

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

G. Baccarani, E. Gnani, A. Gnudi, S. Reggiani, M. Rudan

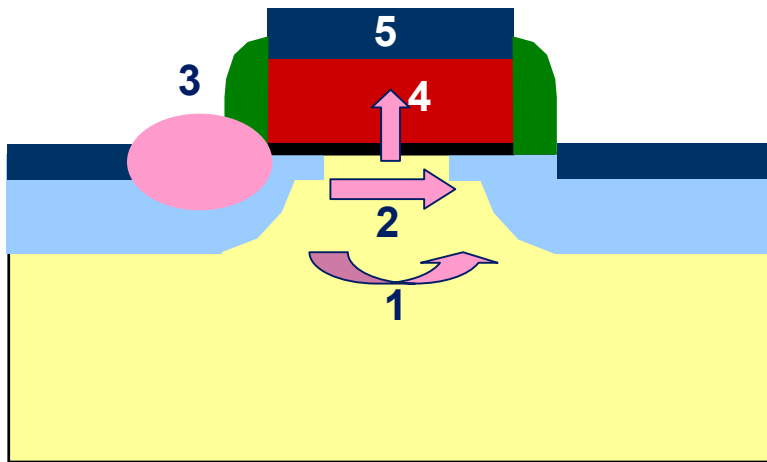
Advanced Research Center on Electronic Systems (ARCES),
Department of Electronics (DEIS) – University of Bologna, Italy

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.



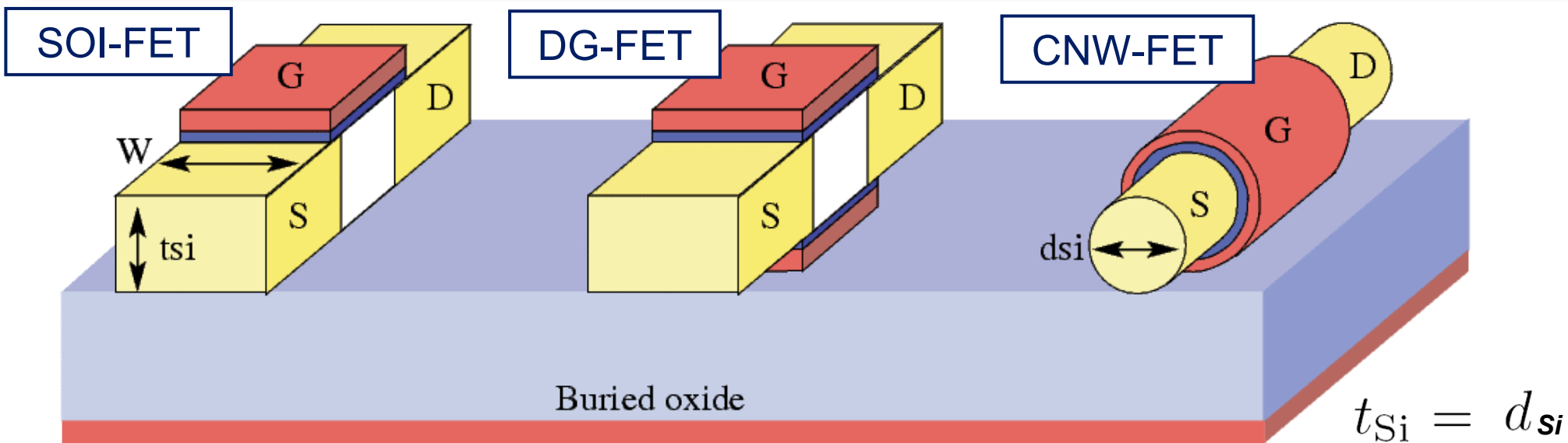
- 1) Poor electrostatics ► increased I_{off}
- 2) Poor channel transport ► decreased I_{on}
- 3) S/D parasitic resistance ► decreased I_{on}
- 4) Gate oxide scaling ► increased J_G
- 5) Gate depletion ► increased EOT

- 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.

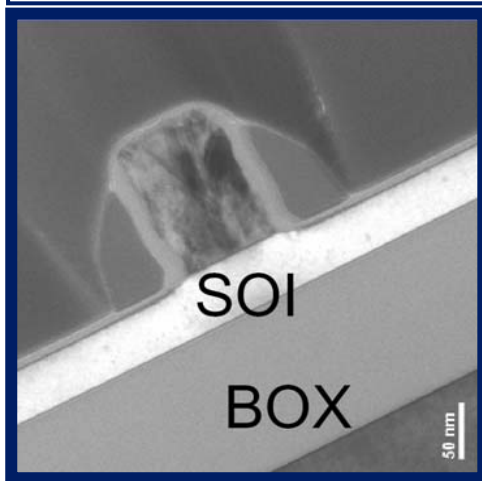


enhanced drive current and acceptable control of SCEs

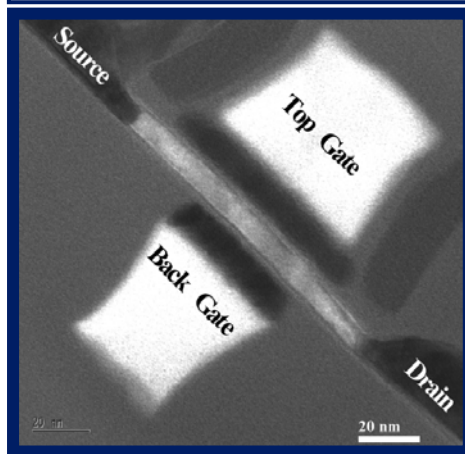
New device architectures



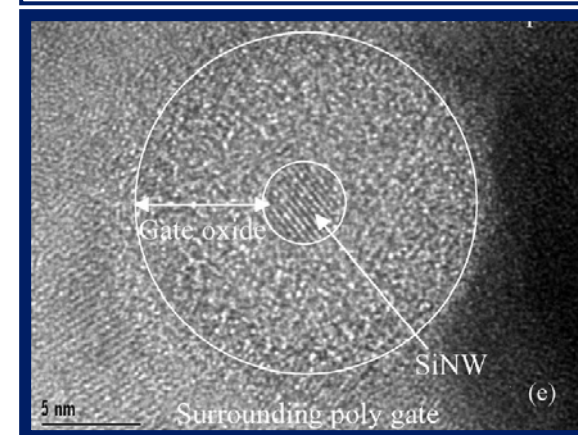
M. Yang et al., IEDM 2003



J. Widiez et al., TED 2005



N. Singh et al., EDL 2006



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

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 confined directions, z 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:

$$\begin{cases} U(x, y, z) \cong U_{\perp}(x, y) + U_{\parallel}(z) \\ \psi(x, y, z) = \chi(x, y) \phi(z) \end{cases}$$

$$\left\{ \begin{array}{l} \left[-\frac{\hbar^2}{2} \left(\frac{1}{m_x} \frac{\partial^2}{\partial x^2} + \frac{1}{m_y} \frac{\partial^2}{\partial y^2} \right) + U(x, y, z) \right] \chi_n(x, y; z) = E_n(z) \chi_n(x, y; z) \\ \hspace{15em} \text{closed boundary 2D SE} \\ \\ \left[-\frac{\hbar^2}{2m_z} \frac{\partial^2}{\partial z^2} + E_n(z) \right] \phi_n(z) = E \phi_n(z) \\ \hspace{15em} \text{open boundary 1D SE} \end{array} \right.$$

Bulk EM quantum-mechanical model (2)

Special case: nanowire uniform in the z direction

$$\begin{cases} U_{\parallel}(z) = 0 \\ E_n(z) \equiv E_n = \text{const} \end{cases}$$

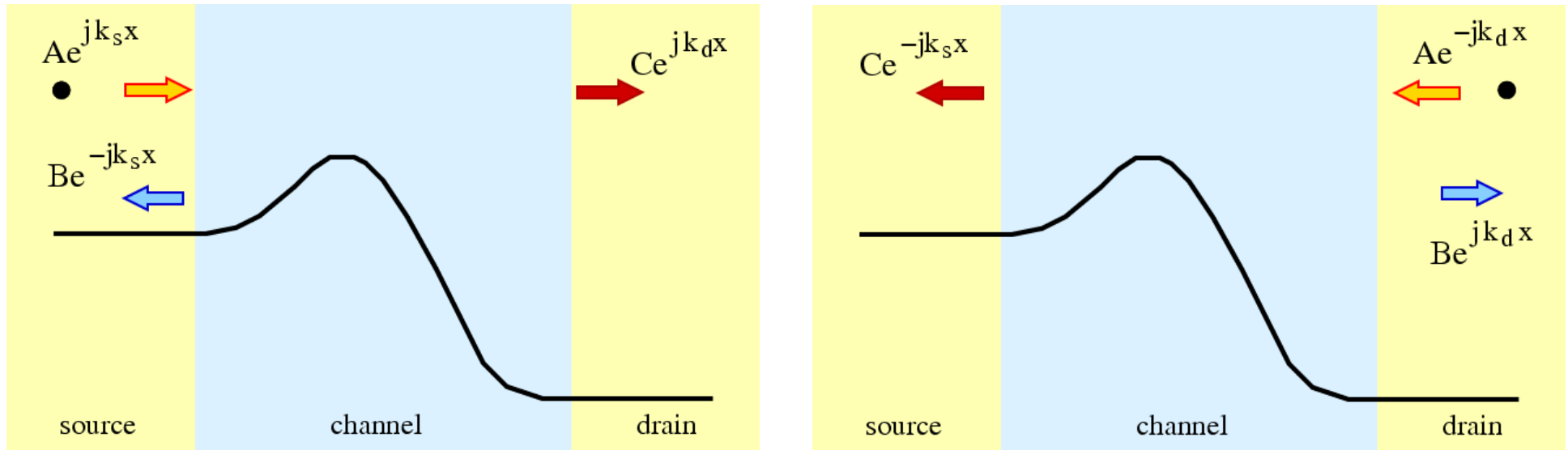
$$\begin{cases} \phi_n(z) = e^{ikz} \\ E = E_n + \frac{\hbar^2 k^2}{2m_z} \end{cases}$$

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

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).



Bulk EM quantum-mechanical model (3)

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

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

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

$$n_{tot} = n_S + n_D$$

Expression of the total current:

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

$T(E)$ 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.

Solve the 2D SE in the transverse direction for each cross-section.

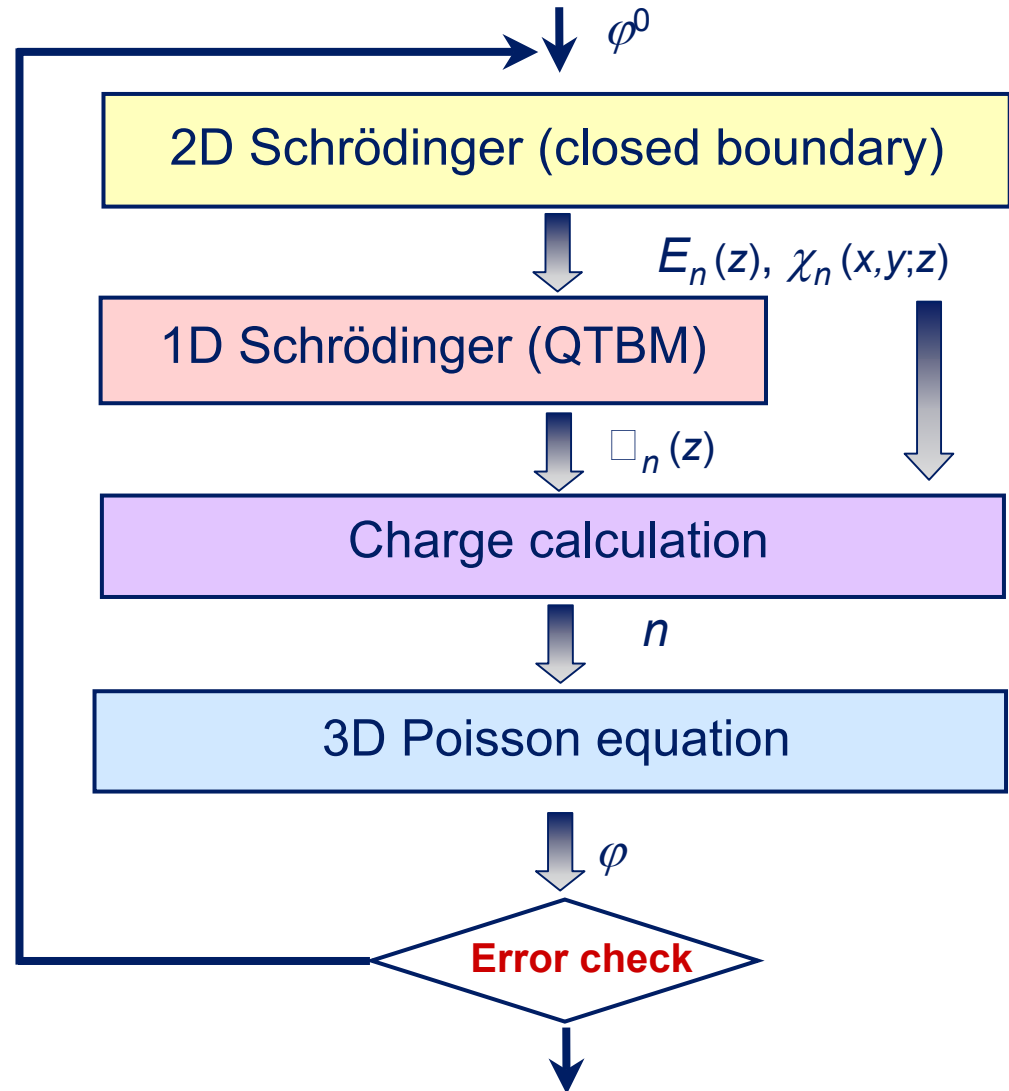
Solve the 1D SE with open boundary conditions.

Calculate the charge density.

Solve the 3D Poisson equation.

φ^0 taken from a classical solution, used only as initial guess.

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



Transverse 2D SE

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.
 - o Very efficient for small physical dimensions, since only a few basis functions are needed in the expansion.
 - o Used for rectangular (sine waves basis functions) and cylindrical (Bessel basis functions) NW.

