Simulation of Tunnel FETs for accurate performance prediction at device and circuit level

P. Palestri, L. Selmi, Univ. of Udine

Many thanks to E. Gnani, M. Luisier, D. Essen, S. Strangio, A. Revelant, C. Alper
Aim of the presentation

- brief overview of the modeling approaches for TFETs
- both device and circuit analysis
- focus on the methodologies employed in the E²SWITCH project
- identification of pros. and cons. of commercial TCAD tools
TFET scenario

- GeSn
- UTB
- nanowires
- broken gap
- strain
- staggered gap
- hetero-junctions
- high- \( k \) dielectrics
- SiGe
- InAs
- InSb
- GaSb
- gate-all-around
- defects
- trap-assisted tunneling
- band-to-band-tunneling

- fabrication process often immature
- modeling needed to help selecting the best architecture/materials
OUTLINE

• Brief introduction to band-to-band tunneling
• Models for device level simulation
• Approaches for circuit level simulation
• Conclusions
Tunneling current vs. BTBT generation

energy bin $\Delta E$

quantum mechanical tunneling

current $\Delta J$

ho. and el. currents $J_p$ $J_n$

ho. and el. gen. rates $G_h$ $G_e$

$\Delta x = \Delta E / (e |F|)$

$\frac{dJ_p}{dx} = eG_h$ $\frac{dJ_n}{dx} = -eG_e$

$|F| \frac{\Delta J}{\Delta E}$
Direct tunneling vs. phonon assisted

- **direct tunneling**: the $k$-vector normal to tunneling is conserved;
- tunneling from top of the VB into CB minima in $\Gamma \rightarrow$ important in direct gap semiconductors (III-V)
- **phonon-assisted tunneling**: scattering with phonons allows to tunnel from VB to CB minima other than $\Gamma \rightarrow$ relevant in Si and Ge
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Model hierarchy

- **Full quantum** based on Non-equilibrium-Green’s Functions
  - Atomistic **tight binding** Hamiltonian
  - $k \cdot p$ Hamiltonian
- **Full quantum** based on post-process of quasi-equilibrium calculations
- **TCAD** with tunneling models based on WKB
Atomistic tight binding approach (1)

- **OMEN** (ETHZ): 3D **Quantum** Transport Solver

- **Empirical Nearest-Neighbor Tight-Binding Method**

**GOOD:**
- bulk CB and VB fitted (BTBT)
- extension to nanostructures
- atomistic description

**BAD:**
- high computational effort
- empirical parametrization
Atomistic tight binding approach (2)

Ballistic simulations of TFETs: InSb devices

• Maximum Current for DG UTB @ $V_{DD}=0.5$ V
• SS below 60 mV/dec:
• GAA (9.2) < DG (20) < SG (34)
• Band Gap increase due to quantization
Atomistic tight binding approach (3)

Ballistic simulations of TFETs: GaSb-InAs BG

- Maximum Current of 900 μA/μm for DG UTB @ $V_{DD} = 0.5$ V
- SS below 60 mV/dec: GAA (7) < DG (11) < SG (17)
- Band Gap increase due to quantization (especially InAs)
# From TB to k·p

<table>
<thead>
<tr>
<th>Tight binding</th>
<th>k·p</th>
</tr>
</thead>
<tbody>
<tr>
<td>In principle all of the core orbitals are needed. But, not all of them contribute in an essential way.</td>
<td>Extrapolate band structure from experimental values obtained at the ( \Gamma ) point.</td>
</tr>
<tr>
<td>Only interactions between two nearest-neighbor atoms are considered</td>
<td>Strain effects and non-standard crystal orientations can be easily included.</td>
</tr>
<tr>
<td>Interactions are treated as empirical parameters ( \rightarrow ) exact knowledge of the atomic orbitals not needed.</td>
<td>Permit to treat hetero-junctions and hetero-structures</td>
</tr>
<tr>
<td>Rigorous multiband description ( \rightarrow ) Band-to-Band-Tunneling automatically taken into account.</td>
<td>Most reliable in the vicinity of the ( \Gamma ) point.</td>
</tr>
<tr>
<td>Atomistic discretization grid needed.</td>
<td></td>
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</tbody>
</table>
k·p approach (IUNET-BO)

- 4x4 (w/o spin-orbit) or 8x8 k·p Hamiltonian for III-Vs

\[
H(\vec{k}) = \begin{pmatrix}
E_c + A_c k^2 & iP_{k_x} & iP_{k_y} & iP_{k_z} \\
-iP_{k_x} & E_v + Lk_z^2 + M (k_y^2 + k_z^2) & Nk_y k_y & Nk_z k_z \\
-iP_{k_y} & Nk_z k_y & E_v + Lk_x^2 + M (k_x^2 + k_z^2) & Nk_x k_x \\
-iP_{k_z} & Nk_x k_z & Nk_y k_z & E_v + Lk_y^2 + M (k_x^2 + k_y^2)
\end{pmatrix}
\]

