Classical:

\[ f_{eq}^{\text{class}}(x, p) = \exp \left( -\frac{\beta |p|^2}{2m^*} - e\beta V(x) \right) \]

Quantum Mechanical:

(a) \[ f_{eq}^{\text{quant}}(x, p) = (2\pi)^{-3} \int_{\mathbb{R}^3} \rho^{eq}(x + \frac{\hbar}{2} \eta, x - \frac{\hbar}{2} \eta) \exp(i\eta \cdot p) d\eta, \]

(b) \[ \rho^{eq}(x, y) = \exp(-\beta H) = \sum_\lambda F(\beta\lambda) \psi^{eq}_\lambda(x)^* \psi^{eq}_\lambda(y), \]

(c) \[ \left( -\frac{\hbar^2}{2m^*} \Delta + V \right) \psi^{eq}_\lambda = \lambda \psi^{eq}_\lambda. \]


\[ \exp \left( -\frac{\beta |p|^2}{2m^*} - e\beta V^Q(x, p, \beta) \right) = (2\pi)^{-3} \int_{\mathbb{R}^3} \rho^{eq}(x + \frac{\hbar}{2} \eta, x - \frac{\hbar}{2} \eta) \exp(i\eta \cdot p) d\eta \]

\[ V^Q(x, p, \beta) = \int \exp \left[ -\beta \frac{\hbar^2 |\xi|^2}{8m^*} \right] \frac{2m^* \sinh \left[ \frac{\beta \hbar p \cdot \xi}{2m^*} \right]}{\beta \hbar p \cdot \xi} \hat{V}(\xi) e^{i\xi \cdot x} d\xi \]

\[ \hat{V}(\xi) = (2\pi)^{-d} \int V(y) e^{-iy \cdot \xi} dy \]

\[ V^Q(s, p, \beta) = V^Q_B(x, p, \beta) + V^Q_H(x, y, p, \beta) \]

\[ e \nabla V^Q_B(x, p, \beta) = \frac{B}{2\pi} (1, 0, 0)^T \int \exp \left[ -\beta \frac{\hbar^2 |\xi|^2}{8m^*} \right] \frac{2m^* \sinh \left[ \frac{\beta \hbar p_y \cdot \xi_y}{2m^*} \right]}{\beta \hbar p_y \cdot \xi_y} e^{i\xi_y \cdot y} d\xi_y \]
(QM2) Quantum Field Approach

LOW-ENERGY ELECTRONS

HIGH-ENERGY ELECTRONS
Model Verification: MOS capacitor

\[ N_A = 10^{18} \text{ cm}^{-3} \]
\[ T_{ox} = 1.5 \text{ nm} \]

Adjusting \( a_0 \) or the form/shape of the wave packet can improve the situation.
Basic idea:

Short-range force is calculated directly from first principles by the implementation of a MD routine and then combined with the Long-range forces found from the mesh.

To avoid double counting:

The corrected Coulomb force is obtained by pre-computing the mesh force from a single ion and then subtracting it from the Coulomb force. This corrected force is then added to the actual mesh force obtained during the real simulation to get the total force.

\[
F_{i \text{Coul}} = \sum_{j=1}^{\text{Nelec}} \frac{q_i^2 \cdot a_{ij}}{4\pi\varepsilon r_i - r_j^2} + \sum_{k=1}^{\text{Nion}} \frac{q_i q_k \cdot a_{ik}}{4\pi\varepsilon r_i - r_k^2}
\]

\[
F_{i \text{corr}} = F_{i \text{Coul}} - F_{i \text{mesh}} \quad \text{(Precomputed)}
\]

\[
F_{i \text{total}} = F_{i \text{corr}} + F_{i \text{mesh}}
\]

(MD2) The P³M Approach

\[ F_{ij}^{corr} = F_{ij}^{Coul} - R_{ij} \]

- Reference force replaces the mesh force and needed to avoid double counting of the short-range force. The reference force should be equal to the mesh force inside the SR domain and equal to the Coulomb force outside the short-range domain.

