Development of Efficient Inelastic Scattering in Atomistic Tight Binding

Master’s Defense

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1. Motivation
2. Acoustic and Optical Phonon Scattering Verification
3. Effect of scattering on MOSFETs
4. Effect of scattering on TFETs
5. Why does scattering increase tunneling current?
6. Numerical Details
7. Conclusions/Future Work
Overview

1) Motivation
2) Acoustic and Optical Phonon Scattering Verification
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7) Conclusions/Future Work
Length Downscaling

Length Scaling:
1) Area ↗ transistor density ↘
2) Capacitance ↗ Delay ↗

Gate Delay $\propto C_{gate} V_{DD}/I_{sat}$

http://www-inst.eecs.berkeley.edu/~ee40/fa03

Length continues to scale smoothly
Voltage Downscaling

Why has voltage scaling saturated around 2000?

Gate Delay $\propto C_{gate}V_{DD}/I_{sat}$

$I_{sat}$ decreases, larger delay

Decrease $V_d, V_t$

Keep off-current constant

Voltage Scaling:
 ✓ Static Power $\propto V_{DD}I_{off}$
 ✓ Dynamic Power $\propto V_{DD}^2$

Voltage scaling has saturated
Importance of Scattering

“that the **reduction [compared to ballistic]** of the device drain current, ...is more important in the ON-state than in the OFF-state of the transistor”


Data from A. Esposito, M. Frey, et. al. JCEL vol. 8 (2009).

![Graph 1](image1)

3 nm circular silicon nanowire, $V_{ds} = 0.6V$

sp$^3$d$^5$s$^*$ tight binding basis

confined phonon model

![Graph 2](image2)

3.2 nm square silicon nanowire, $V_{ds} = 0.5V$

non-parabolic effective mass basis

bulk phonon model

Conflicting trends for subthreshold current in literature. How to resolve this?
Critical Questions:
1) How to increase electrostatic gate control?
2) What is the limit of gate length scaling?
3) How to continue supply voltage scaling?
4) What is the importance of scattering in gate length and supply voltage scaling?
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Capacitance by Oxide Thickness Scaling

_capacitance ✓ oxide thickness

IEEE TRANSACTIONS ON ELECTRON DEVICES, VOL. 50, NO. 4, APRIL 2003
Geometry Trend

increased electrostatic control

Nanowires candidate for best electrostatic control

ESSDERC 2012

Bulk

SOI

IEEE Spectrum

Nanowire increased drive current and reduced delay

Experimental evidence of nearly perfect S.S achieved for nanowires

“delivering more than 30% and 40% reduced SS over FinFETs and planar MOSFETS”

nanowires have excellent gate control
Critical Questions:

1) How to increase electrostatic gate control?
2) What is the limit of gate length scaling?
3) How to continue supply voltage scaling?
4) What is the importance of scattering in gate length and supply voltage scaling?
ITRS demands scaling of gate length

J. Wang, M. Lundstrom, IEDM 2002: “The results show that source-to-drain tunneling does set an ultimate scaling limit

Bandgap engineering shown to decrease tunneling leakage.

Phonon

(1) Thermionic
(2) Thermally assisted source-to-drain tunneling
(3) Direct source-to-drain tunneling

Need to include scattering to account for thermally assisted source-to-drain tunneling.
Critical Questions:

1) How to increase electrostatic gate control?
2) What is the limit of gate length scaling?
3) How to continue supply voltage scaling?
4) What is the importance of scattering in gate length and supply voltage scaling?
Supply Voltage Scaling

Note: prediction of EOT depends on scaled voltage (dictated by ITRS)

Reality:
Since ~2000, supply voltage is no longer scaling. Why?

