Numerical simulation of ballistic quantum transport in silicon nanowires accounting for full band effects

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Outline

- Toward silicon nanowire (SNW) transistors
- Modeling quantum-mechanical effects in SNW-FETs:
  - bulk EM approximation
  - limits of the bulk EM approximation
- Engineering approaches
  - constant EM with non parabolic corrections
  - non parabolic 1D transport
  - full band 1D transport approach
  - applications to device simulations
- Conclusions
Why new device architectures?

- The difficulty in scaling conventional MOSFETs makes it necessary to search for alternative device structures → new structural and technological solutions.

- Advanced non-classical devices like ultra-thin body fully depleted SOI and multiple-gate FETs will be needed to effectively scale the MOSFET gate length.

1. Poor electrostatics → increased $I_{\text{off}}$
2. Poor channel transport → decreased $I_{\text{on}}$
3. S/D parasitic resistance → decreased $I_{\text{on}}$
4. Gate oxide scaling → increased $J_G$
5. Gate depletion → increased EOT

enhanced drive current and acceptable control of SCEs
New device architectures

- SOI-FET
- DG-FET
- CNW-FET

M. Yang et al., IEDM 2003
J. Widiez et al., TED 2005
N. Singh et al., EDL 2006

Buried oxide

$t_{Si} = d_{si}$
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Quantum effects in NW-FETs

- **Structural-quantum confinement:**
  - Quantization effects in the direction perpendicular to the Si/SiO₂ interface ⇒ Schrödinger equation

- **Channel length reduction:**
  - Full-quantum ballistic transport ⇒ open boundary
    Schrödinger equation
Bulk EM quantum-mechanical model (1)

Schrödinger equation with **constant bulk** effective mass (EM) \((x,y\text{ confined directions}, z\text{ transport direction})\):

\[
\left\{-\frac{\hbar^2}{2} \left( \frac{1}{m_x} \frac{\partial^2}{\partial x^2} + \frac{1}{m_y} \frac{\partial^2}{\partial y^2} + \frac{1}{m_z} \frac{\partial^2}{\partial z^2} \right) + U(x, y, z) \right\} \psi(x, y, z) = E \psi(x, y, z)
\]

Quasi-separable potential approximation:

\[
\left\{-\frac{\hbar^2}{2} \left( \frac{1}{m_x} \frac{\partial^2}{\partial x^2} + \frac{1}{m_y} \frac{\partial^2}{\partial y^2} \right) + U(x, y, z) \right\} \chi_n(x, y; z) = E_n(z) \chi_n(x, y; z)
\]

\[
\left\{-\frac{\hbar^2}{2m_z} \frac{\partial^2}{\partial z^2} + E_n(z) \right\} \phi_n(z) = E \phi_n(z)
\]

**closed boundary 2D SE**

**open boundary 1D SE**
Bulk EM quantum-mechanical model (2)

Special case: nanowire uniform in the z direction

\[
\begin{align*}
U_\parallel(z) &= 0 \\
E_n(z) &\equiv E_n = \text{const}
\end{align*}
\]

\[
\phi_n(z) = e^{ikz}
\]

\[
g(E) = \frac{\sqrt{2m_z}}{\hbar \pi} \frac{1}{\sqrt{E - E_n}}
\]

1DEG n-th subband

In general \( \phi_n(z) \) is the solution of the open boundary 1D SE.

Constant potential in the injection leads (charge reservoirs) (QTBM).

\[
E = E_n + \frac{\hbar^2 k^2}{2m_z}
\]

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Bulk EM quantum-mechanical model (3)

Expression of the electron charge density (injection from the source):

\[ n_S = q \sum_n |\chi_n(x, y, z)|^2 \int_{E_n^S} |\phi_n^S(z; E)|^2 g_n^S(E) f(E, E_{FS}) \, dE \]

Similarly for the drain injection. Total density (to Poisson equation):

\[ n_{tot} = n_S + n_D \]

Expression of the total current:

\[ I = \frac{q}{\pi \hbar} \int T(E) \left[ f(E, E_{FS}) - f(E, E_{FD}) \right] \, dE \]

\( T(E) \) is the total (sum over all subbands) transmission coefficient
Bulk EM quantum-mechanical model (4)

The problem is solved by separating the Schrödinger equation along the transverse and longitudinal coordinates.