- Smoothing of the total interparticle force between the long- and short-range domains can be thought of as ascribing a finite size to particle \( i \). A sphere with uniformly decreasing density profile, \( S(r) \) is a good choice for smoothing in three dimensions.

\[
S(r) = \begin{cases} 
48 \frac{r_{sr}}{\pi r_{sr}^4} \left( \frac{r_{sr}}{2} - r \right), & r \leq r_{sr} / 2 \\
0, & \text{otherwise}
\end{cases}
\]

\[
R_y(r) = \begin{cases} 
\frac{q_i q_j}{4\pi \epsilon} \times \frac{1}{35 r_{sr}^2} (224\xi - 224\xi^3 + 70\xi^4 + 48\xi^5 - 21\xi^6), & 0 \leq r \leq r_{sr} / 2 \\
\frac{12}{\xi^2} - 224 + 896\xi - 840\xi^2 + 224\xi^3 + 70\xi^4 - 48\xi^5 + 7\xi^6, & r_{sr} / 2 \leq r \leq r_{sr} \\
\frac{q_i q_j}{4\pi \epsilon} \times \frac{1}{r^2}, & r > r_{sr}
\end{cases}
\]

\[
\xi = \frac{2r}{r_{sr}} \quad \text{and} \quad 0 \leq r \leq r_{sr} / 2
\]

Central Strategy of the FMM: How does the FMM speed up the computation?

\[
\Phi(x) = \sum_{i=1}^{N} \frac{q_i}{|x - y_i|}
\]

\[
= \sum_{i=1}^{N} q_i \sum_{k=1}^{p} \psi_k(y_i) \phi_k(x)
\]

\[
= \sum_{k=1}^{p} \phi_k(x) \sum_{i=1}^{N} q_i \psi_k(y_i)
\]

\[
= \sum_{k=1}^{p} \phi_k(x) A_k
\]

\[O(N \times N) \rightarrow O(N \times p)\]


In FMM one uses *multipole moments* to represent distant particle groups and introduces a *local expansion* to evaluate the contribution from distant particles in the form of a series. The multipole moment associated with a distant group can be translated into the coefficient of the local expansion associated with a local group. Interactions with particles which are nearby are handled directly.
The FMM

Uniform mesh (40 x 25 x 25)

An external field of 1kV/cm was applied to ensure linear region of operation.

The drift velocity was averaged over 5ps with an interval time of 0.1 ps. The first 1.5 ps data were discarded.

<table>
<thead>
<tr>
<th>Method</th>
<th>Time/iteration</th>
</tr>
</thead>
<tbody>
<tr>
<td>P³M</td>
<td>39 sec</td>
</tr>
<tr>
<td>FMM</td>
<td>17 sec</td>
</tr>
</tbody>
</table>

No. of monopole charges: ~22000
Mesh: 40 x 25 x 25
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Results for the SOI device

A. Quantum Mechanical Narrow Channel Effect
B. Coulomb Effects

Results for the SOI device

Size Quantization Effect:

- Experimental
- Simulation

Channel Width [nm] vs. Threshold Voltage [V]
Results for the SOI device

Unintentional Dopant: How It Affects the Total Picture

Due to the unintentional dopant both the electrostatics and the transport are affected.

Dip due to the presence of the impurity. This affects the transport of the carriers.
Results for the SOI device

Unintentional Dopant:

Impurity located at the very source-end, due to the availability of increasing number of electrons screening the impurity ion, has reduced impact on the overall drain current.

Impurity position varying along the center of the channel

$V_G = 1.0\ \text{V}$

$V_D = 0.2\ \text{V}$

Source end

Drain end

Impurity located at the very source-end, due to the availability of increasing number of electrons screening the impurity ion, has reduced impact on the overall drain current.
Results for the SOI device

Unintentional Dopant:

Results for the SOI device

Electron-Electron Interactions:

- Electron Velocity vs. Distance Along the Channel [nm]
  - PM
  - FMM
  - $V_G = 1.0 \text{ V}$
  - $V_D = 0.3 \text{ V}$

- Distribution Function vs. Electron Kinetic Energy [eV]
  - PM
  - FMM
  - $V_G = 1.0 \text{ V}$
  - $V_D = 0.3 \text{ V}$
More Results on Quantum Effects

Diagram:

- $N^+$
- $N^+$
- $p$-Substrate
- Source
- Drain
- Si Channel
- Front Gate
- Back Gate
- BOX
- Substrate
- $L_{G}$
- $L_{sd}$
- $T_{si}$
- $L_{T}$
More Results on Quantum Effects

Electron Distribution:

Without Quantization

Charge Set-Back With Quantization (New Approach)

Vg = Vd = 1.0 V
More Results on Quantum Effects

Transfer and Output Characteristics:

More Results on Quantum Effects

15 nm MOSFET: Sheet Density

\[ V_G = V_D = 0.8 \, \text{V} \]
More Results on Quantum Effects

Average Carrier Distance:

Distance Along the Channel [nm]

% Change in Distance

Classical (1.5x)  QM (1.5x)  Classical (2x)  QM (2x)  % Change (1.5x)  % Change (2x)
More Results on Quantum Effects