Decrease $V_d$

Off-current increases
Typical MOSFETs: Barrier controlled device

- Sub-threshold slope: fundamental limit of how fast the device can turn on
- This is limited by the Fermi band-tail

\[
S.S = \ln(10) \frac{kT}{q} \left(1 + \frac{C_{ch}}{C_{ox}}\right)
\]

\[
\text{min}(S.S) = 60 \text{ mV/dec}
\]

How can we overcome this limit?
The Need for Tunneling Dominated Transistors

Spectral current for InAs TFET

High energy filtering

Fermi tail suppressed

$V_g = 0V$

Current magnitude related to tunneling probability

tunneling

unwanted ambipolar

transport direction

p++

n--

n++
Gate-all-around (GAA) nanowire TFET

1. Excellent Gate Control
   $I_{on}$ increases with steeper source to channel transition
   (decreased tunneling distance $\lambda_{tunn}$.)

2. Best subthreshold-slope compared to MOSFET

What is the importance of scattering in TFETs?
Critical Questions:

1) How to increase electrostatic gate control?
2) What is the limit of gate length scaling?
3) How to continue supply voltage scaling?
4) What is the importance of scattering in gate length and supply voltage scaling?
Method:
Non-equilibrium Green’s Function (NEGF) + scattering in the Self-consistent Born Approximation (SCBA)

Atomistic Resolution with Semi-empirical tight binding


Schematic of Gate All Around (GAA) Nanowire
What is a scattering self-energy?
• Contribution to particle’s energy due to interaction with the system.
• Complex matrix
  Real Part $\Sigma^R \sim \Delta E$
  Imaginary Part $\Sigma^R \sim$ related to lifetime of particle.

What is self-consistent Born?
• Interactions treated as (weak) perturbations
• Leads to self-consistent loop to stabilize charge/current

Why include scattering?
Three Major Effects from scattering:
- Resistive (decreases on-current)
- Increases tunneling current
- Broadens/fills resonant states

Tunneling mechanisms for TFET:
(0) Direct, coherent tunneling
(1) Thermally excited carriers tunneling
(2) Tunneling via channel band-tails

Khayer, JAP 110, 074508 (2011).
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• With bulk phonons, the perturbing potential (electron-phonon interaction strength) is solved analytically

• Assume:
  o linear dispersion
  o bulk phonons in equilibrium
  o elastic
  o high temperature

Scattering Parameters:
• ion mass density
• sound velocity
• deformation potential

http://exafs.ucsc.edu/simulations
• With bulk phonons, the perturbing potential (electron-phonon interaction strength) is solved analytically.

• Assume:
  o flat dispersion
  o bulk phonons in equilibrium
  o inelastic

Optical phonon

Scattering Parameters:
• ion mass density
• phonon frequency
• optical deformation constant

http://exafs.ucsc.edu/simulations
Both can be verified against analytical expressions for scattering rate

\[ \Gamma_{N E G F}(E) = -\frac{2}{\hbar} \text{Im}\{\Sigma_{\text{scatt}}^R(E)\} \]

**Acoustic**

\[ \Gamma_{F G R} = \frac{\sqrt{2}m^*2D_{ac}^2k_BT}{\pi\hbar\rho v_s^2}\sqrt{E} \]

**Optical**

\[ \Gamma_{F G R} = \frac{m^*3D_{op}^2}{\sqrt{2\pi\hbar^2\rho E_0}} \left\{ \frac{n_0(E+E_0)^{1/2}}{2} + [n_0 + 1] \right\} \times (E - E_0)^{1/2} \times \theta(E - E_0) \]

### Bulk GaAs Material Parameters:
- Deformation potential \( D_{ac} = 8.8 \)
- Sound velocity \( v_s = 4726 \text{ m/s} \)
- Material density \( \rho = 5317 \text{ kg/m}^3 \)
- Phonon energy \( E_0 = 35 \text{ meV} \)
- Optical Coupling constant \( D_{op} = 110 \text{ eV/nm} \)
Device: homogeneous silicon bar in effective mass

Steps:
1. Calculate current of different lengths with small applied potential (5 meV)
2. Calculate slope of resistance vs. length

Matches well for phonon-limited range

Deviation due to neglect of electron-electron and impurity scattering

Experimental data from NIST
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Effect of scattering on MOSFETs

Si, 2nm cross section sp$^3$d$^5$s$^*$

NIN nanowire elastic acoustic + optical

Scattering increases subthreshold current

Scattering decreases on-current
Varying Scattering Strength

Si, 2nm cross section sp$^3$d$^5$s$^*$
NIN nanowire elastic acoustic

$$\lambda = \frac{k_B T D_{ac}^2}{\hbar v_s^2 \rho} \delta_\alpha,$$

$$\lambda_{\text{bulk, Si}} \approx 0.1 \text{ eV}^2$$
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Question: What is the impact of scattering on TFETs?