1. Solve the 2D SE in the transverse direction for each cross-section.
2. Solve the 1D SE with open boundary conditions.
3. Calculate the charge density.
4. Solve the 3D Poisson equation.

$\phi^0$ taken from a classical solution, used only as initial guess.

The Fermi level is prescribed at the S and D leads.

$\phi^0 = \phi$
The transverse 2D Schrödinger equation is solved numerically using different approaches:

- **Direct spatial discretization**
- **Expansion of the unknown wave function in the eigenfunctions of the well potential problem, when known analytically.**
  - Very efficient for small physical dimensions, since only a few basis functions are needed in the expansion.
  - Used for rectangular (sine waves basis functions) and cylindrical (Bessel basis functions) NW.
Example: cylindrical SNW (1)

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \varphi^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m^*}{\hbar^2} \left[ E - V(r) \right] \psi = 0
\]

\[
\begin{cases}
V(r) = 0 \text{ for } r \leq R \\
V(r) = \infty \text{ for } r > R
\end{cases}
\]

The solution is given by:

\[
E_{m,n,k}^{(0)} = \frac{\hbar^2 \mu_{m,n}^2}{2m^*_r k_R R^2}
\]

\[
\psi_{m,n}^{(0)}(r, \varphi, z) = A_{m,n} J_m \left( k_r^{(m,n)} r \right) \exp (j m \varphi) \exp (j k_z z)
\]

where \( \mu_{m,n} \) are the zeros of the Bessel function \( J_m(x) \) and \( k_r^{(m,n)} = \frac{\mu_{m,n}}{R} \).
Example: cylindrical SNW (2)

**BASICS**

\( \langle 001 \rangle \)-direction

- \( R \) – radius of the circle

\[ \mu_{0,1} = 2.405 \]

\[ E_C = E_{0,1,1} = \frac{(\mu_{0,1} \hbar)^2}{2m_{r1} R^2} \]

\[ E'_C = E_{0,1,2} = \frac{(\mu_{0,1} \hbar)^2}{2m_{r2} R^2} \]

\[ m_{r1} = 2 \frac{m_t m_l}{m_t + m_l} = 0.315 \text{ } m_0 \]

\[ m_{r2} = m_t = 0.19 \text{ } m_0 \]

\[ \text{Area (nm}^2\text{)} \]

\[ \text{Energy (eV)} \]

\[ 8.57\% \]

\( \langle 001 \rangle \)-direction

Ellipsoid 1

Ellipsoid 2

Ellipsoid 3

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Example: cylindrical SNW (3)

Self consistent charge calculation

Si

SiO₂

R=10nm

R=5nm

R=2.5nm

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Limits of the bulk EM approximation

- The strong quantization due to the lateral dimensions pushes the eigenvalues up in energy ➔ non parabolic effects.
- Limited number of atoms in the transverse cross-section.
- The nature of the interface and the termination of the dangling bonds have an influence on the band structure.
- Conclusion: the band structure is no longer a material property but, rather, a device property ➔ it must be computed for every device geometry using atomistic computations.
The reduction of the structure size forces $k$ to shift to higher values $\rightarrow E(k)$ is not parabolic anymore.
Limited number of atoms in the cross-section

(100)-Si wafer/(001)-Si wire

(a) [110]-Si wafer/(001)-Si wire

(b) [100]-Si wafer/(001)-Si wire

(c) [010]-Si wafer/(001)-Si wire

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An extreme solution

Full 3D atomistic tight binding (TB) simulation.