Example: cylindrical SNW (1)

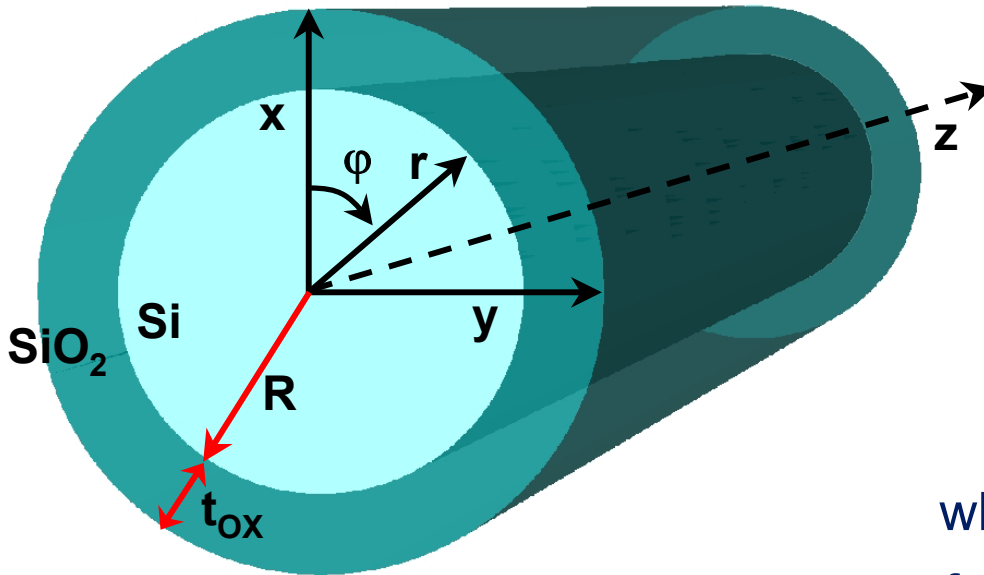
$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \varphi^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m^*}{\hbar^2} [E - V(r)] \psi = 0 \begin{cases} V(r) = 0 \text{ for } r \leq R \\ V(r) = \infty \text{ for } r > R \end{cases}$$

The solution is given by:

$$E_{m,n,k}^{(0)} = \frac{\hbar^2 \mu_{m,n}^2}{2m_r^* k R^2}$$

$$\psi_{m,n}^{(0)}(r, \varphi, z) = A_{m,n} J_m(k_r^{(m,n)} r) \exp(jm\varphi) \exp(jk_z z)$$

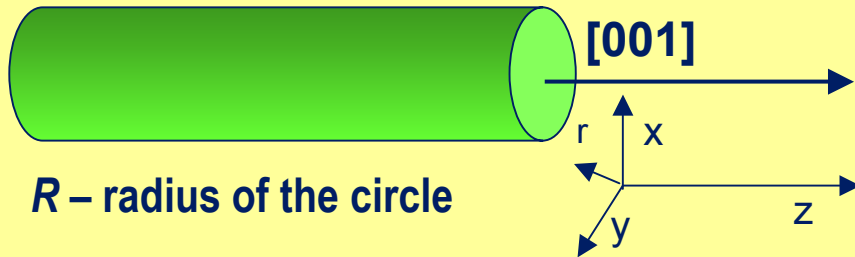
where $\mu_{m,n}$ are the zeros of the Bessel function $J_m(x)$ and $k_r^{(m,n)} = \frac{\mu_{m,n}}{R}$



Example: cylindrical SNW (2)

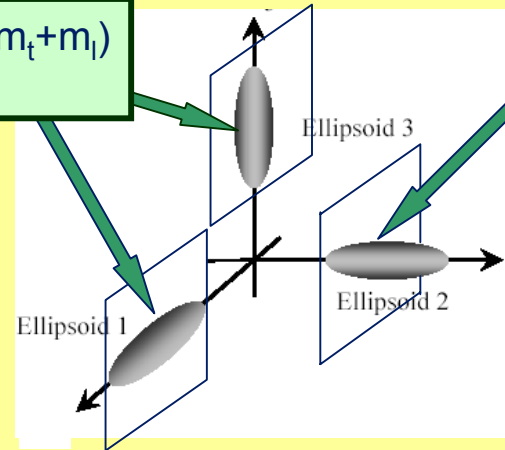
BASICS

$\langle 001 \rangle$ -direction



$$m_{r1} = 2 m_t m_l / (m_t + m_l) = 0.315 m_0$$

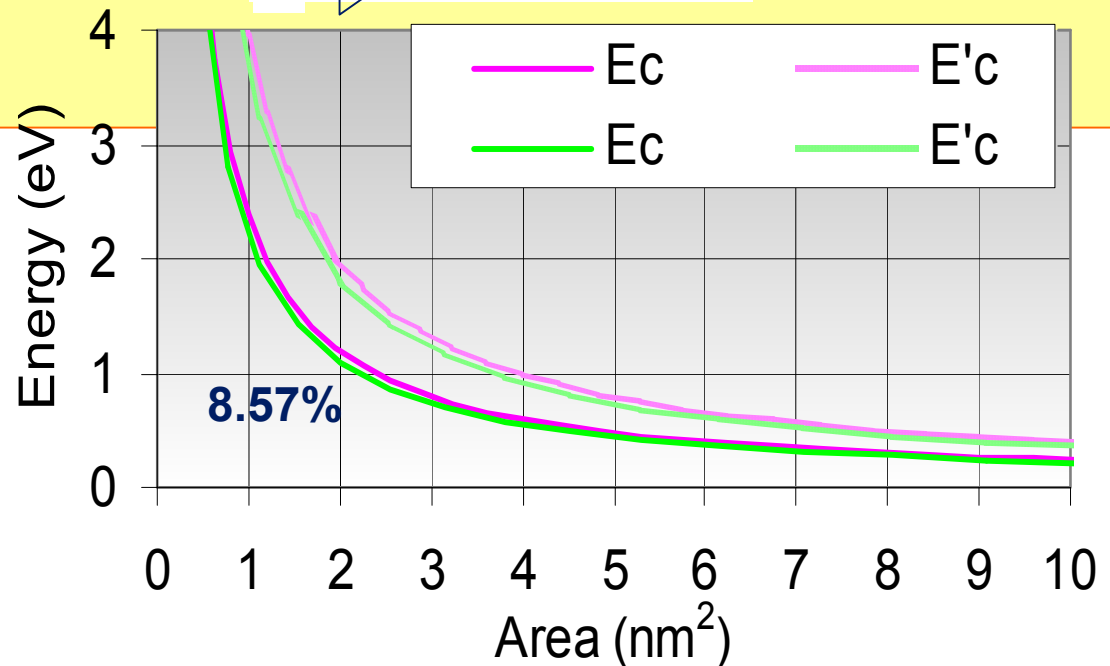
$$m_{r2} = m_t = 0.19 m_0$$



$$\mu_{0,1} = 2.405$$

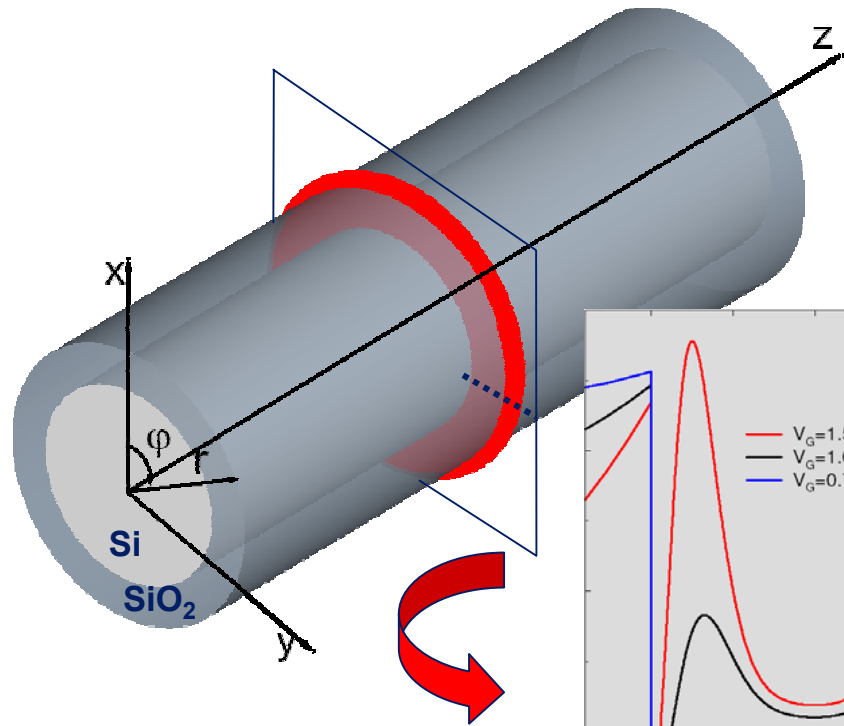
$$E_c = E_{0,1,1} = \frac{(\mu_{0,1} \hbar)^2}{2m_{r1} R^2}$$

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

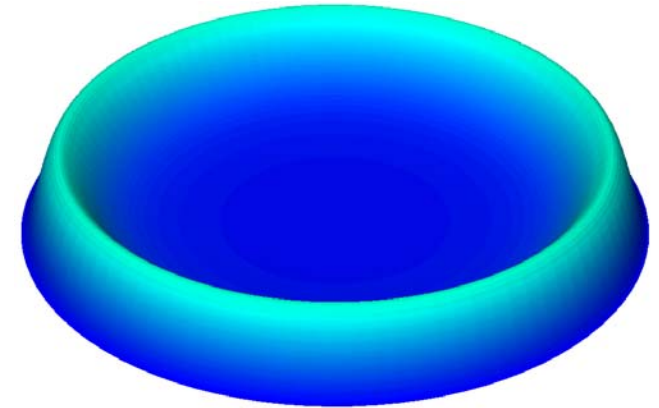


Example: cylindrical SNW (3)

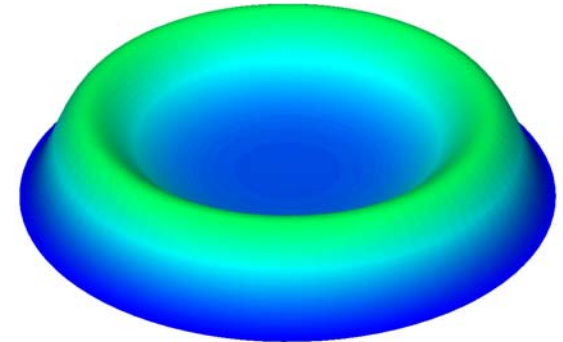
Self consistent charge calculation



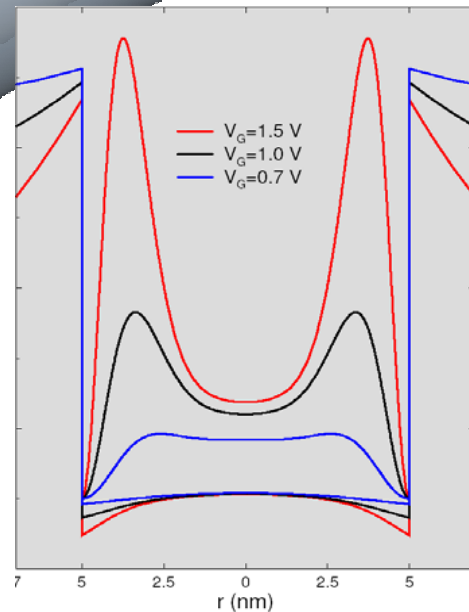
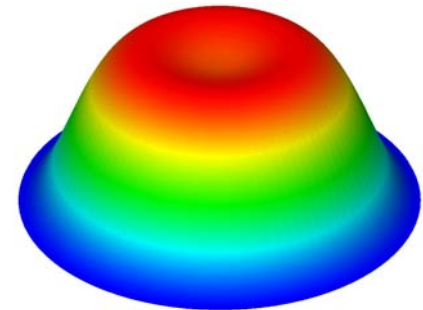
R=10nm



R=5nm



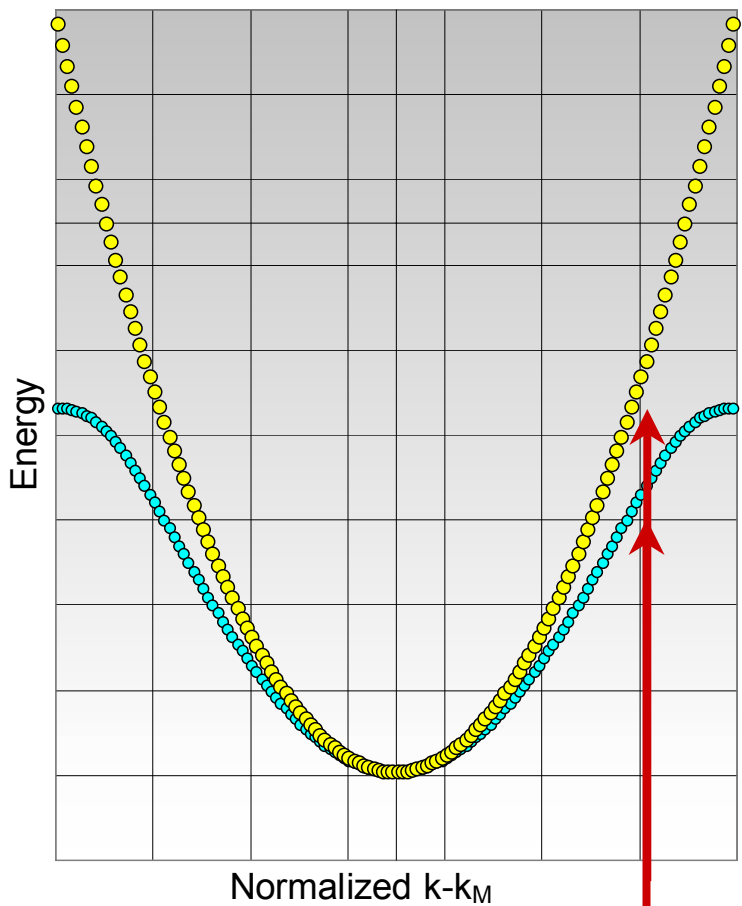
R=2.5nm



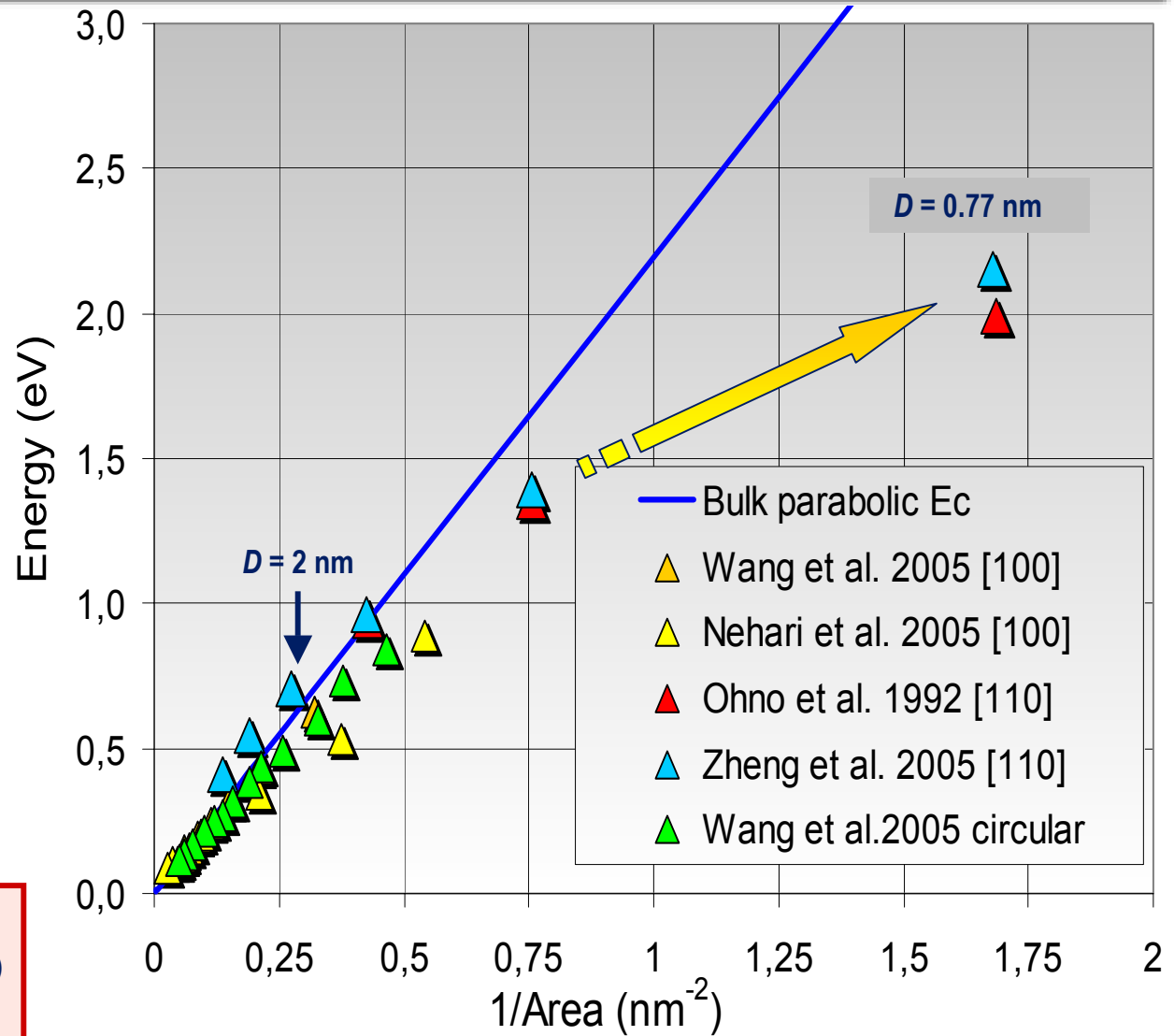
Limits of the bulk EM approximation

- ❑ 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.