- only Γ valleys are considered
- 3D NEGF + 3D Poisson
- Wavefunction set to zero at the semiconductor/oxide interface
- Parameters from Vurgaftman et al., JAP 89, 5815, 2001
- Alteration of \( P \) and \( A_c \) to avoid spurious solutions (similar to Foreman, PRB 56, R12748, 1997)
- periodic boundary conditions for planar devices
**k·p vs. tight binding**

**5nm x 5nm InAs wire**

- **Blue:** tight-binding
- **Red:** $k \cdot p$

**InAs NW-TFET**

- $V_{ds} = 0.2V$
- $SS = 60mV/\text{dec}$

- $5 \times 5 \text{nm}^2 L_G = 20\text{nm}$
- $T_{ox} = 1\text{nm} \quad \varepsilon_{ox} = 12.7$
- $N_A = N_D = 5 \times 10^{19} \text{cm}^{-3}$
- 100 transport, [100] confinement
- GAA structure
Effective mass + post-processing (1)

- quasi-equilibrium solution assuming that the BTBT current is not affecting the charge in the device w.r.t. equilibrium

\[
\begin{align*}
\left( E_{c0} - \frac{\hbar^2}{2m^*_c} \nabla^2 + U_{\text{ext}}(\mathbf{r}) \right) \chi_c(\mathbf{r}) &= E \chi_c(\mathbf{r}) , \\
\left( E_{v0} + \frac{\hbar^2}{2m^*_v} \nabla^2 + U_{\text{ext}}(\mathbf{r}) \right) \chi_v(\mathbf{r}) &= E \chi_v(\mathbf{r}).
\end{align*}
\]

\[ A_{v,c}(\mathbf{r}, \mathbf{r}'; E) = 2\pi \delta(E - H_{v,c}) = 2\pi \sum_\ell \chi_{v,c\ell}(\mathbf{r}) \delta(E - E_{v,c\ell}) \chi_{v,c\ell}^*(\mathbf{r}'). \]

\[ T_{v}^{\text{abs,em}}(\mathbf{R}; E) = \Omega |M_0|^2 \sum_{\alpha,\alpha'} A_{v\alpha}(\mathbf{r}, \mathbf{r}; E) \times A_{\alpha'\alpha}(\mathbf{r}, \mathbf{r}; E \pm \hbar \omega_0) \quad (\Omega = \text{total volume}), \quad (5) \]

\[ G(\mathbf{R}) = -\frac{2}{\hbar} \int \frac{dE}{2\pi} \left( \left( f_v(E) (1 - \frac{f_c(E - \hbar \omega_0)}{1 + \nu(\hbar \omega_0)}) \nu(\hbar \omega_0) \right) - f_c(E - \hbar \omega_0) (1 - f_v(E)) \nu(\hbar \omega_0) \right) T_v^{\text{em}}(\mathbf{R}; E) \\
- \frac{(f_v(E) (1 - f_c(E + \hbar \omega_0)) \nu(\hbar \omega_0) - f_c(E + \hbar \omega_0) (1 - f_v(E)) \nu(\hbar \omega_0) + 1) T_v^{\text{abs}}(\mathbf{R}; E)}, \quad (6) \]

\[ I_{ds} = qW \int d^2 R G(\mathbf{R}). \quad (7) \]

[W.Vandenberghe et al., IEDM 2011]
[W.Vandenberghe et al., JAP, v.109, p.124503 2011]
Effective mass + post-processing (2)

- models also for direct tunneling. Example: direct tunneling in EHBTFET, assuming 1D profile

\[
I_{\text{dir}} = -\frac{eE_G L G W}{2\hbar} \sum_k \sum_{\alpha', k' \in \nu} \psi_{kG}^2 \psi_{k'\alpha'}^2 C_{\alpha, \alpha'}(\theta)(f_0(E_T) - f_c(E_T)) \Theta(E_{k'\alpha'} - E_{kG})
\]

[C. Alper et al., TED, v.60, p.2754 2013]
Commercial TCAD (1)

- old “local” models have been replaced by non-local models
- example: non-local dynamic path model for direct tunneling in SDevice

\[ R_{net}^d = |\nabla E_V(0)| C_d \exp \left( -2 \int_0^l \kappa dx \right) \left( \exp \left[ \frac{\varepsilon - E_{F,n}(l)}{kT(l)} \right] + 1 \right)^{-1} - \left( \exp \left[ \frac{\varepsilon - E_{F,p}(0)}{kT(0)} \right] + 1 \right)^{-1} \]