Circular Si TFET 3nm cross section

Source, P-doped 2E20 /cm³

Drain, N-doped 1E20 /cm³

1nm thick oxide covers entire device (not shown)

$V_{ds} = 1.0V$

Deformation potential phonons included:
Elastic acoustic and inelastic optical phonon self-energies
Silicon TFET with scattering

**Impact of incoherent scattering:**
- Increase and shift of band tails
- Increase of tunneling current by ~4x

**Realistic TFET performance prediction questionable without scattering**

**TFET IV characteristics**

$I_{on, scatt} = 0.46 \, nA$
$I_{on, ball.} = 0.10 \, nA$
$SS_{scatt} = 114 \, mV/dec$
$SS_{ball.} = 130 \, mV/dec$

**Density of states along cut**

Scattering lowers DOS tail below band-edge
Question:
What is the impact of scattering on a III-V resonant TFET?

Dominant scattering in III-Vs is polar optical phonon (POP) scattering

Assumptions:
Treat POP scattering as diagonal (non-polar optical) with increased scattering strength. Why? It is numerically feasible but loses nonlocality information.

TFET design by Pengyu Long, et. al. DRC (2016).
Scattering Effective on Resonance TFET

Optical phonon energy 35 meV

<table>
<thead>
<tr>
<th></th>
<th>Strength</th>
</tr>
</thead>
<tbody>
<tr>
<td>ballistic</td>
<td></td>
</tr>
<tr>
<td>Optical A</td>
<td>Optical C * 4</td>
</tr>
<tr>
<td>Optical B</td>
<td>Optical C * 1.85</td>
</tr>
<tr>
<td>Optical C</td>
<td>Si non-polar def. const.</td>
</tr>
<tr>
<td>acoustic</td>
<td>Bulk GaAs parameters</td>
</tr>
</tbody>
</table>

Simulations ran by Devin Verrick

![Graph showing I [µA/µm] vs Vgs [V] for ballistic, optical A, optical B, optical C, and acoustic phases with 60 mV/dec slope.]

- Increased scattering strength
- Scattering degrades subthreshold slope

Simulations ran by Devin Verrick

![Graph showing I [µA/µm] vs Vgs [V] for ballistic, optical A, optical B, optical C, and acoustic phases with 60 mV/dec slope.]

- Increased scattering strength
- Scattering degrades subthreshold slope
Inelastic scattering increases:
(1) Tunneling below band edge
(2) Penetration of resonance state into bandgap
(3) Coupling of source hole states to resonance states
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Approximation I: Neglect $Re\{\Sigma^R\}$ completely. Solve $\Sigma^>$ and $\Sigma^<$

\[ \Sigma^R \approx \frac{1}{2} (\Sigma^> - \Sigma^<) \]
then neglecting the principal value integral.

Approximation II: Keep part of $Re\{\Sigma^R\}$ by solving $\Sigma^R$ and $\Sigma^<$ then neglecting the (partial) principal value integral.

Full: Solve principal value integral

Using Approximation II is a compromise between efficiency and accuracy
Comparing Results from Literature

Maybe the difference in approximations made lead to conflicting trends?


Data from A. Esposito, M. Frey, et. al. JCEL vol. 8 (2009).