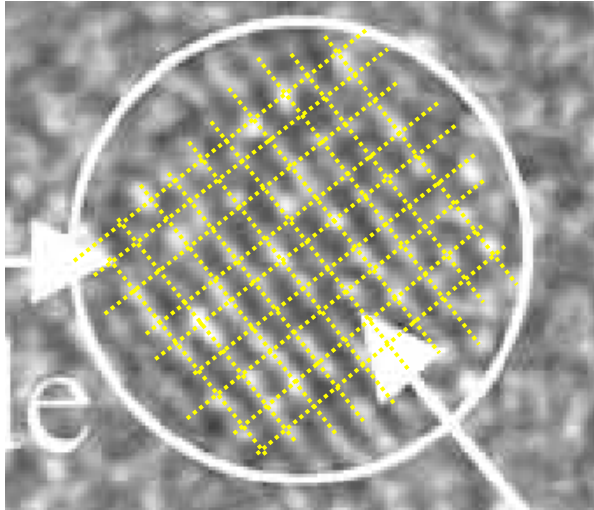
Non-parabolicity & energy gap



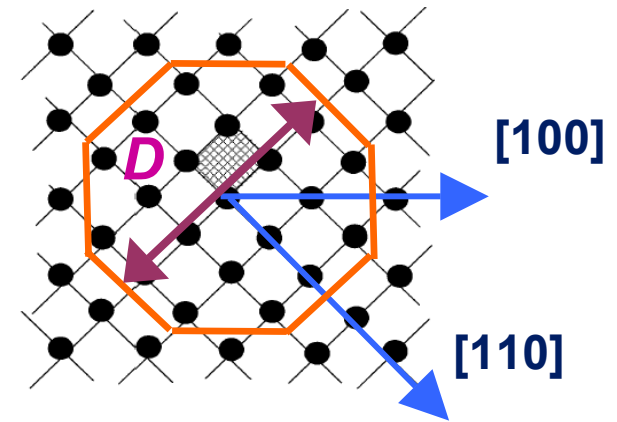
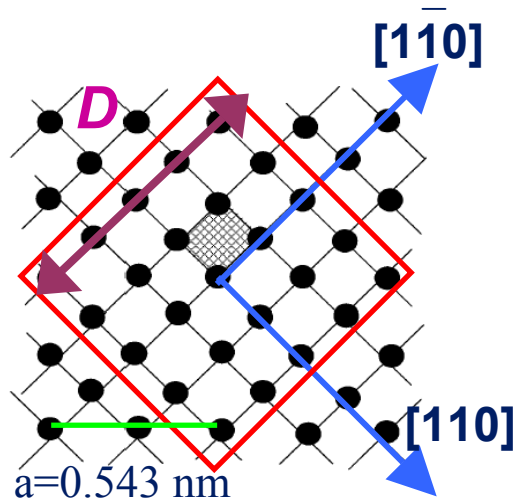
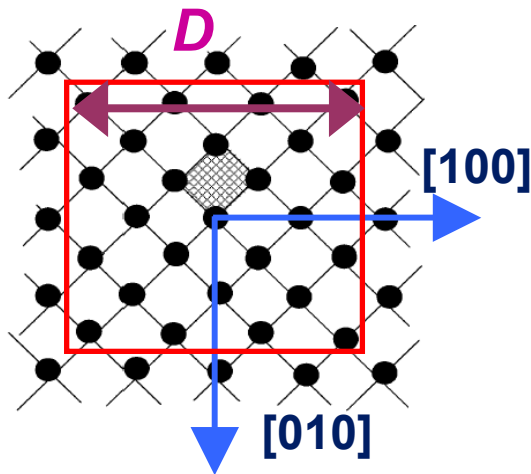
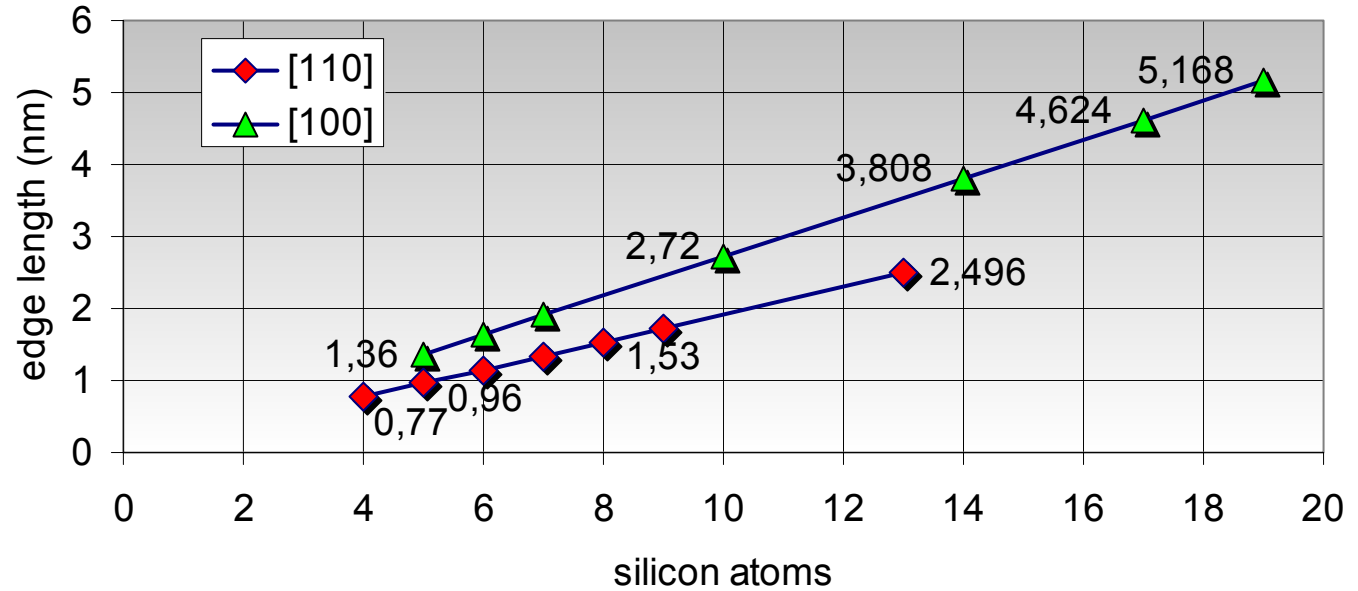
The reduction of the structure size forces k to shift to higher values $\rightarrow E(k)$ is not parabolic anymore.



Limited number of atoms in the cross-section



(100)-Si wafer/⟨001⟩-Si wire



An extreme solution

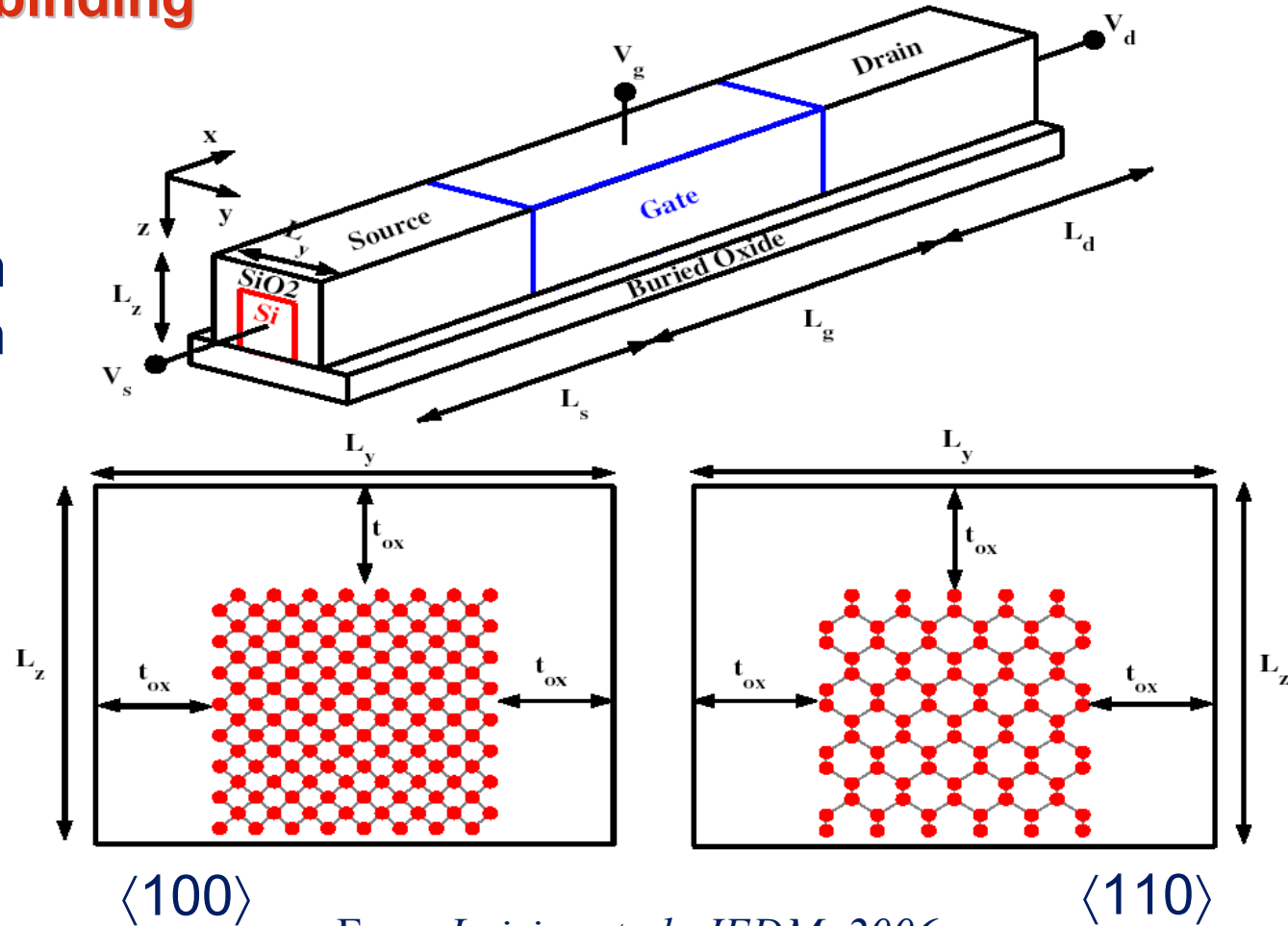
Full 3D atomistic tight binding (TB) simulation.

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

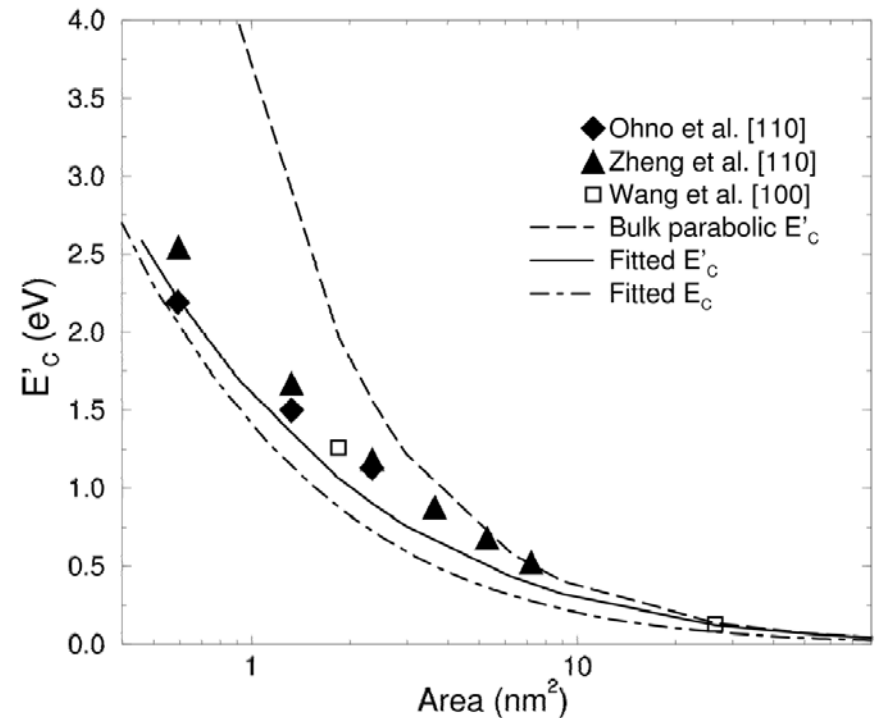
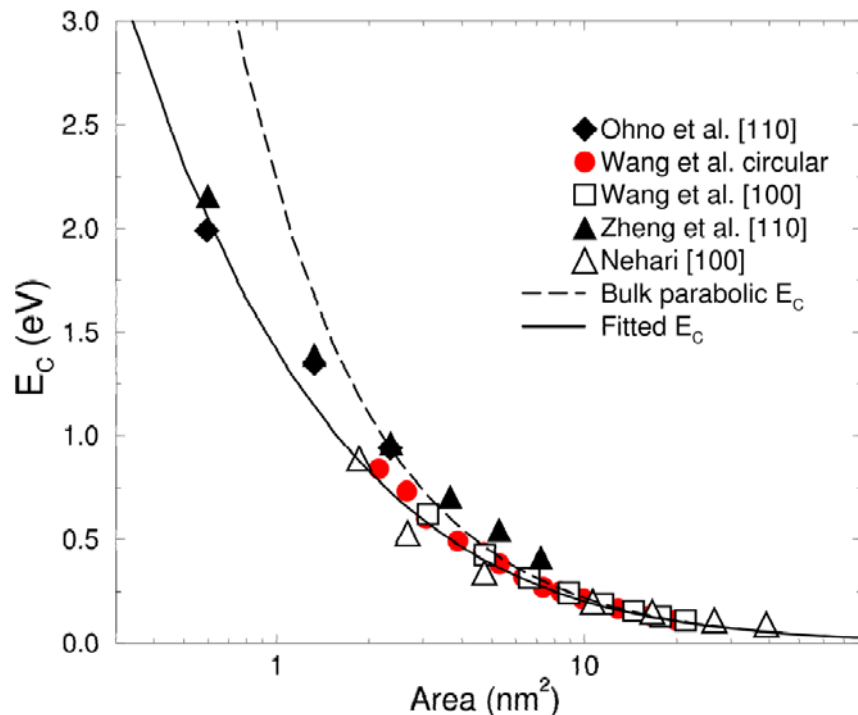
Outline

- ❑ 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

An engineering approach (1)

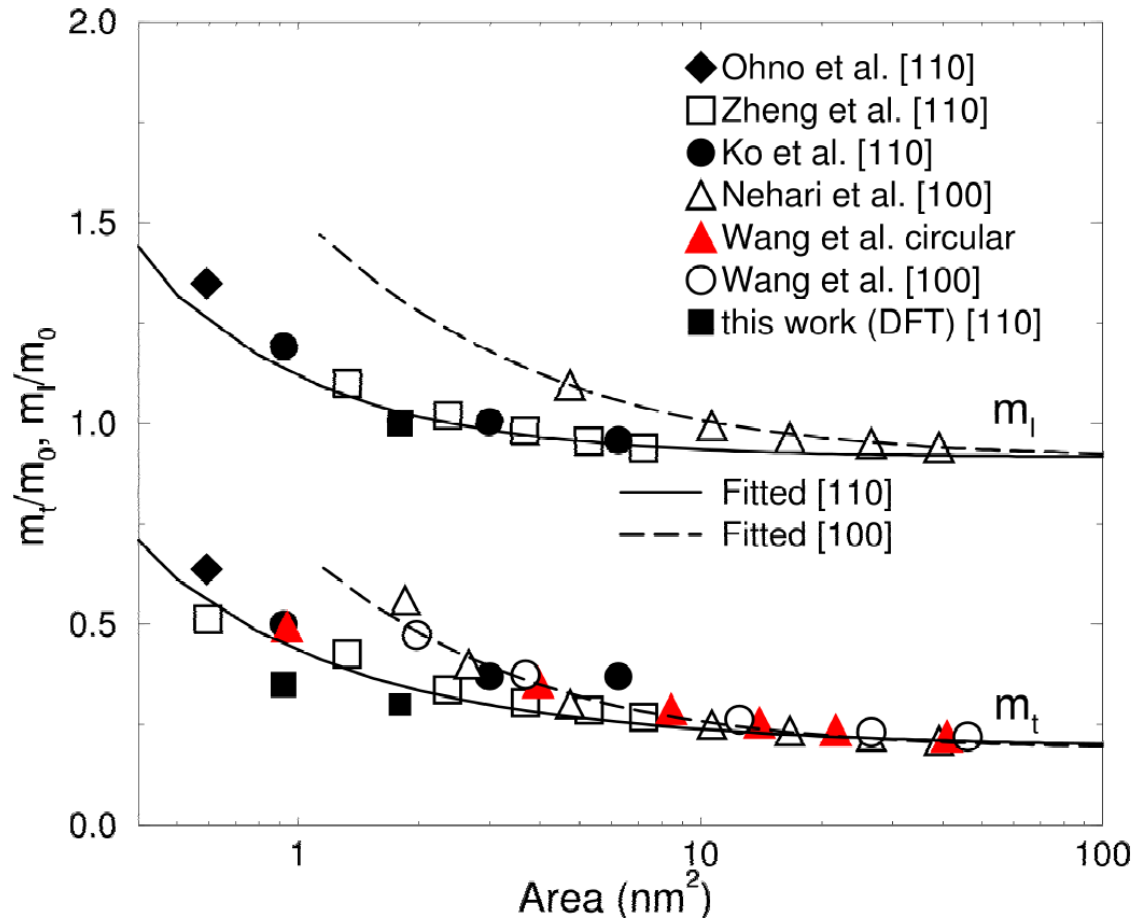
Inject non parabolic corrections into the **constant** EM model scheme:
abandon the bulk EM and use EMs function of the cross-section area,
fitted upon atomistic band calculations for well potentials.