In this example:
2.1 nm x 2.1 nm x 32 nm
20 orbitals for each atom
≈ 7000 atoms

Easy to account for different orientations and surface roughness.

Very time consuming, prohibitive for device optimization

From Luisier et al., IEDM, 2006
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An engineering approach (1)

Inject non parabolic corrections into the **constant** EM model scheme: abandon the bulk EM and use EMs function of the cross-section area, fitted upon atomistic band calculations for well potentials. Quantization masses used in the 2D transverse SE (cylinder) are fitted on subband bottom energies.
Transport masses used in the 1D longitudinal SE are fitted on the parabolic part of the 1DEG subbands.
Electrical characteristics: threshold shift

From ITRS 2005: $t_{ox} = 1$ nm & $V_{DD} = 0.7$ V. Analysis at fixed $L_G = 10$ nm:

- $d_{Si} = 2$ nm
- $V_{DS} = V_{DD}$

$V_{t(bulk)} - V_{t(new)} (V)$, $E_{c(bulk)} - E_{c(new)} (eV)$
Electrical characteristics: effects on $I_{ON}$

- $d_{Si} = 2$ nm
- $V_{DS} = V_{DD}$
- $I_{ON(new)} - I_{ON(bulk)}$

Graphs showing current ($I$) versus gate voltage ($V$) and diameter (nm) with comparison between bulk parabolic model and new model.

Relative difference %

- 0%
- 5%
- 10%
- 15%
- 20%
- 25%
- 30%
- 35%
- 40%
- 45%

$V_{DS} = V_{DD}$

$V_{GS}$ vs. $I_{ON}$ for different diameters.
Electrical characteristics: subthreshold slope

\[ d_{\text{Si}} = 1 \text{ nm} \]

New model

Bulk parabolic model

\[ T(E) \propto \exp \left[ -2 \sqrt{\frac{2m(V_0 - E)}{\hbar}} L \right] \]
A higher order engineering approach

As before + **non parabolic** transport model in the 1D longitudinal SE.

E.g.: 6\(^{th}\) order expansion of \(E(k) = \gamma - \alpha \gamma^2 + \beta \gamma^3\), where \(\gamma = (\hbar k)^2/(2m^*)\).

\(\alpha\) and \(\beta\) fitted on the 1DEG subbands
Example of 1DEG subband fitting

$d_{Si} = 1 \text{ nm (5 atoms)}$

Symbols = DFT

Red squares: twofold degenerate

Solid lines = 6\textsuperscript{th} order fitting
A non-parabolic $E(k)$ relationship can always be expanded in series of $k^2$ due to the parity of the dispersion relationship.

$$E(k) = \frac{\hbar^2 k^2}{2m^*}$$

Following the effective-mass theorem, we perform the substitution $k \rightarrow -j \nabla$

$$E(-j \nabla) = \frac{\hbar^2}{2m^*} \sum_{n=1}^{\infty} b_n \left(-\frac{d^{2n}}{dx^{2n}}\right)$$

The probability current becomes (generalization of the constant EM case):

$$J = -\frac{j}{\hbar} \frac{dE}{dk^2} \left[ \psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right]$$
Non-parabolic Hamiltonian: problems (1)

- A direct discretization scheme (central differences) does not seem to work properly.
- The transfer matrix method (TMM) provides much more reliable results (at least up to the 6th order). However…
- The TMM approach (from the literature) is based on:
  1. staircase potential
  2. in each element with $k_i$ in the first Brillouin zone
  3. continuity of $\psi$ and $J$ at each potential step

$$
J = -\frac{j}{\hbar} \frac{dE}{dk^2} \left[ \psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right]
$$
Non-parabolic Hamiltonian: problems (2)

Problems:

- $J$ is continuous, but not $d\psi/dx$.
- If $E(k)$ is non monotonic, the local transfer matrix is singular at the points where $dE(k)/dk = 0$.
- What to do when 4 $k$s (or more) exist in the first Brillouin zone?
- In principle, for an expansion of order $N$, in each element there are $N$ plane waves, and the wave function and its derivatives up to order $N-1$ should be matched, but …
- … if the expansion is truncated to reasonably low order, junk $k$s
- … if one tries to fit $E(k)$ over the full Brillouin zone, a very high order expansion is required.
A full 1DEG band engineering approach

\[
\begin{align*}
\left\{ \begin{array}{l}
\varepsilon \left( -j \frac{d}{dx} \right) + U(x) \end{array} \right\} \psi(x) &= E \psi(x) \\
\varepsilon(k) &= \sum_n \varepsilon_n e^{j k n a}
\end{align*}
\]

1D open-boundary SE

generic subband: use Fourier expansion!!

\[
\left[ e^{n a \frac{d}{dx}} \right] \psi(x) = \left[ \sum_l \frac{1}{l!} \left( na \frac{d}{dx} \right)^l \right] \psi(x) = \psi(x + n a)
\]

\[
\sum_n \varepsilon_n \psi(x + n a) + U(x) \psi(x) = E \psi(x)
\]

Discrete form:

\[
\sum_n \varepsilon_n \psi_{i+n} + (U_i - E) \psi_i = 0
\]

SOURCE

LEAD

\( x = 0 \)

\( i = 0 \)

\( a \)

DRAIN

LEAD

\( x = L \)

\( N_l + 1 \)
Subband features and Fourier expansion

- 8x8 atoms cell octagonal \langle 100 \rangle SNW
- KS-DFT atomistic energy calculation by code CRYSTAL2003
- H-passivated structural relaxed SNW

![Graph showing subband features and Fourier expansion](image)

- Missed crossing
- Unprimed ladder splitting
Boundary conditions (1)

Characteristic equation in the source lead:

\[ \varepsilon(k_S) + U_S = E \]

If \( N \) is the Fourier expansion order, there are \( 2N \) complex solutions \( k_{Sn} \) symmetric around the origin, with the real part in the first Brillouin zone:

\[ \varepsilon(k) = \sum_{n=0}^{N} 2\varepsilon_n \cos(nka) = \sum_{n=0}^{N} A_n \cos^{N-n}(ka) = \text{polynomial of order N in } \cos(ka) \]

Expression of the wave function within the source lead:

\[ \psi_S(x; k_{Sn}^{\text{inj}}) = A e^{jk_{Sn}^{\text{inj}}x} + \sum_{n=1}^{N} \sum_{l=-\infty}^{+\infty} B_{ln} e^{jk_{Sn}^{\text{inj}}[l\frac{2\pi}{a}]} \]

The \( k_{Sn} \) are selected corresponding to back propagating waves (negative group velocity), or vanishing modes in the source lead (complex with positive real part)
Boundary conditions (2)

\[ \psi_S(x; k_S^{inj}) = A e^{jk_S^{inj}x} + \sum_{n=1}^{N} \sum_{l=-\infty}^{+\infty} B_{ln} e^{jk_{Sn} + l\frac{2\pi}{a}x} \]

\[ = A e^{jk_S^{inj}x} + \sum_{n=1}^{N} e^{jk_{Sn}x} \phi_n(x) \]

\[ \phi_n(x+a) = \phi_n(x) \quad \text{N additional periodic unknown functions} \]

- The wave function in the lead is expressed by a superposition of Bloch functions, even if the injected electron is a plane wave.