3 nm circular silicon nanowire, $V_{ds} = 0.6V$
sp$^3$d$^5$s$^*$ tight binding basis confined phonon model

3.2 nm square silicon nanowire, $V_{ds} = 0.5V$
non-parabolic effective mass basis bulk phonon model

subthreshold current

subthreshold current
Comparing Approximation I and II for MOSFETs

Si, 2nm cross section $sp^3d^5s^*$
NIN nanowire

Relative Error $\frac{(I_{\text{scatt}} - I_{\text{ball}})}{I_{\text{ball}}}$

Neglecting $\text{Re}\{\Sigma^R\}$ (Approximation I) underestimates subthreshold current
$V_{gs} = 0.2 \text{V}, \ V_{ds} = 0.8 \text{V}$

1D conduction band edge through center of device

DOS lowered beneath band edge

$\frac{3}{4}$ Peak – Full Maximum
Ballistic 38 meV
With $Re\{\Sigma^R\}$ 50 meV
Without $Re\{\Sigma^R\}$ 45 meV
Comparing Approximation I and II for Si TFET

Si, 3nm diameter sp$^3$d$^5$s$^*$

PIN nanowire TFET

Source, P-doped 2E20/cm$^3$

Drain, N-doped 1E20/cm$^3$

Neglecting Re{$\Sigma^R$} underestimates current
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Scattering self-energies requires energies that can be on different MPI processes:

$$\Sigma^<(E) = \frac{\hbar}{2\rho \omega_o} \delta(x_3 - x_4) \left[ N_{op} G^<(E - E_{op}) ight.$$  

$$+ (N_{op} + 1) G^<(E + E_{op}) \right]$$

Requires communication of diagonal matrices

Note: for UTB simulations there is an additional wave-vector k integral that increases communication

Reasonable scaling despite complex communication
Other Development Work for Electron-Phonon Scattering in NEMO5

- Stabilized Recursive Green’s Function algorithm
- Improved Poisson convergence with improved Jacobian
- Interpolated scattering self-energies to decrease number of scattering iterations needed and improve current conservation
- Implemented dynamical convergence to decrease number of scattering iterations needed
- Current conservation in optical phonon scattering with inhomogeneous energy grid
- Improved resonance mesh suitable for resonant devices
**Objective:**
Efficient implementation of recursive Green’s function (RGF) algorithm suitable for scattering

**Problem:**
Initial implementation of RGF in NEMO5 following OMEN was unstable when scattering was included.

**Approach:**
- Systematic analysis of RGF equations to find source of instability.
- Remove assumptions of symmetries only valid with infinite precision
- Preserve symmetry of equations in each recursive iteration

**Results/Impact:**
Found instabilities and improved RGF algorithm to allow scattering simulations.

Before:
\[ G_{i,i}^{<} = g_{i,i}^{<} + g_{i,i}^{R} H_{i,i+1} G_{i+1,i+1}^{<} + g_{i,i}^{R} H_{i,i+1} G_{i+1,i+1}^{R} + g_{i,i}^{R} H_{i,i+1} G_{i+1,i+1}^{R} + g_{i,i}^{<} \]
\[ -(g_{i,i}^{R} H_{i,i+1} G_{i+1,i+1}^{<} + g_{i,i}^{<})^\dagger \]

After:
\[ G_{i,i}^{<} = g_{i,i}^{<} + g_{i,i}^{R} H_{i,i+1} G_{i+1,i+1}^{<} + g_{i,i}^{R} H_{i,i+1} G_{i+1,i+1}^{R} + g_{i,i}^{R} H_{i,i+1} G_{i+1,i+1}^{R} + g_{i,i}^{<} \]
\[ +(g_{i,i}^{R} H_{i,i+1} G_{i+1,i+1}^{<} + g_{i,i}^{<})^\dagger \]

Additionally: \( G_{i,i}^{<} \) is anti-symmetrized each iteration.
Objective:
Convergence of NEGF-Poisson equations with minimum number of iterations

Problem:
Ballistic Jacobian typically used in NEMO5 is not suitable for scattering

Approach:
• Balance between number of iterations needed and calculation time of Jacobian
• Found best balance is to use a mixture of ballistic Jacobian (extra NEGF solution) and approximate scattering Jacobian

Results/Impact:
Convergence achieved for previously not converging simulations.