Quantization masses used in the 2D transverse SE (cylinder) are fitted on
subband bottom energies.



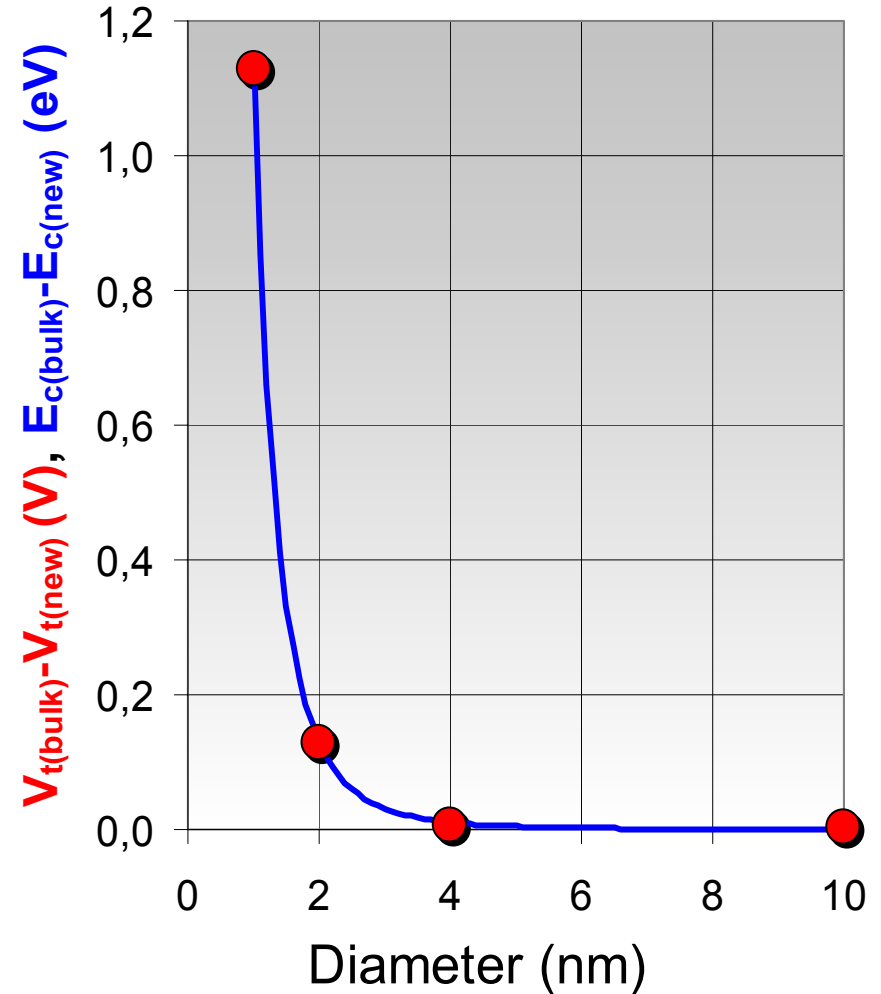
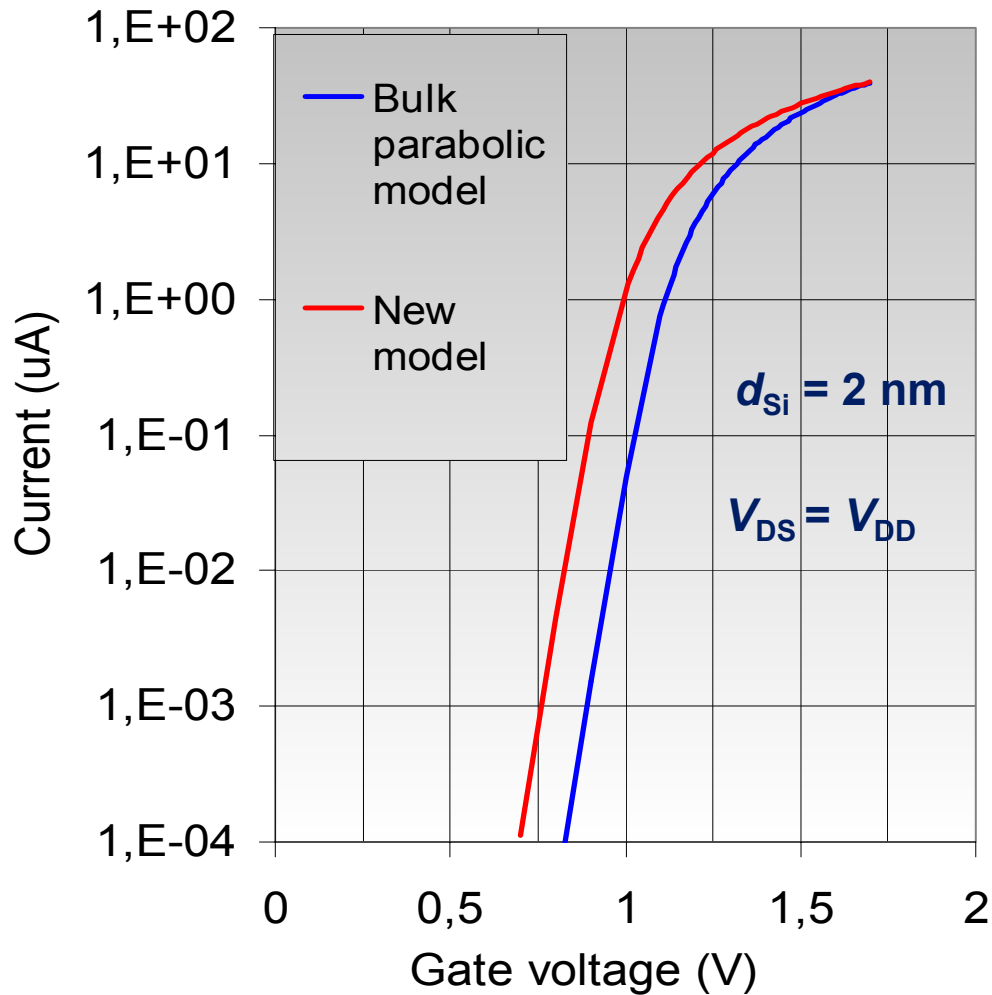
An engineering approach (2)

Transport masses used in the 1D longitudinal SE are fitted on the parabolic part of the 1DEG subbands.

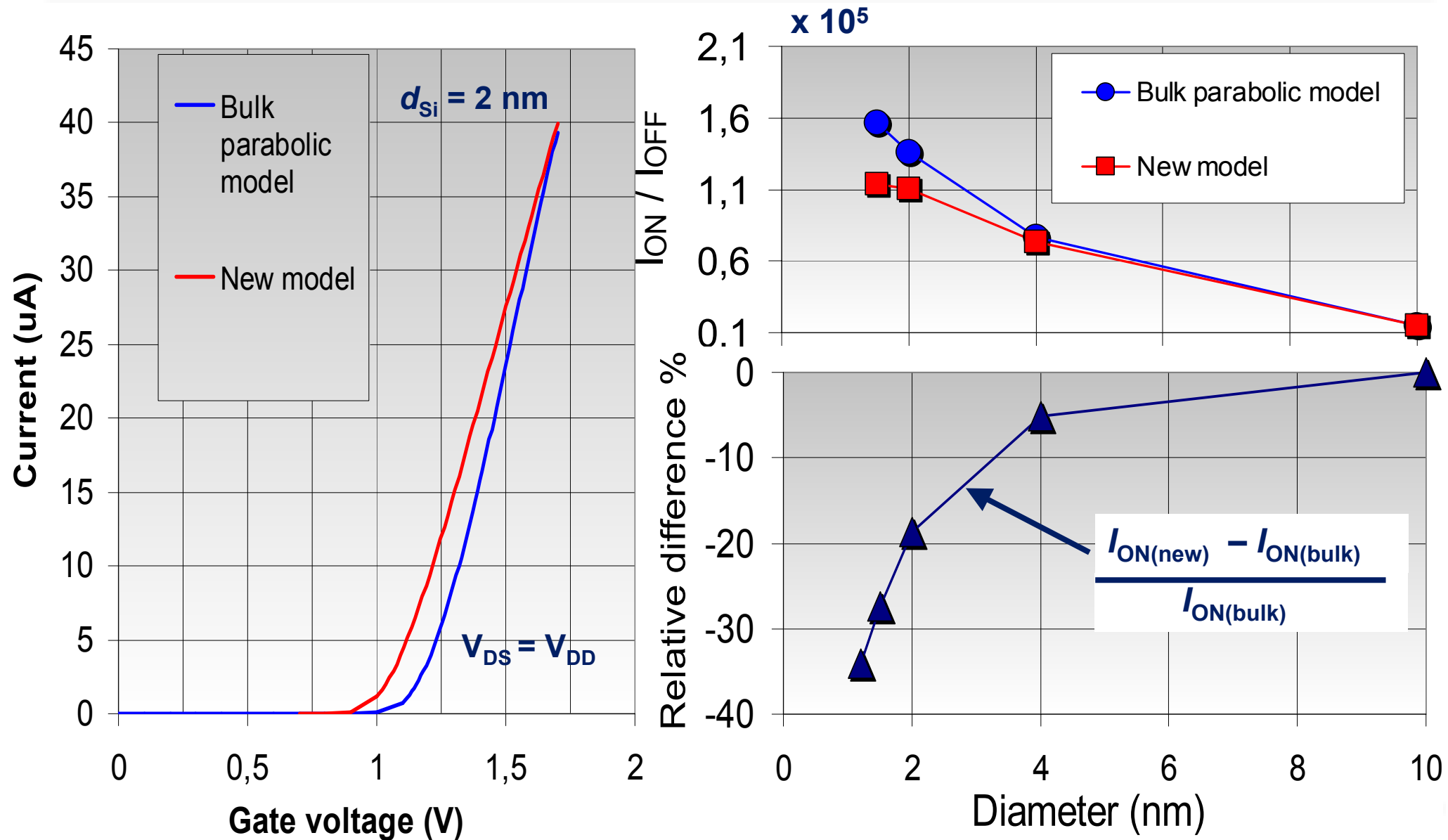


Electrical characteristics: threshold shift

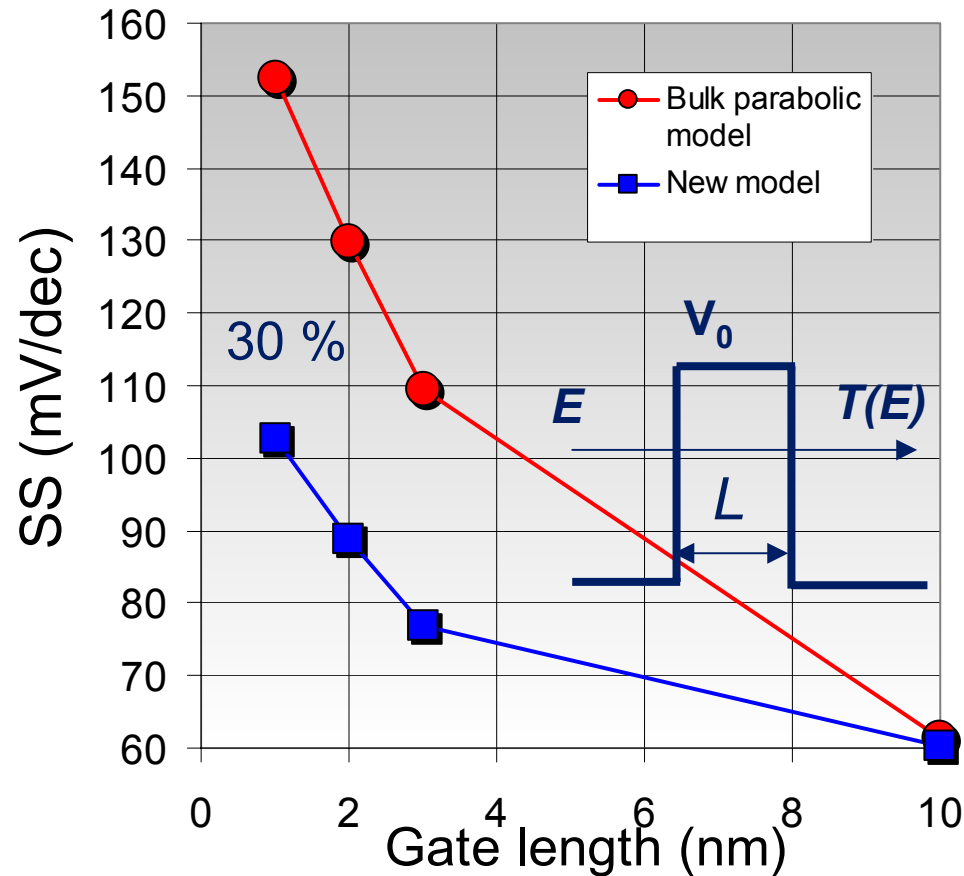
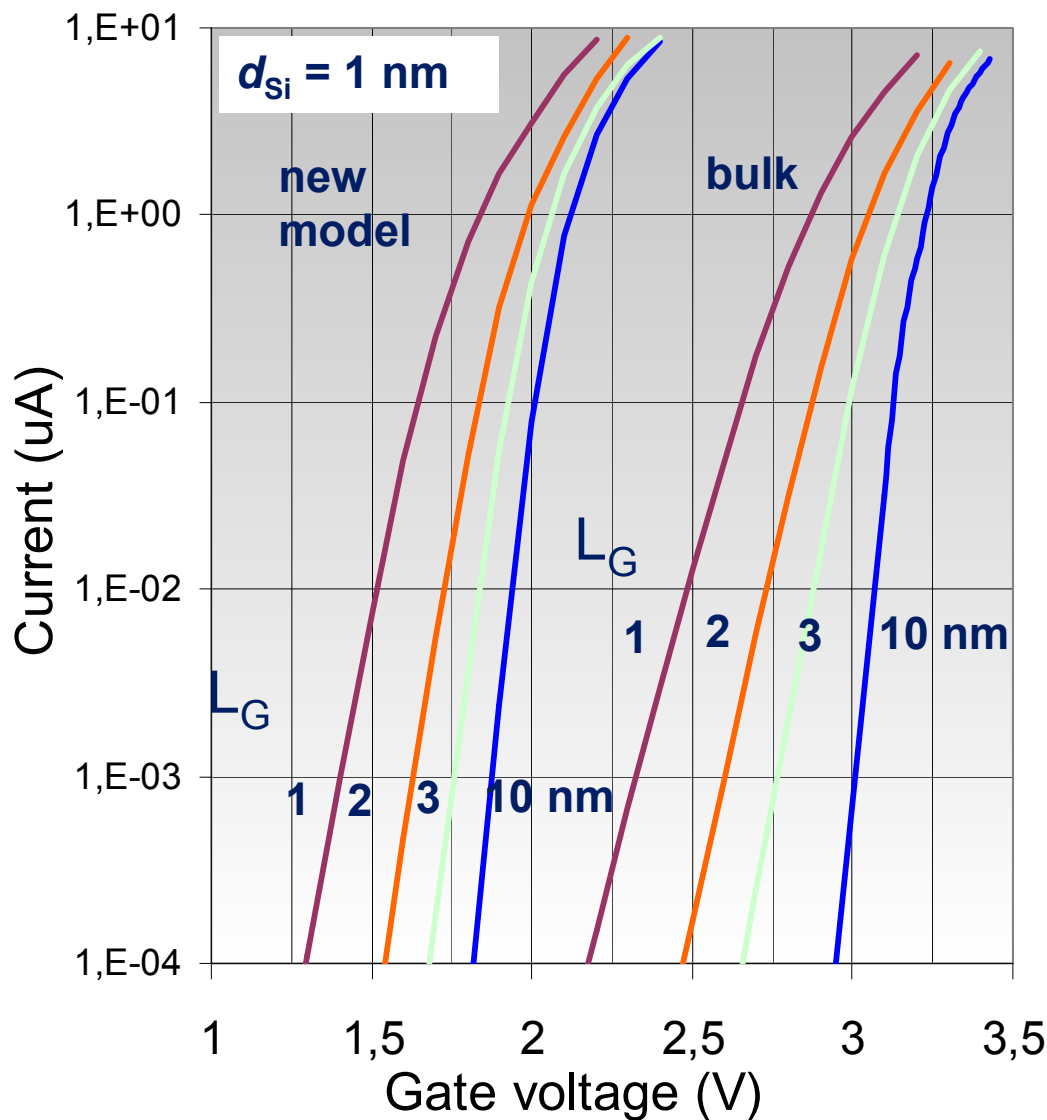
From ITRS 2005: $t_{ox} = 1$ nm & $V_{DD} = 0.7$ V. Analysis at fixed $L_G = 10$ nm:



Electrical characteristics: effects on I_{ON}



Electrical characteristics: subthreshold slope



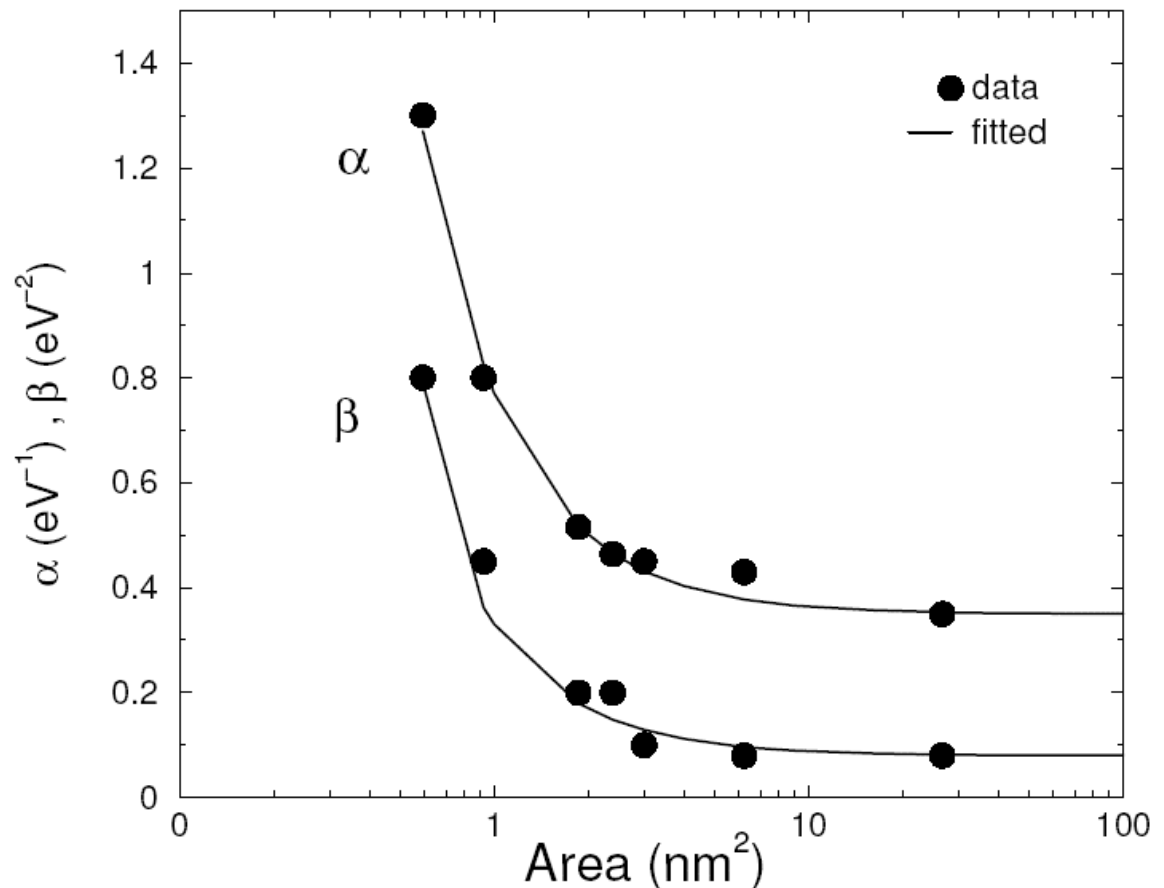
$$T(E) \propto \exp \left[-2 \frac{\sqrt{2m(V_0 - E)}}{\hbar} L \right]$$

A higher order engineering approach

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

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

α and β fitted on the
1DEG subbands



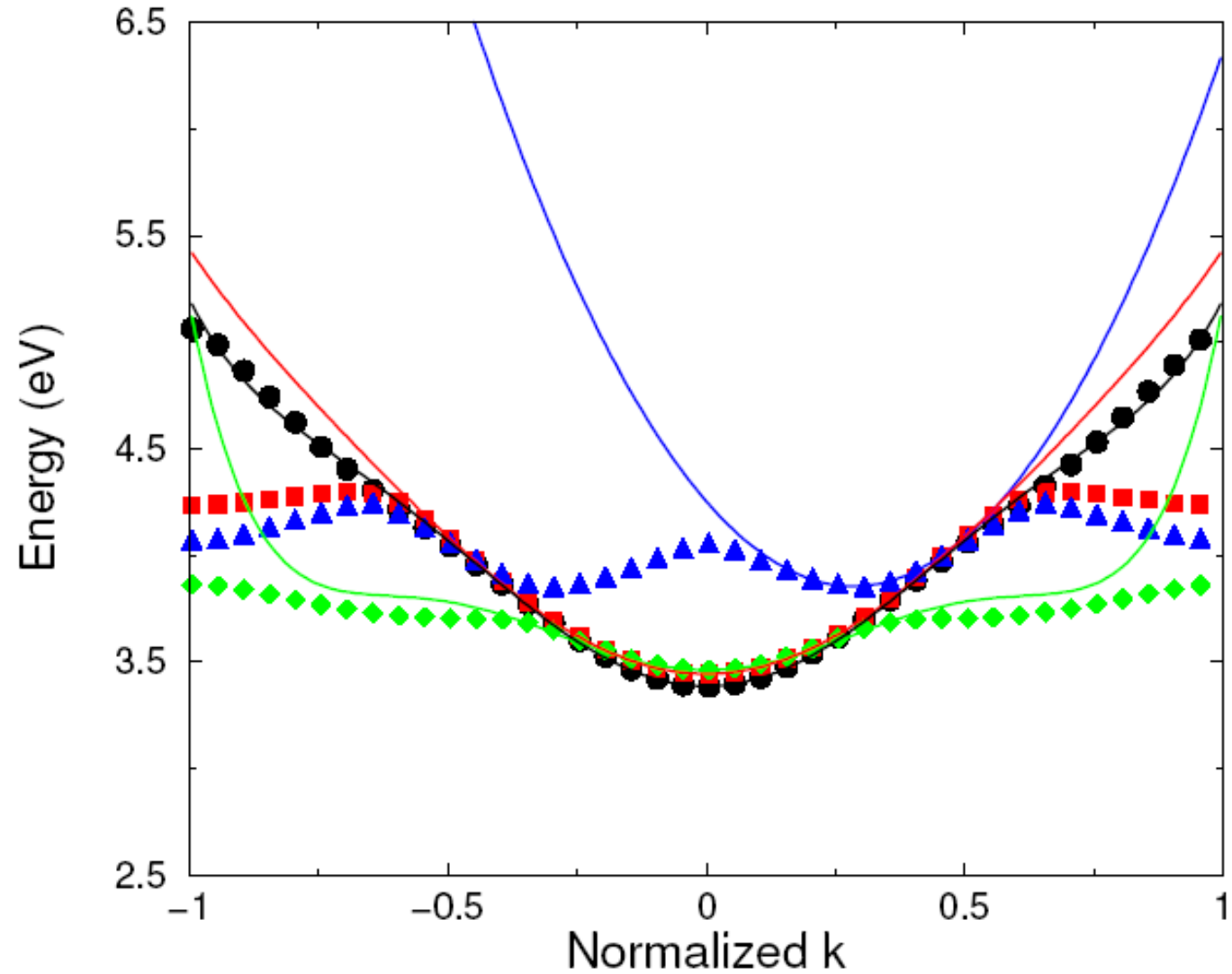
Example of 1DEG subband fitting

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

Symbols = DFT

Red squares:
twofold degenerate

Solid lines =
6th order fitting



Non-parabolic Hamiltonian: formulation

A **non-parabolic** $E(k)$ relationship can always be expanded in series of k^2 due to the parity of the dispersion relationship

$$E(k) = \frac{\hbar^2 k^2}{2m^*} \quad \longrightarrow \quad E(k) = \frac{\hbar^2}{2m^*} \sum_{n=1}^{\infty} b_n k^{2n}$$

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

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

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)

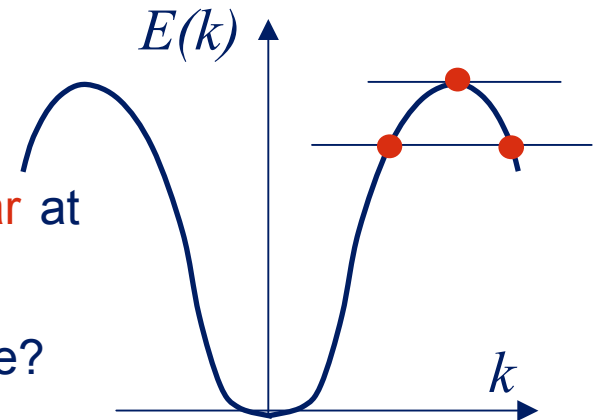
- ❑ A direct discretization scheme (central differences) does not seem to work properly.
- ❑ The transfer matrix method (TMM) provides much more reliable results (at least up to the 6th order). However...
- ❑ The TMM approach (from the literature) is based on:
 1. **staircase potential**
 2. in each element $\psi_i = A_i e^{jk_i x} + B_i e^{-jk_i x}$ with k_i in the first Brillouin zone
 3. **continuity of ψ 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 ks (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 ks**
- ❑ ... 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

$$\left\{ \begin{array}{l} \left[\varepsilon \left(-j \frac{d}{dx} \right) + U(x) \right] \psi(x) = E\psi(x) \quad \text{1D open-boundary SE} \\ \varepsilon(k) = \sum_n \varepsilon_n e^{jkna} \end{array} \right.$$

generic subband: use Fourier expansion!!

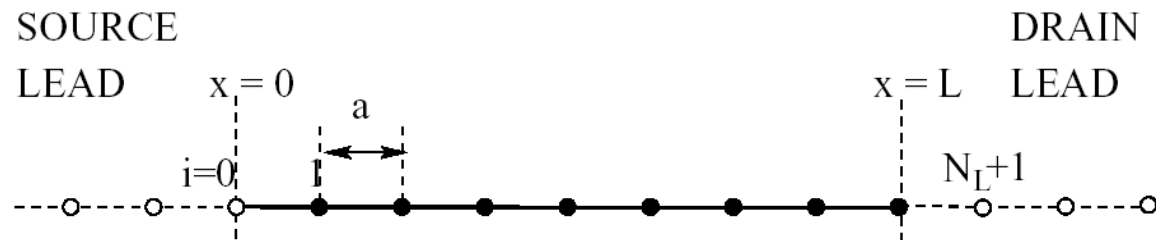
$$\left[e^{na \frac{d}{dx}} \right] \psi(x) = \left[\sum_l \frac{1}{l!} \left(na \frac{d}{dx} \right)^l \right] \psi(x) = \psi(x + na)$$



$$\sum_n \varepsilon_n \psi(x + na) + U(x)\psi(x) = E\psi(x)$$

Discrete form:

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

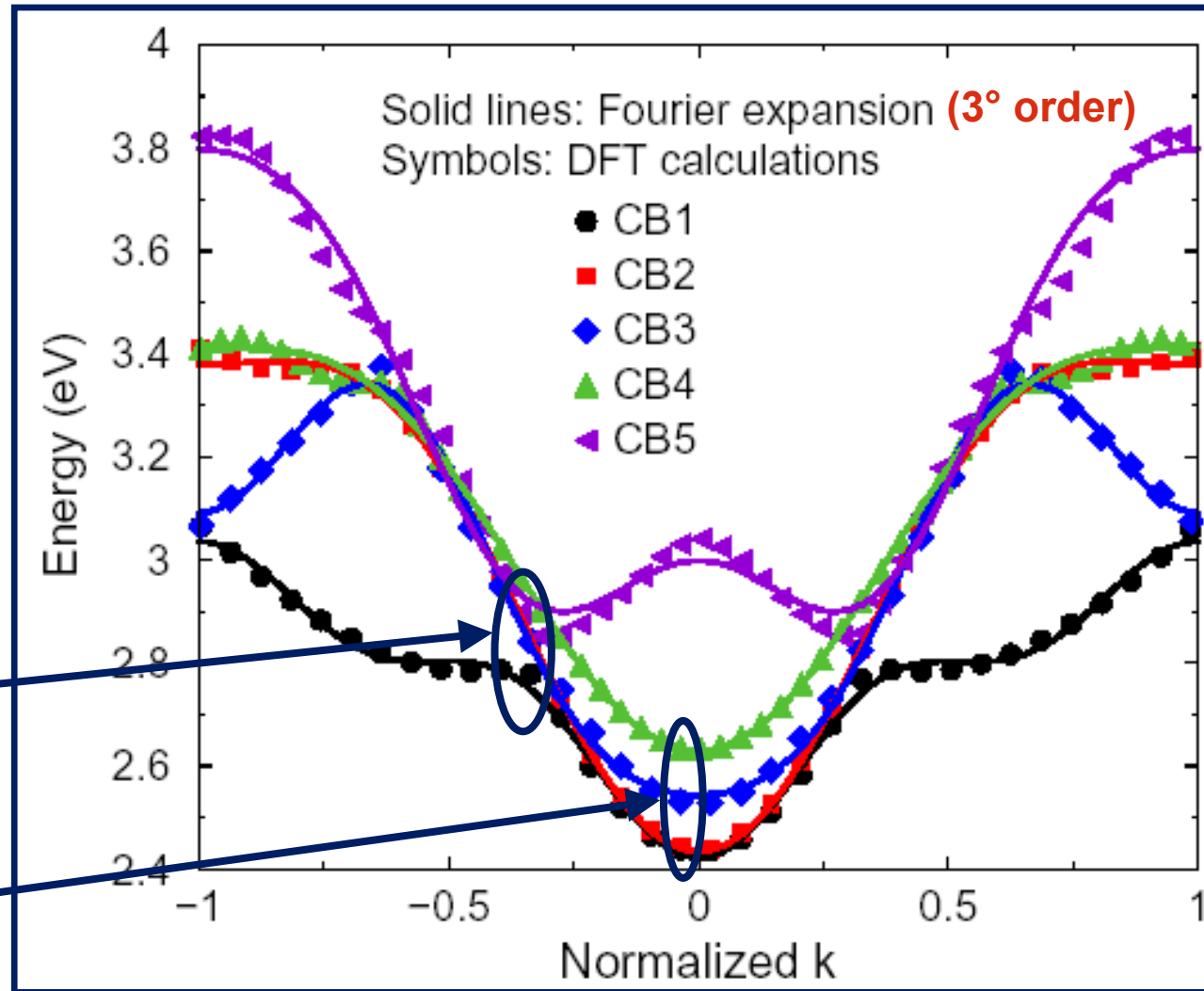


Subband features and Fourier expansion

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

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:

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

Expression of the wave function within the source lead:

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

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)

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

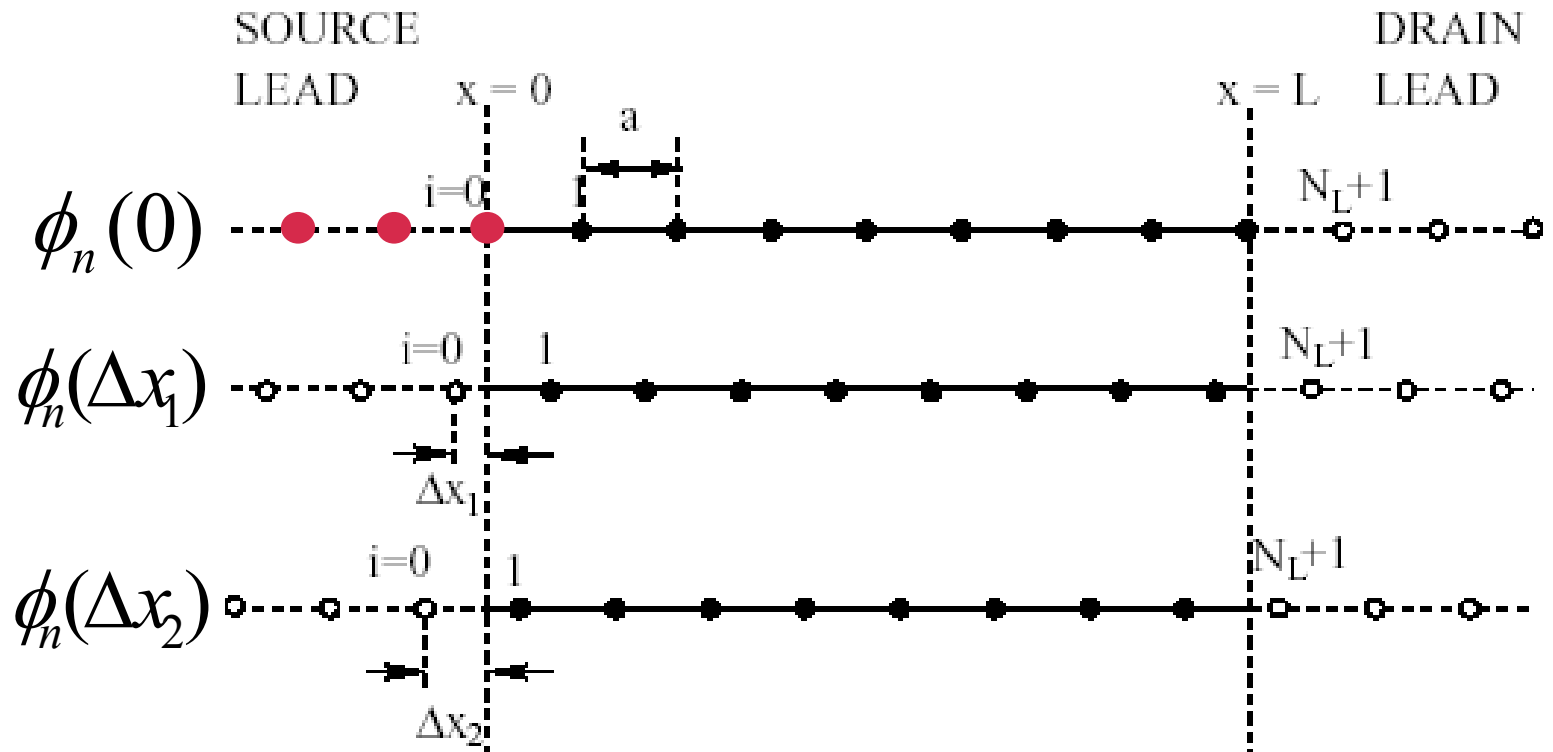
$\phi_n(x+a) = \phi_n(x)$ **N additional periodic unknown functions**

- ❑ 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 $\phi_n(x)$ 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)

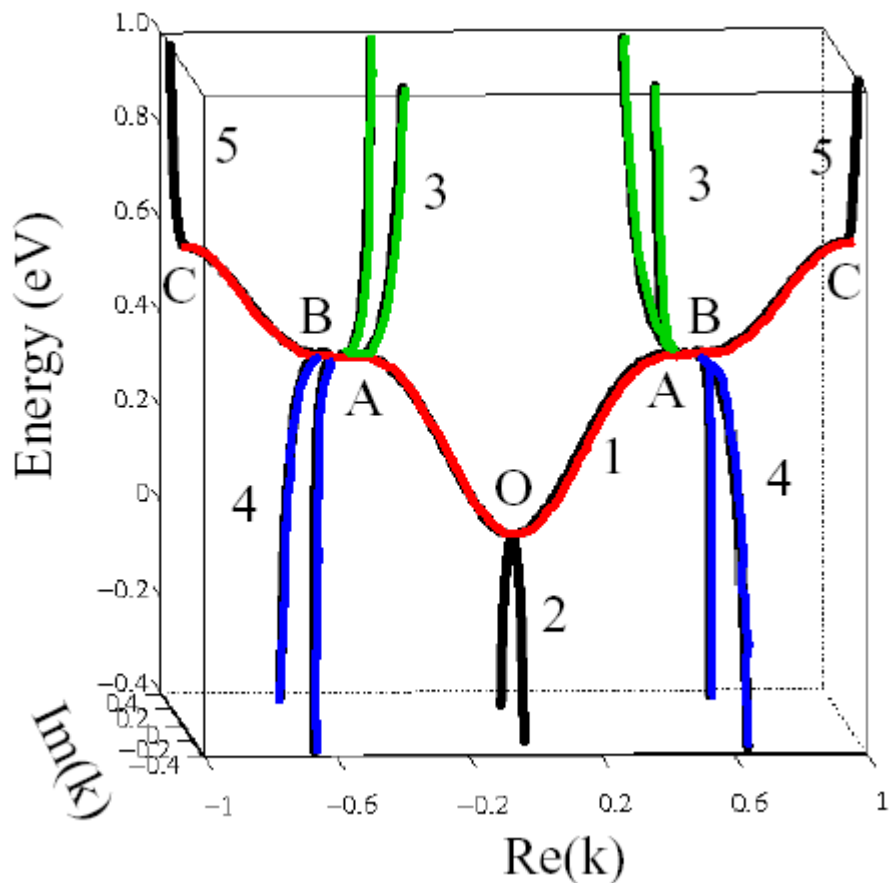


Boundary conditions (4)

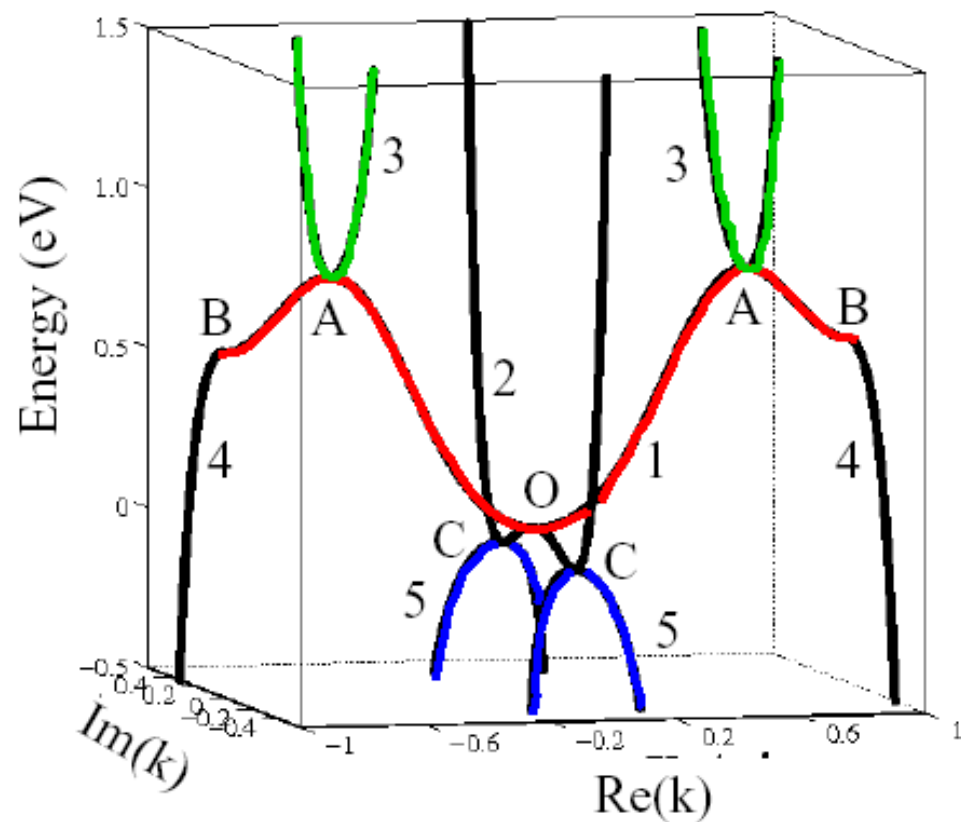
Examples of root *loci* of the characteristic equation $\varepsilon(k_s) = E$

$N = 3$

CB_1



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 $\varepsilon(k)$

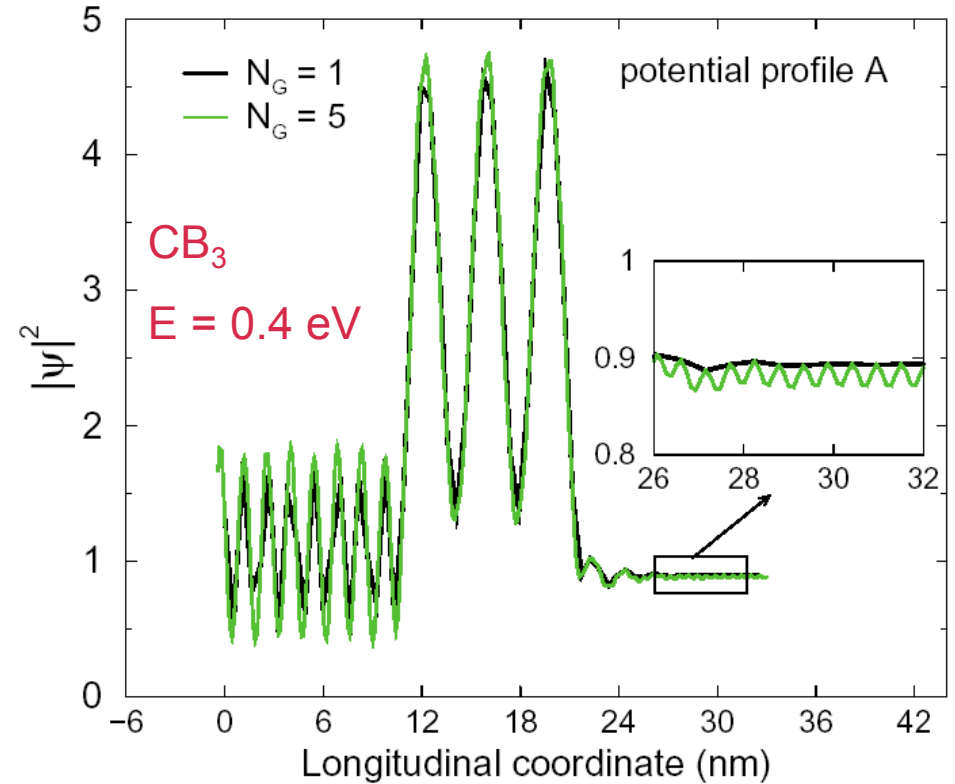
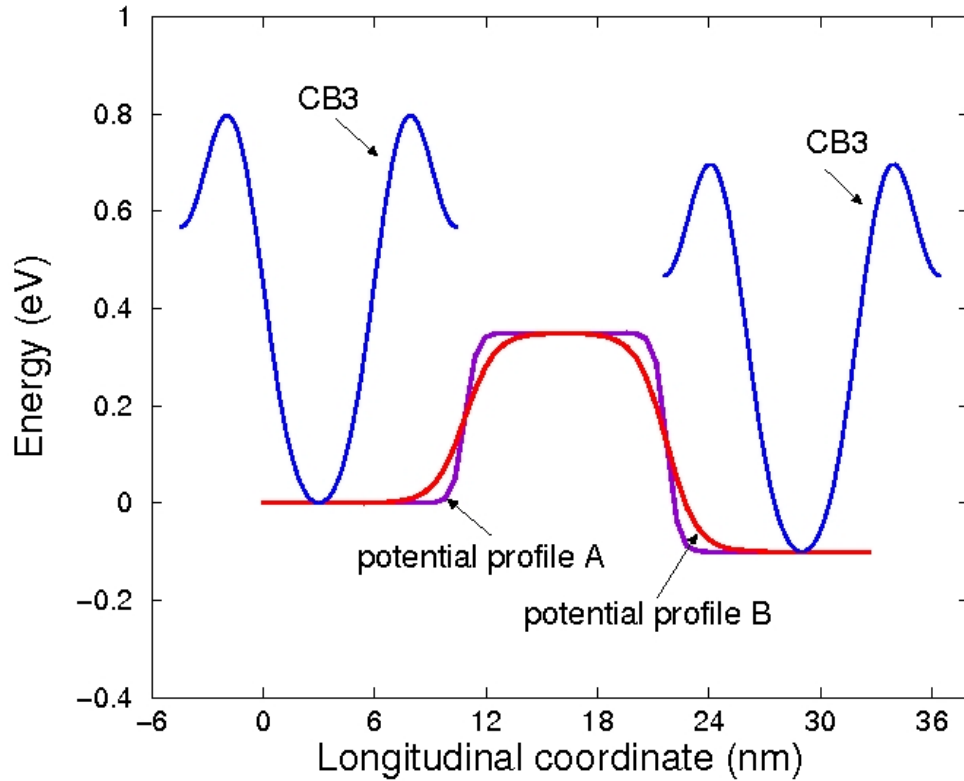
$$\varepsilon(k) = \sum_{s=0}^{\infty} c_s (k^2)^s$$