Electron Velocity:

- Classical (1.5x)
- QM (1.5x)
- Classical (2x)
- QM (2x)
More Results on Quantum Effects

Transfer and Output Characteristics:

- Drain Current [uA/um]
- Drain Voltage [V]

Graph showing various curves for different models and experimental results, with labels indicating

- W/o quant. (1.5x)
- Barrier (1.5x)
- Barrier+Hartree (1.5x)
- SILVACO (1.5x)
- Experimental
- W/o quant. (2x)
- Barrier (2x)
- Barrier+Hartree (2x)
- % Reduction (1.5x)
- % Reduction (2x)

Legend:

- $V_G = 0.8$ V
More Results on Quantum Effects

Importance of Hartree Corrections:

- $T_{OX} = 0.8\text{nm}$
- $N_{SUB} = 1.0 \times 10^{18}\text{cm}^{-3}$
- $V_G = V_D = 0.8\text{ V}$
- $L_G = 15\text{ nm}$

![Graph showing % change in current vs. channel doping density.](image-url)
More Results on Quantum Effects

SG SOI: Variation of Threshold Voltage with $T_{SOI}$:

More Results on Quantum Effects

DG SOI Device:

![Diagram of DG SOI Device]

- $T_{ox} = 1 \text{ nm}$
- $L_G = 9 \text{ nm}$
- $L_{sd} = 10 \text{ nm}$
- $N_b = 0$
- $\Phi_G = 4.188$
- $T_{si} = 3 \text{ nm}$
- $L_T = 17 \text{ nm}$
- $N_{sd} = 2 \times 10^{20} \text{ cm}^{-3}$
- $g = 1 \text{ nm/decade}$
- $V_G = 0.4 \text{ V}$

% Change in Current

- W/o quant. (3nm)
- QM (3nm)
- NEGF (3nm)
- W/o quant. (1nm)
- QM (1nm)

- 3 nm
- 1 nm

Drain Current [uA/um]

Drain Voltage [V]
Event-Biasing Experiments

Aims at reduction of the computation time: faster convergence of the stochastic process. Especially useful when the transport is governed by rare events.

Statistical enhancement

Population control techniques
Based on the heuristic idea for splitting of the particles entering a given phase space region $\Omega$ of interest

Event-biasing approach
Guiding the particles towards $\Omega$ by biasing the probabilities associated with the transport of classical carriers

Random variable $\Psi$ takes values $\Psi(Q)$ with probability density $p_\Psi(Q)$: $E_\Psi = \int dQ p_\Psi(Q) \psi(Q)$

$N$ realizations of $p_\Psi(Q)$ generates $Q_1, \ldots, Q_N$ sampling points.

Expectation value (MC): $E_\Psi = \frac{1}{N} \sum_{i=1}^{N} \psi(Q_i)$

$$\langle A \rangle = \sum_i \langle A \rangle_i$$

$$\langle A \rangle_2 = \int dQ' dQ_1 dQ_2 P_0(Q') P(Q', Q_1) P(Q_1, Q_2) \frac{f_0(Q')}{P_0(Q')} \frac{K(Q', Q_1)}{P(Q', Q_1)} \frac{K(Q_1, Q_2)}{P(Q_1, Q_2)} A(Q_2)$$

Realization of $N$ trajectories $(Q' \rightarrow Q_1 \rightarrow Q_2)_n, n = 1 \ldots N$ estimates the mean value $\langle A \rangle_2$

Event-Biasing Experiments

1. \( T_b = \text{Bias} \times T \)

Equilibrium distribution: 
\[
f_{eq}(\varepsilon, T) = \frac{1}{\varepsilon} e^{-\frac{\varepsilon}{\varepsilon}}
\]

\( \varepsilon = 1.5k_B T \)

Choose biased distribution: 
\[
f_0^b(\varepsilon, T_b) = \frac{1}{\varepsilon_b} e^{-\frac{\varepsilon}{\varepsilon_b}}
\]

Corresponds to a higher temperature \( T_b = \text{bias} \times T \)
\[
\varepsilon_b = \text{bias} \times 1.5k_B T
\]

Having higher kinetic energy, the numerical particles readily overcome the source potential barrier and enrich the statistics in the channel.

Weight, \( W = \text{bias} \times \frac{\exp\left(-\frac{\varepsilon}{\varepsilon}\right)}{\exp\left(-\frac{\varepsilon}{\varepsilon_b}\right)} \)
Event-Biasing Experiments

Weight distribution:

\[ T = 450K \]
\[ N \sim 100000 \]

Enhancing Channel Statistics:

Particle number increases in the channel and decreases in the source/drain with biasing.