Jacobian where $\lambda$ is a mixing parameter

$$J(\tilde{x}) = \Re \left\{ \lambda \int G_{\text{ballistic}}^{<} (\tilde{x}, E, \frac{\partial f_{S,D}}{\partial E}) dE \right\}$$

$$+ \int (1 - \lambda) G_{\text{scattered}}^{<} (\tilde{x}, E, f_{S,D}) dE$$

Si circular nanowire TFET
Interpolate Scattering Self-energy

**Objective:**
Minimum number of self-consistent Born approximation (SCBA) iterations to reach converged result

**Problem:**
Typically for current conservation, self-consistent Born needs 20-40 computationally expensive iterations

**Results/Impact:**
- Discovered that when Poisson-NEGF loop is close to convergence previously scattered results can be interpolated on to the updated energy mesh
- Reduced number of SCBA iterations by about 3

**Approach:**
- Reuse previously converged SCBA results to accelerate convergence of updated Poisson potentials

Diagram:
- Is previous scattering self-energy valid?
  - Yes: Skip ballistic RGF, Use previous scattering self-energies
  - No: Solve ballistic RGF

Interpolate self-energies on to new energy mesh $\Sigma(E_{\text{new}}) \approx \Sigma(E_{\text{old}})$.
1. Find which MPI process has $\Sigma(E_{\text{old}})$
2. Find $E_{\text{old}}$ closest to $E_{\text{new}}$
3. Communicate $\Sigma(E_{\text{old}})$ found from 1 to get $\Sigma(E_{\text{new}})$
Objective:
Minimum number of self-consistent Born approximation (SCBA) iterations to reach converged result.

Problem:
Typically for current conservation, self-consistent Born needs 20-40 computationally expensive iterations.

Results/Impact:
Reduced number of SCBA iterations by approximately half.

Approach:
- Reduce the number of SCBA iterations without making additional approximations.

Input: charge criterion (set in input deck)
Ratio = current Poisson residual / Poisson absolute tolerance

If Ratio > 5 and Ratio ≤ 10
Convergence criterion = 2 * charge criterion

Else if Ratio > 10 and Ratio ≤ 100
Convergence criterion = 5 * charge criterion
Use previous scattering self-energies

Else if Ratio > 10 and Ratio ≤ 100
Convergence criterion = 5 * charge criterion
Use previous scattering self-energies

Output:
New convergence criterion
Objective:
Current conservation criterion for converged self-consistent Born results

Problem:
For efficient simulations, an inhomogeneous energy mesh must be used but the energy mesh will not be commensurate with phonon energies, thus current conservation is not trivial.

Approach:
• Ensure detailed balance is always met and use this constraint to form constraints on interpretation of scattering self-energies

\[ \int (\Sigma^{<}(E)G^{>}(E) - G^{<}(E)\Sigma^{>}(E))dE = 0 \]

“in-scattering must balance out-scattering”

Results/Impact:
Current Conservation with general energy mesh

2nm silicon nanowire
Objective:
Convergence of NEGF-Poisson equations with minimum number of iterations

Problem:
Scattering introduces resonance shifts that must be properly resolved

Approach:
- Use device information in order to resolve resonances due to scattering
- Adapt energies to shifts in resonances

Results/Impact:
- Improved convergence of NEGF-Poisson loop.
- Resonances due to scattering are properly resolved
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Conclusions

• Efficient implementation of scattering introduced
• Verification of implementation with comparison to Fermi’s golden rule and to experimental resistivity

• Effect of certain approximations made in literature assessed
• MOSFET IV results with and without scattering

• TFET IV results with and without scattering compared
Future Work

• Further assessment of approximations made e.g. local POP, bulk phonons.
• Comparison to heuristic models e.g. Klimeck’s 1994 model “equilibrium-nonequilibrium” model
• Include other scattering mechanisms as scattering self-energies (e.g. roughness)
• Scattering model (phonons, roughness etc.) suitable for 2D materials e.g. TMDs
Thanks to:
my committee members: Professors Gerhard Klimeck, Supriyo Datta, Tillmann Kubis
Administrative Staff
My groupmates and friends