and using the previous expression of ψ_S

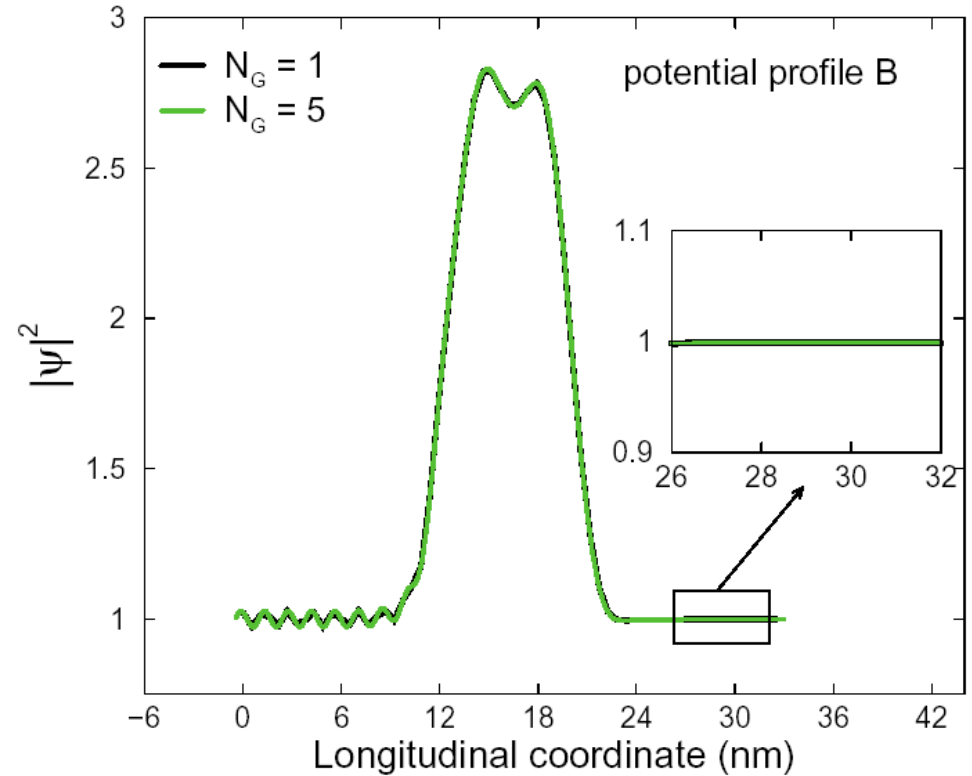
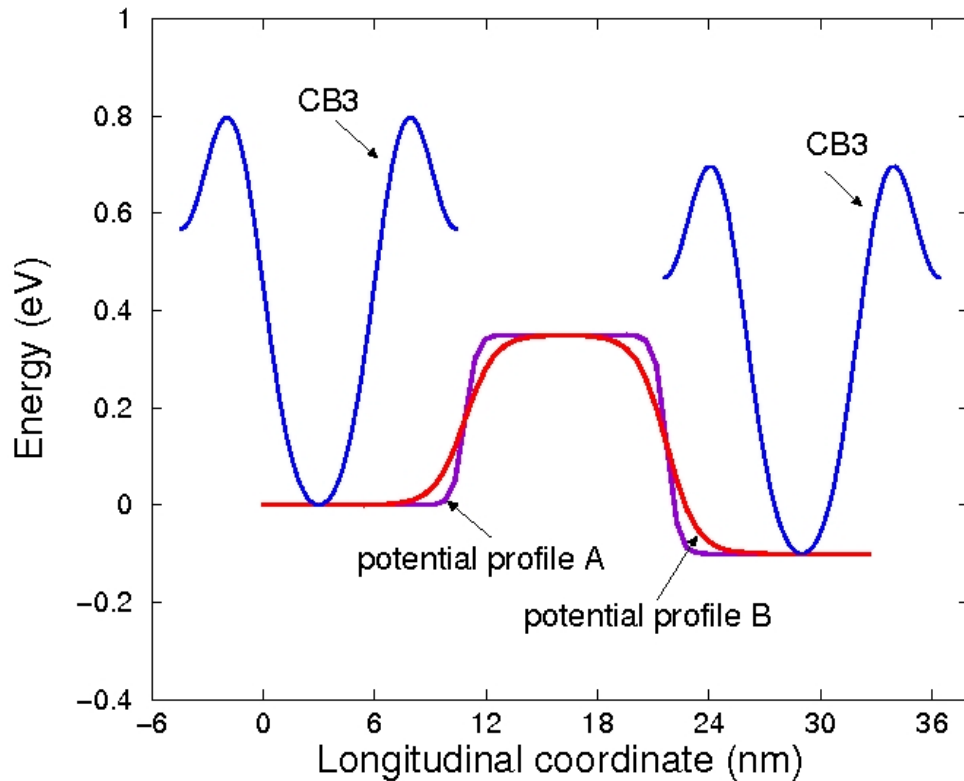
$$\psi_S(x; k_S^{inj}) = A e^{jk_S^{inj} x} + \sum_{n=1}^N e^{jk_S n x} \phi_n(x)$$

with $\phi_n(x)$ approximated with the truncated Fourier series through $\phi_n(0)$, $\phi_n(\Delta x_1)$, ...

Are multiple grids really needed?

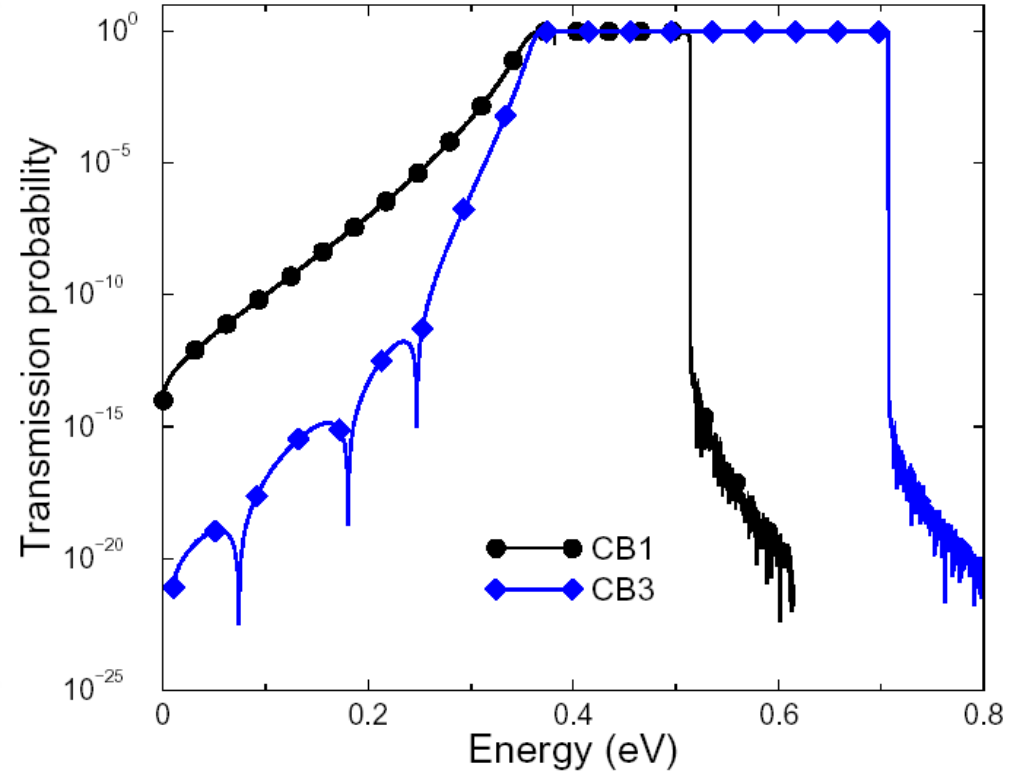
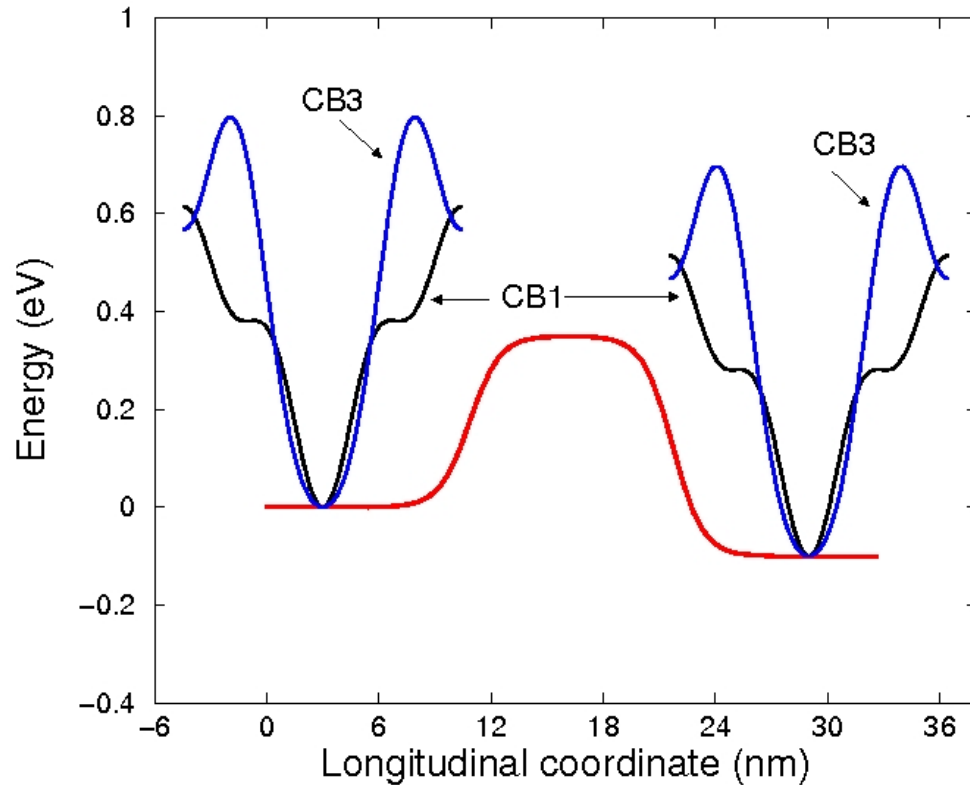


Are multiple grids really needed?



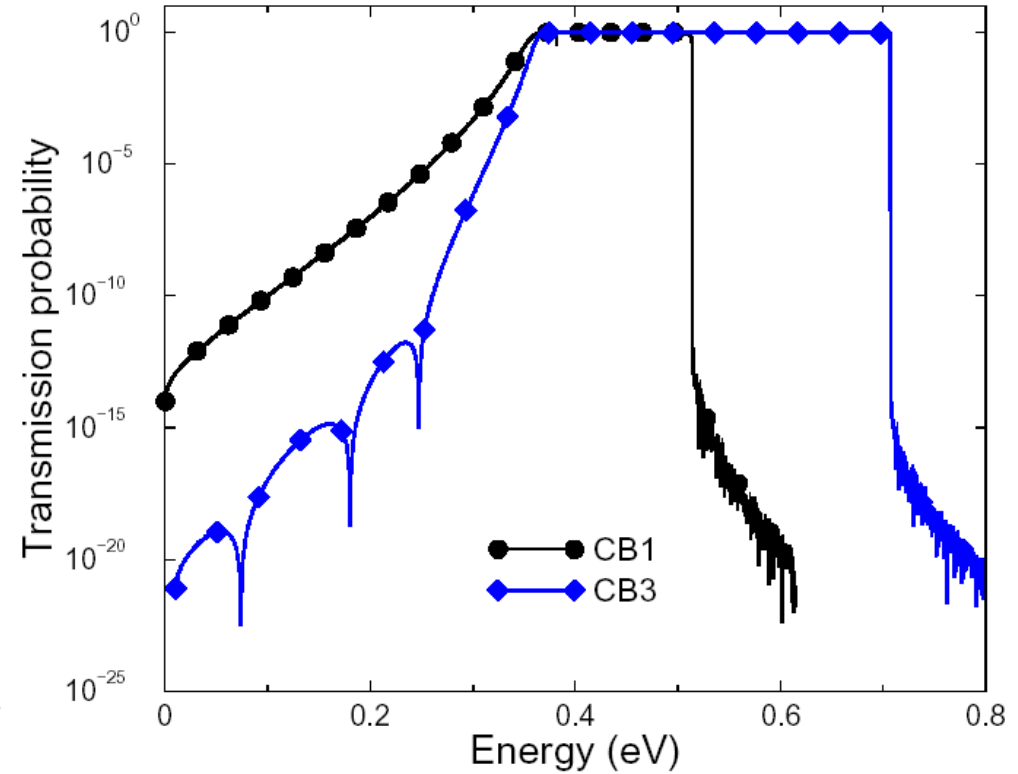
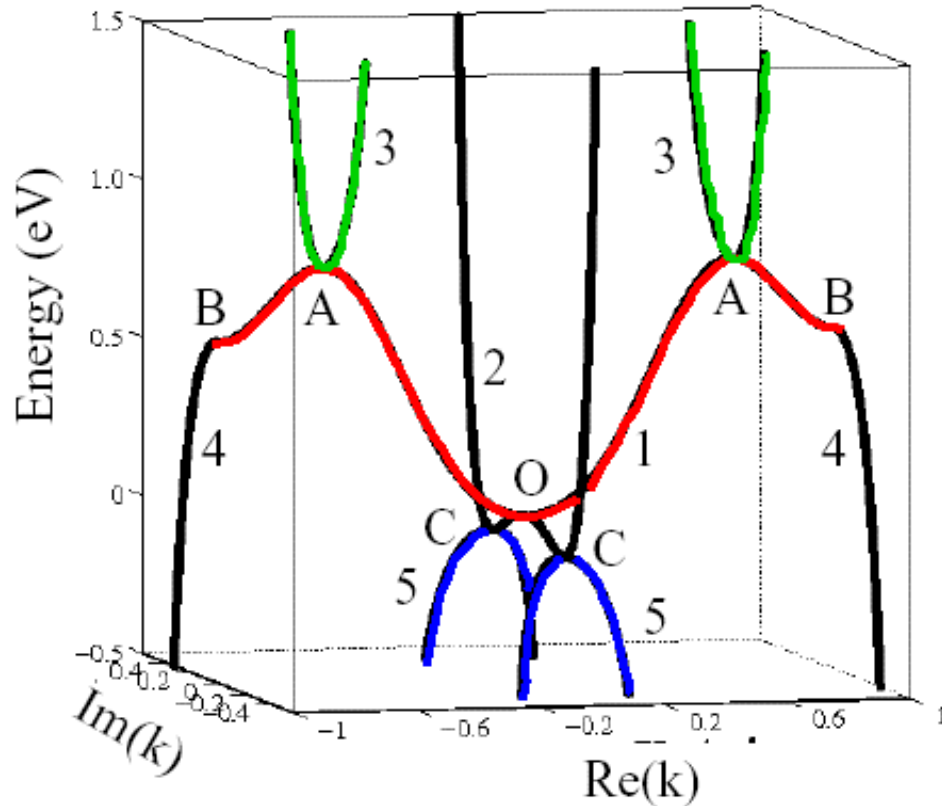
With typical potential profiles one grid is generally sufficient, unless very high charge resolution is required

Band effects on transport



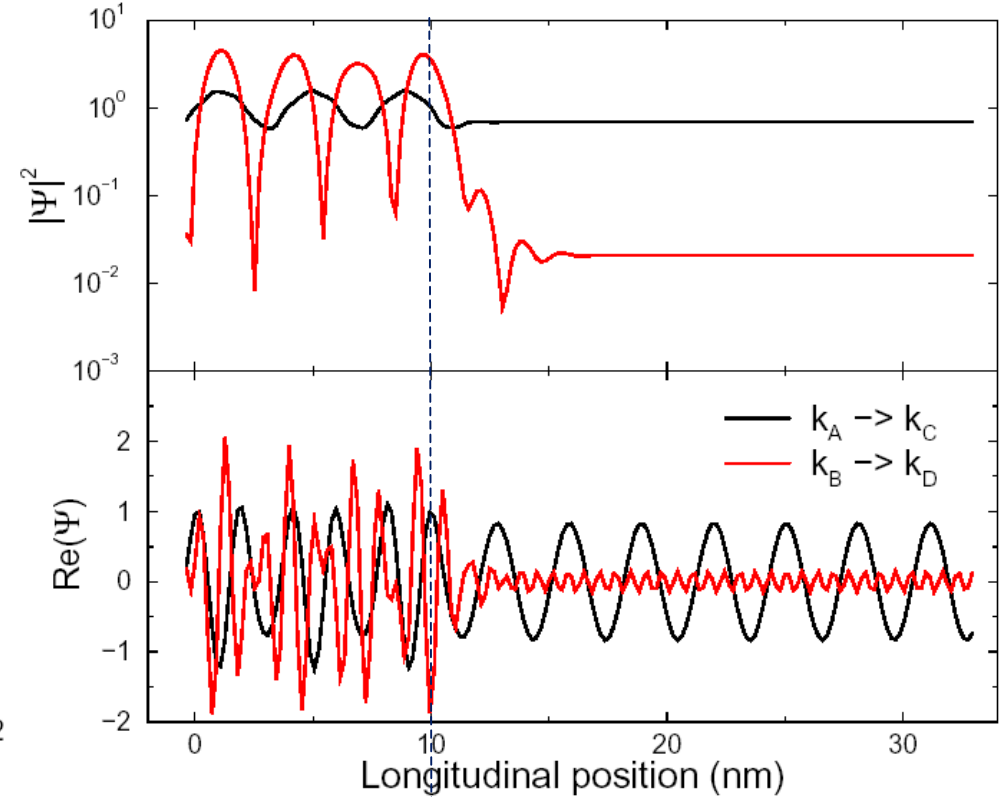
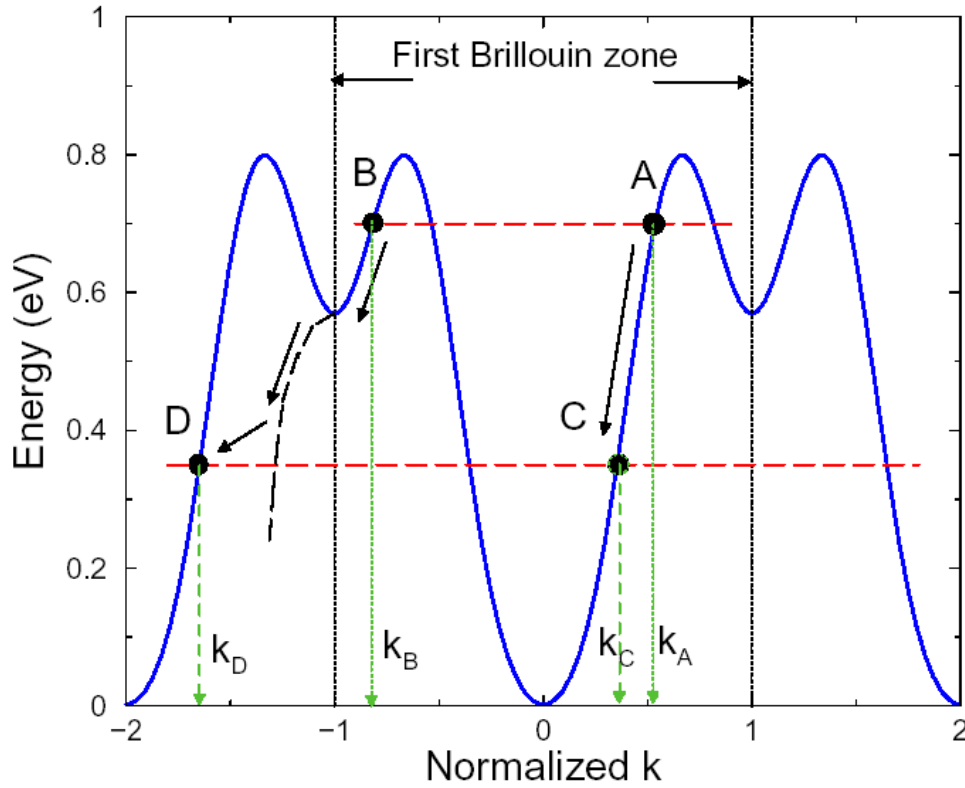
- **T(E) drop due to finite energy extension of the subbands**
- **different SS due to different effective masses**
- **transmission zeros for CB₃ in deep subthreshold**