- It is expected the fine structure \( (x) \) to be nearly flat for reasonably smooth potential profiles.
Boundary conditions (3)

\( \phi_n(x + a) = \phi_n(x) \)  
N additional periodic unknown functions

- add N extra equations in the lead
- repeat the solution on additional shifted grids (uncoupled)
Boundary conditions (4)

Examples of root loci of the characteristic equation $\varepsilon(k_S) = E$

$N = 3$

$\text{CB}_1$

$\text{CB}_3$
Calculation of the probability current

From Gomez-Campos et al., J. Appl. Phys., 2005

\[ J_S = \frac{j}{\hbar} \sum_{m=1}^{\infty} (-1)^m c_m \sum_{r=0}^{2m-1} (-1)^r \frac{d^r \psi^*_S}{dx^r} \frac{d^{2m-r-1} \psi_S}{dx^{2m-r-1}} \]

based on the \( k^2 \) power series expansion of \( \varepsilon(k) \)

\[ \varepsilon(k) = \sum_{s=0}^{\infty} c_s (k^2)^s \]

and using the previous expression of \( \psi_S \)

\[ \psi_S(x; k_{S}^{inj}) = A e^{j k_{S}^{inj} x} + \sum_{n=1}^{N} e^{j k_{S}^{inj} x} \phi_n(x) \]

with \( (x) \) approximated with the truncated Fourier series through \( (0), (\Delta x_1), \ldots \)
Are multiple grids really needed?

CB3

$E = 0.4 \text{ eV}$
Are multiple grids really needed?

With typical potential profiles one grid is generally sufficient, unless very high charge resolution is required.
Band effects on transport

- \( T(E) \) drop due to finite energy extension of the subbands
- different SS due to different effective masses
- transmission zeros for \( \text{CB}_3 \) in deep subthreshold
Band effects on transport

- $T(E)$ drop due to finite energy extension of the subbands
- different SS due to different effective masses
- transmission zeros for CB$_3$ in deep subthreshold
Intervalley transitions: test case

subband CB$_3$

0.35 V potential step
Application to device simulation: flow chart

Atomistic calculation of 1D subbands with well potential

- subbands $\varepsilon_i(k)$

3D potential initial guess $\varphi^0(r,x)$

Transverse 2D Schrödinger eq. for each $x$ (fitted const. quantization EM)

- potential energy profiles $U_i(x)$
- transverse wavefunctions $\chi_i(r;x)$

Longitudinal 1D Schrödinger eq. with full $\varepsilon_i(k)$

- longitudinal wavefunctions $\psi_i(x)$

Charge calculation

- electron density $n(r,x)$

Poisson equation

- 3D electrostatic potential $\varphi(r,x)$

Error check

Fermi distributions at source/drain

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Transmission coefficient – 1\textsuperscript{st} subband

\[ V_{DS} = 0.4 \text{ V} \]
\[ L_{G} = 11 \text{ nm} \]
Transmission coefficient – 2\textsuperscript{nd} subband

$V_{DS} = 0.4 \text{ V}$
$L_G = 11 \text{ nm}$
Transmission coefficient – 3rd subband

Potential energy (eV)

FBH second

FBH first

$V_{DS}=0.4 \text{ V}$

$L_G=11 \text{ nm}$
Output characteristics

- Two negative output conductance intervals are clearly visible.
- The drop at $V_{DS} = 0.8$ V is larger because of the 2-fold degeneracy of the 2nd subband.
Summary and conclusions (1)

- The importance of quantum effects in ultra scaled SNWs has been highlighted, both for electrostatics and transport.
- The bulk EM approximation turns out to be inaccurate for very thin NWs.
- A hierarchy of models with an increasing order of complexity has been presented to account for band effects.
- A method has been described to deal with the 1D transport open boundary SE including the full subband structure.
- The drop of the transmission coefficient due to the limited energy extension of the subbands, the possibility of tunneling transmission zeros and intervalley transitions have been discussed.
- The preliminary use of this method for full device simulation has been presented.
- Possibility of negative output conductance.
Summary and conclusions (2)

Open problems:

- How far can the uncoupled subband method be pushed?
- Is tunneling in the energy gap correctly described?
- The kinetic part of the Hamiltonian in principle is not separable any more when non parabolic bands are considered. What are we loosing by still forcing the separation?

An extensive comparison with more accurate methods (full 3D and atomistic simulations) and with experiments is necessary.

Are full band effects on transport really important in practical devices?