Questions?
Neglecting $Re\{\Sigma^R\}$ leads to underestimation of off-current. NEMO5 uses Approx. II

Si Nanowire in effective mass
Lc = 15 nm, D = 3.26 nm

NP – ballistic nonparabolic EM
NPSC – Nonparabolic EM + Approx II
Re{Σ^R} ≦ 0 But neglect PVI

Same trend as seen in NEMO5!

\[ \Sigma_{ac}^< (\alpha, \beta, E) = \frac{D^2 k_b T}{\rho v_s^2} \delta_{\alpha,\beta} G^< (\alpha, \beta, E) \]
Optical Phonon Scattering Self-energies

\( N_{op} \) is independent of \( q \) (flat optical phonon band)

Long wavelength limit \( q \to 0 \)

Discrete energies for emission and absorption \((E \pm E_{op})\) where \( E_{op} = \hbar \omega_o \)

\[
\Sigma^<(E) = \frac{\hbar}{2\rho \omega_o} \delta(\vec{x}_3 - \vec{x}_4) \left[ N_{op} G^<(E - E_{op}) + (N_{op} + 1) G^<(E + E_{op}) \right]
\]

\[
\Sigma^R(E) = \frac{\hbar}{2\rho \omega_o} \delta(\vec{x}_3 - \vec{x}_4) \left[ N_{op} G^R(E + E_{op}) + (N_{op} + 1) G^<(E - E_{ac}) \right.
\]
\[
+ \frac{1}{2} G^<(E - E_{ac}) - \frac{1}{2} G^<(E + E_{ac}) \right]
\]

Neglecting principal value integral

Approximations for Scattering Real/Imag. Part

Approximation I:

\[ \Sigma^R(E) = \frac{1}{2} (\Sigma^>(E) - \Sigma^<(E)) + iP \int \frac{dE'}{2\pi} \frac{(\Sigma^>(E') - \Sigma^<(E'))}{E - E'} \]

Approximation II:

\[ \Sigma^<(E) = \frac{\hbar}{2\rho\omega_o} \delta(x_3 - x_4) [N_{op}G^<(E - E_{op}) + (N_{op} + 1) G^<(E + E_{op})] \]

\[ \Sigma^R(E) = \frac{\hbar}{2\rho\omega_o} \delta(x_3 - x_4) [N_{op}G^R(E + E_{op}) + (N_{op} + 1) G^<(E - E_{ac}) \]

\[ + \frac{1}{2} G^<(E - E_{ac}) - \frac{1}{2} G^<(E + E_{ac}) \]

\[ + iP \int \frac{dE'}{2\pi} \frac{G^<(E - E')}{E' - \hbar\omega_o} - \frac{G^<(E - E')}{E' - \hbar\omega_o} \]

**"Quantum Transport in Semiconductor Nanostructures", T. Kubis PhD thesis (2009).**
<table>
<thead>
<tr>
<th>Region-Material</th>
<th>Length [nm]</th>
<th>Doping [cm$^{-3}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - AlSb</td>
<td>4.57</td>
<td>3x10$^{19}$</td>
</tr>
<tr>
<td>2 - Al$<em>{0.5}$Ga$</em>{0.5}$Sb</td>
<td>1.2</td>
<td>6x10$^{19}$</td>
</tr>
<tr>
<td>3 - GaSb</td>
<td>3.2</td>
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<td>4 - InAs</td>
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<tr>
<td>5 - AlInAsSb</td>
<td>27.1</td>
<td>1x10$^{15}$</td>
</tr>
<tr>
<td>6 - AlInAsSb</td>
<td>17.3</td>
<td>5x10$^{19}$</td>
</tr>
</tbody>
</table>
Mobility calculations

Simulations and figures by Devin Verrick

Scattering strength still too weak by ~2.