Average Electron Number

Source

Drain

Distance Along the Channel [nm]

Distance [nm]

Distance [nm]
Event-Biasing Experiments

2. Particle Split

Weight control by choosing a desired weight \( w_1 \) of the numerical particles with kinetic energy below given level \( \varepsilon_1 \) and weight \( w_2 \) with kinetic energy above \( \varepsilon_1 \).

\( f^b \) is obtained from \( f_{eq} \) as follows:

\[
f^b_0(\varepsilon) = \frac{f_{eq}(\varepsilon)}{w_1}, \quad \varepsilon \leq \varepsilon_1
\]

\[
f^b_0(\varepsilon) = \frac{f_{eq}(\varepsilon)}{w_2}, \quad \varepsilon > \varepsilon_1
\]

\( w_2 \) is obtained as a function of \( w_1 \) and \( \varepsilon_1 \) from the condition for normalization of \( f^b \):

\[
w_2 = \frac{w_1 \cdot e^{-\frac{\varepsilon}{\varepsilon_1}}}{w_1 - 1 + e^{-\frac{\varepsilon}{\varepsilon_1}}}
\]

A choice of \( w_1 > 1 \) effectively reduces the number of particles below \( \varepsilon_1 \) as compared to the unbiased case.
3. Biasing the Scattering Event (e-a)

Artificial carrier heating can be achieved by biasing the phonon scattering rates.

For a given scattering mechanism, the probability for phonon absorption is increased at the expense of phonon emission, controlled by a parameter $w_1$,

$$\lambda_{e,m}^b = \frac{\lambda_{e,m}}{w}, \quad w > 1$$

$$\lambda_{a,b}^b = \lambda_{a,b} + \left( \frac{\lambda_{e,m} - \lambda_{e,m}}{w} \right)$$

If in the course of the simulation a phonon absorption is selected, the particle weight is updated by a multiplication with $\lambda_{a,b} / \lambda_{a,b}^b$, otherwise with $\lambda_{e,m} / \lambda_{e,m}^b$.

The distribution of the flight time is not affected, because the sum of emission and absorption rate is not changed.
Event-Biasing Experiments

Sheet Electron Density:

Average Electron Energy:

Sheet Density [cm$^{-2}$]

Distance Along the Channel [nm]

Average Energy [eV]

Distance Along the Channel [nm]
Event-Biasing Experiments

Enhancement of Statistics: Reducing Standard Deviation

Conventional

\[ T = 450K \]

Split

bias e-a

\[ \text{STD} = 1.402 \]

\[ \text{STD} = 1.15 \]

\[ \text{STD} = 1.26 \]

\[ \text{STD} = 1.37 \]
Event-Biasing Experiments

Faster Convergence: Channel Current Evolution

Current Density [µA/µm]

- PARTICLES 100000 CURRENT FROM CHANNEL VELOCITY
- conventional EMC
- bias T = 450

- PARTICLES 100000 CURRENT FROM CHANNEL VELOCITY
- conventional EMC
- bias e-a
Event-Biasing Experiments

Faster Convergence: Contact Current Evolution

Current Density [µA/µm]

Particle: 100000
Current from S/D Particles

- Conventional EMC
- Bias T = 450K
- Split

Particle: 100000
Current from S/D Particles

- Conventional EMC
- Bias e-a
- Bias e-a/split
Conclusion

- The experimentally observed *quantum mechanical narrow-channel effect* in a FD SOI device structure has been successfully accounted for by the effective potential approach.

- Three different MD approaches have applied in the investigations of the role of unintentional doping on the operation of narrow-width SOI devices. We find significant correlation between the location of the impurity atom and the magnitude of the drain current. Impurities near the source end of the channel have maximum influence on the drain current. We have also investigated in depth the fluctuations in the threshold voltage due to discrete distribution of the impurity atoms.

- A novel *parameter-free quantum field approach* for use in conjunction with particle-based simulations has been proposed. The method is based on a perturbation theory around thermodynamic equilibrium and leads to a quantum field formalism in which the size of an electron depends upon its energy. The approach when used in the simulations of a conventional nanoscale *n*-channel MOSFET devices and novel nanoscale DG SOI devices is found to produce correct experimental/theoretical trend. *In some cases, faster simulation can be achieved with the incorporation of only the barrier field that is pre-computed in the initial stages of the simulation and does not require additional CPU time.*

- It is found that *event-biasing* experiments recover precisely the physical averages and the self-consistent field and reduces the time necessary for computation of the desired device characteristics.
Questions or Comments?