Integration over a suitable tunneling path

\[ \kappa = \frac{1}{h^2} \sqrt{\frac{m_r E_{g,tun}}{1 - \alpha^2}} \]

\[ \alpha = - \frac{m_0}{2m_r} + \frac{1}{2} \sqrt{\frac{m_0}{2m_r} \left( \frac{\varepsilon - E_V}{E_{g,tun}} - \frac{1}{2} \right) \left( \frac{m_0^2}{16m_r^2} + \frac{1}{4} \right)} \]

\[ \frac{1}{m_r} = \frac{1}{m_V} + \frac{1}{m_C} \]

\[ k_m^2 = \min(k_{vm}^2, k_{cm}^2) \]

\[ k_{vm}^2 = \frac{2m_V(e_{\text{max}} - \varepsilon)}{h^2} \]

\[ k_{cm}^2 = \frac{2m_C(\varepsilon - e_{\text{min}})}{h^2} \]

E-k inside the energy gap
Commercial TCAD (2)

- similar expressions also for phonon-assisted and trap-assisted BTBT
- proper definition of tunneling path and E-k inside the gap are the main ingredients of such models
- example: impact of the choice of the tunneling path

 horizontal path: lower current w.r.t. path following the gradient of the VB

[L.DeMichielis, SSE, v.71, p.7 2012]
Commercial TCAD (3)

- use effective gap [Revelant, SSE, v.88, p.54] to account for size-induced quantization

- 1D Schrödinger equation in each section is needed
- approach so far not included in commercial TCAD
Commercial TCAD (4)

- effective gap [Revelant, SSE, v.88, p.54]:

  good agreement vs. QM [Vandenberghe IEDM 2011]

  good agreement vs. exp. [Dewey IEDM 2011]
Commercial TCAD (5)

- calibration required for **alloys** and **strain**
- BTBT in SiGe is not a pure interpolation between Si and Ge
  - Ge is dominated by direct tunneling but default calibration associates BTBT to indirect tunneling, Si by indirect
  - SiGe up to high Ge conc. is Si-like

**Example:**

- template homo-junction TFET
- default Sentaurus calibration vs. [Kao, TED, 2012]

[Revelant, ESSDERC 2013]
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Approaches

- Mixed device/circuit simulations
- Circuit analysis with Verilog-A models
- Circuit analysis with SPICE models
Example of mixed device/circuit simulation (1)

mesh and parameters calibrated on [Knoll, EDL, 2013]

simulation of a TFET inverter
Example of mixed device/circuit simulation (2)

- SRAM performance using TFETs [Strangio, ESSDERC 2014]

![OUTWARD TFET cell diagram]

Write and read transients

Node Voltages [V]

Write & Read Delays [s]

Write (V_DD)
Read (V_DD/2)

6T SRAM CELL
(Outward-AT)
Issues (e.g. SDevice)

• the most accurate model for BTBT (non-local dynamic tunnel) does not work with mixed device/circuits
  – AC simulations not working, too → issue also in generating look-up tables
• simple models require ad-hoc calibration often with unphysical parameters
• almost impossible to use 3D devices in mixed device/circuit
• limited number of devices → use look-up tables in Verilog-A
Verilog-A models based on lookup tables

\[ I_d(t) = I_{DC}(V_{gs}, V_{ds}) + \frac{\partial Q_d}{\partial v_d} \frac{\partial v_d}{\partial t} + \frac{\partial Q_d}{\partial v_g} \frac{\partial v_g}{\partial t} + \frac{\partial Q_d}{\partial v_s} \frac{\partial v_s}{\partial t} \]

- table must contain DC current and AC capacitances vs. bias
- sample results from [Alper, ESSDERC 2012] (EPFL)

high-k at the inj. point, and then low-k

high-k over whole gate
Compact models for TFETs

- Example from [Biswas, ULIS2014] (EPFL)
  - conformal mapping for 2D poisson
  - bias-dependent characteristic length
  - BTBT model: WKB as in SDevice

\[
\frac{1}{\lambda^2} = \frac{1}{\lambda_0^2} + \left( \beta N_{\text{inv}} / \varepsilon_{\text{Si}} t_{\text{Si}} \phi_S \right)
\]

\[
\beta = \beta_0 \left[ 1 - c \times \exp\left( - \left( V_G^* - V_{\text{th,inv}} - \eta / \sigma \right)^2 \right) \right]
\]

Good agreement with TCAD (solid lines)
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Conclusions

- huge efforts over the last 5 years to improve modeling of BTBT
- models/tools with different accuracy/field of applicability available today
- most experimental data dominated by TAT \(\rightarrow\) accurate models are needed
- inclusion of band tails
- main open issues with commercial TCAD
  - calibration
  - quantum corrections
  - accurate models and 3D mesh should work also in mixed device/circuits