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

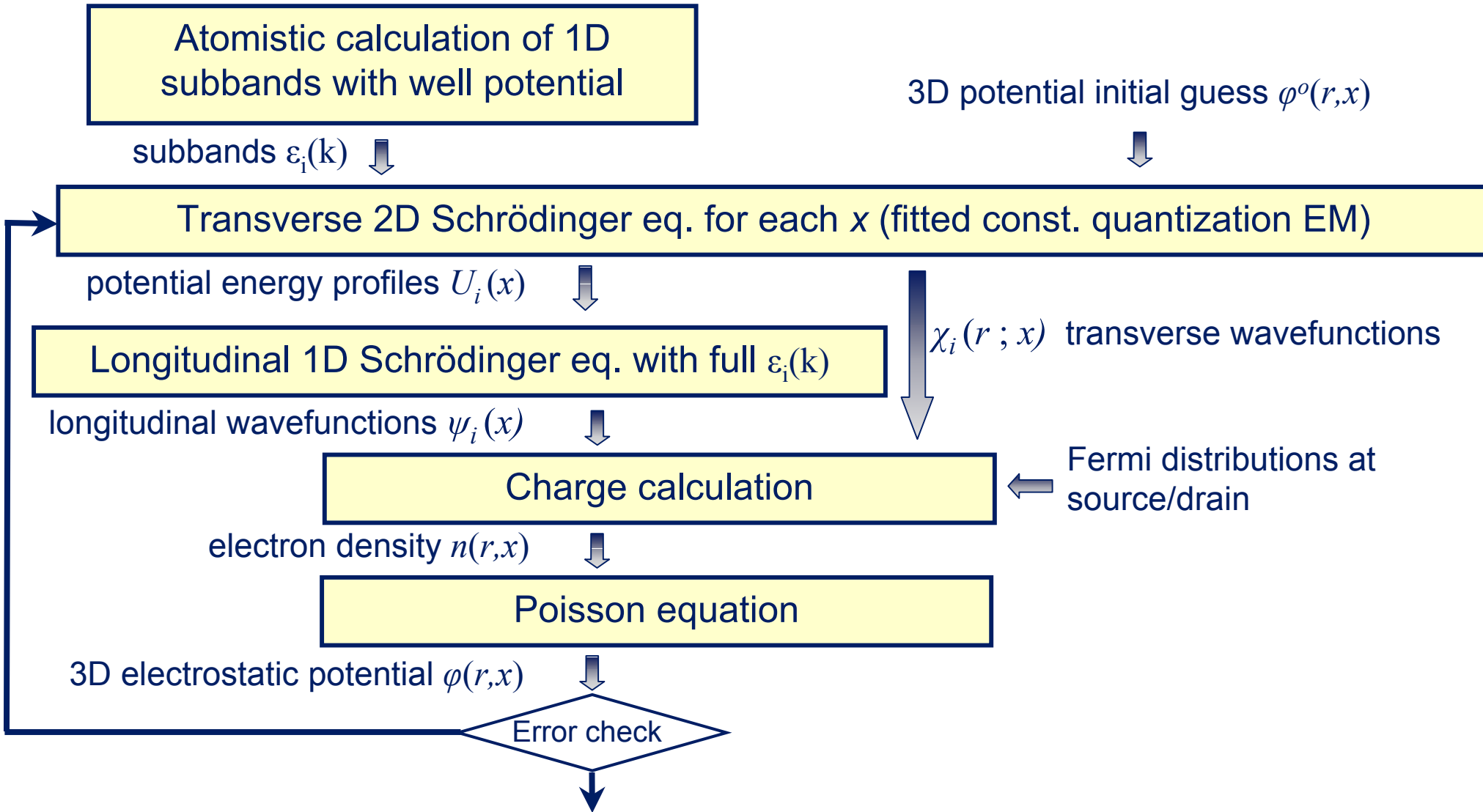
Intervalley transitions: test case



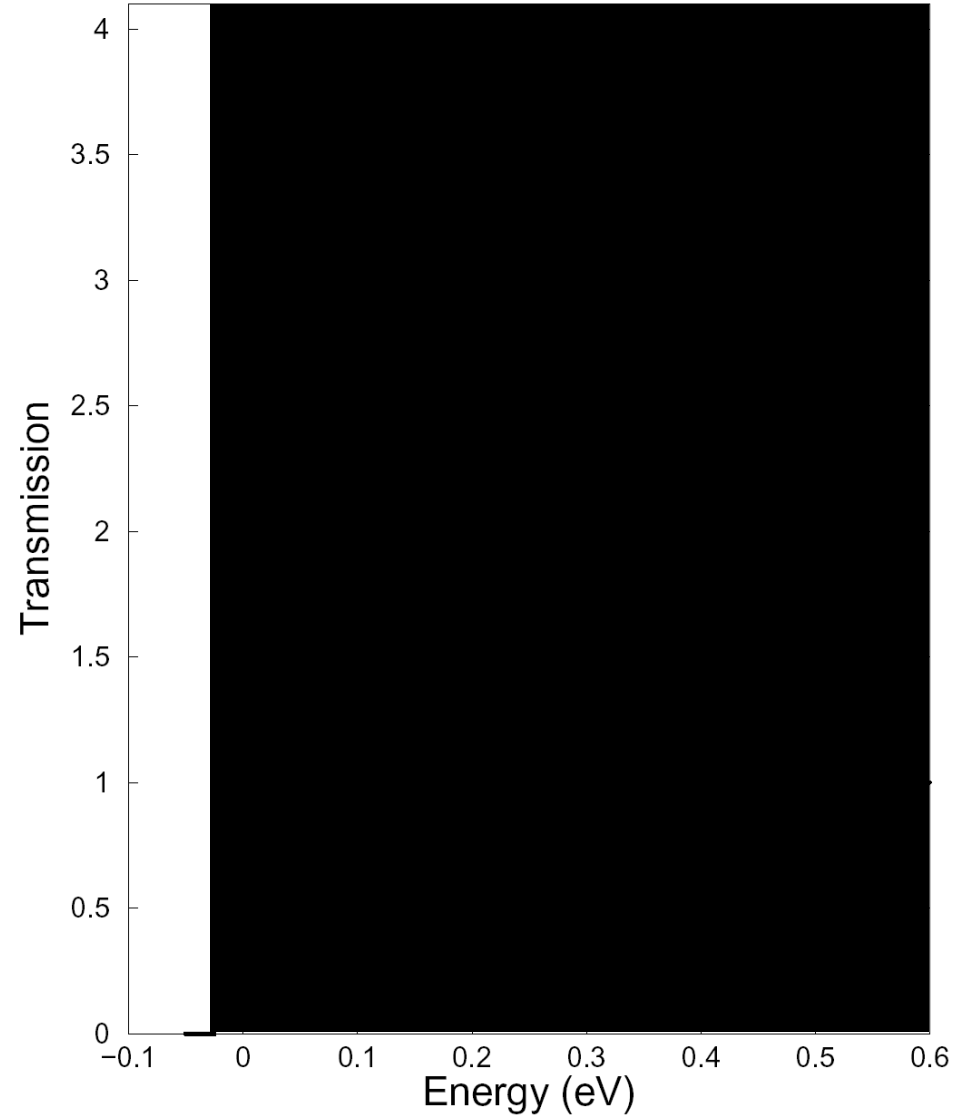
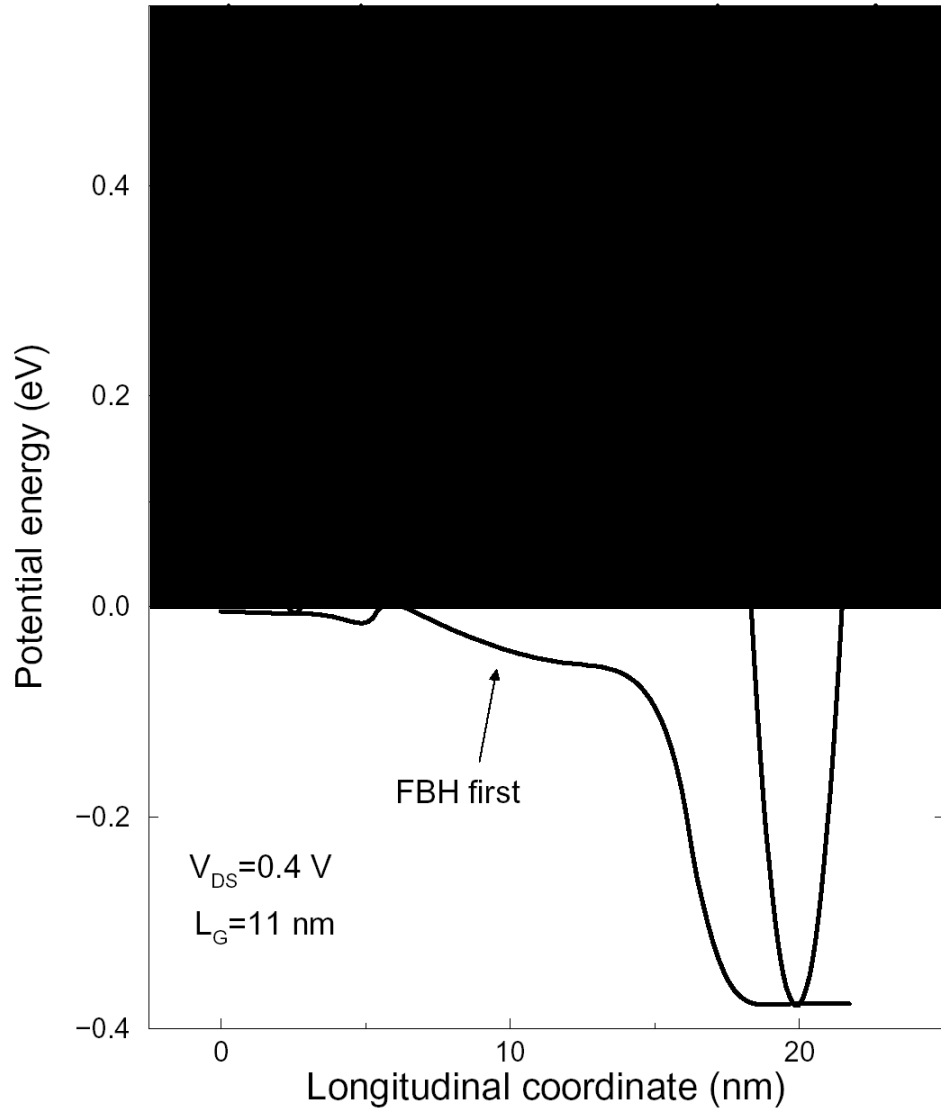
subband CB_3

0.35 V potential step

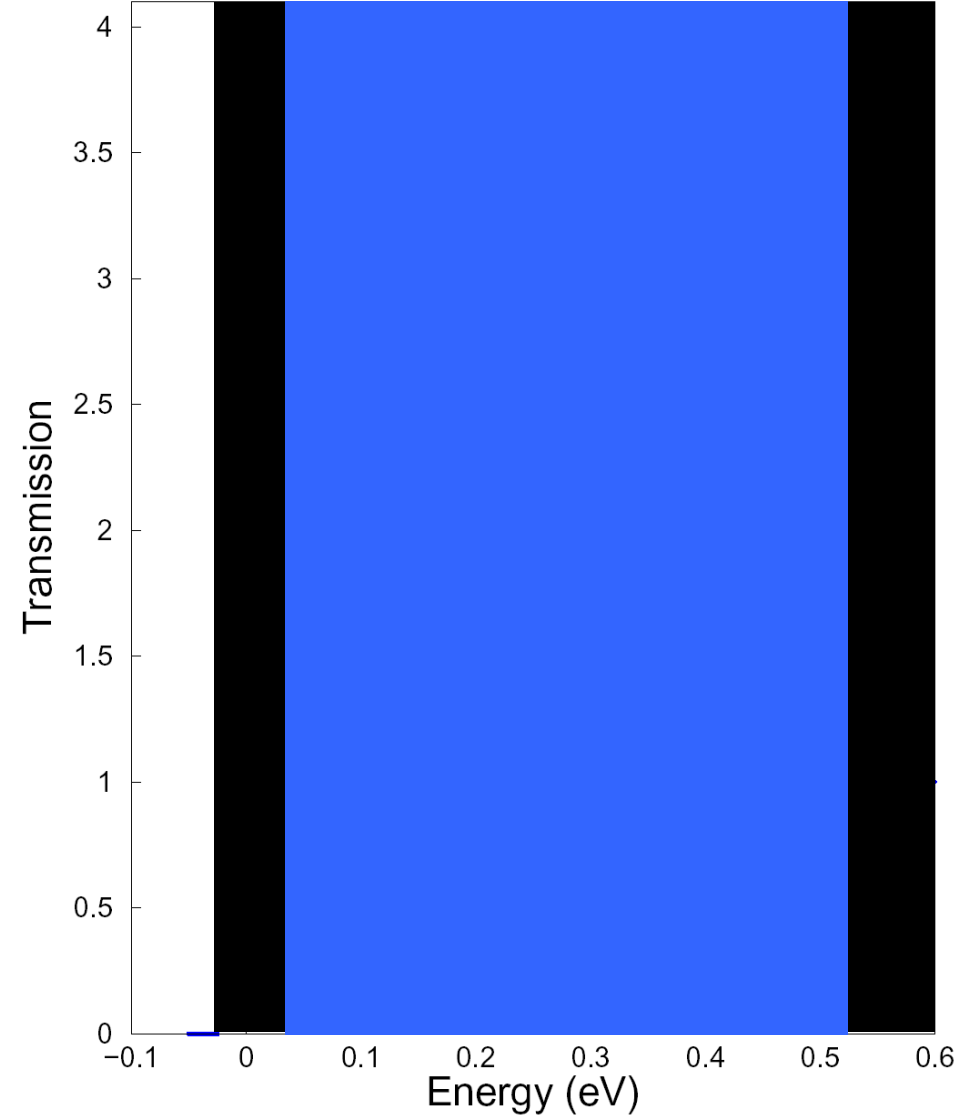
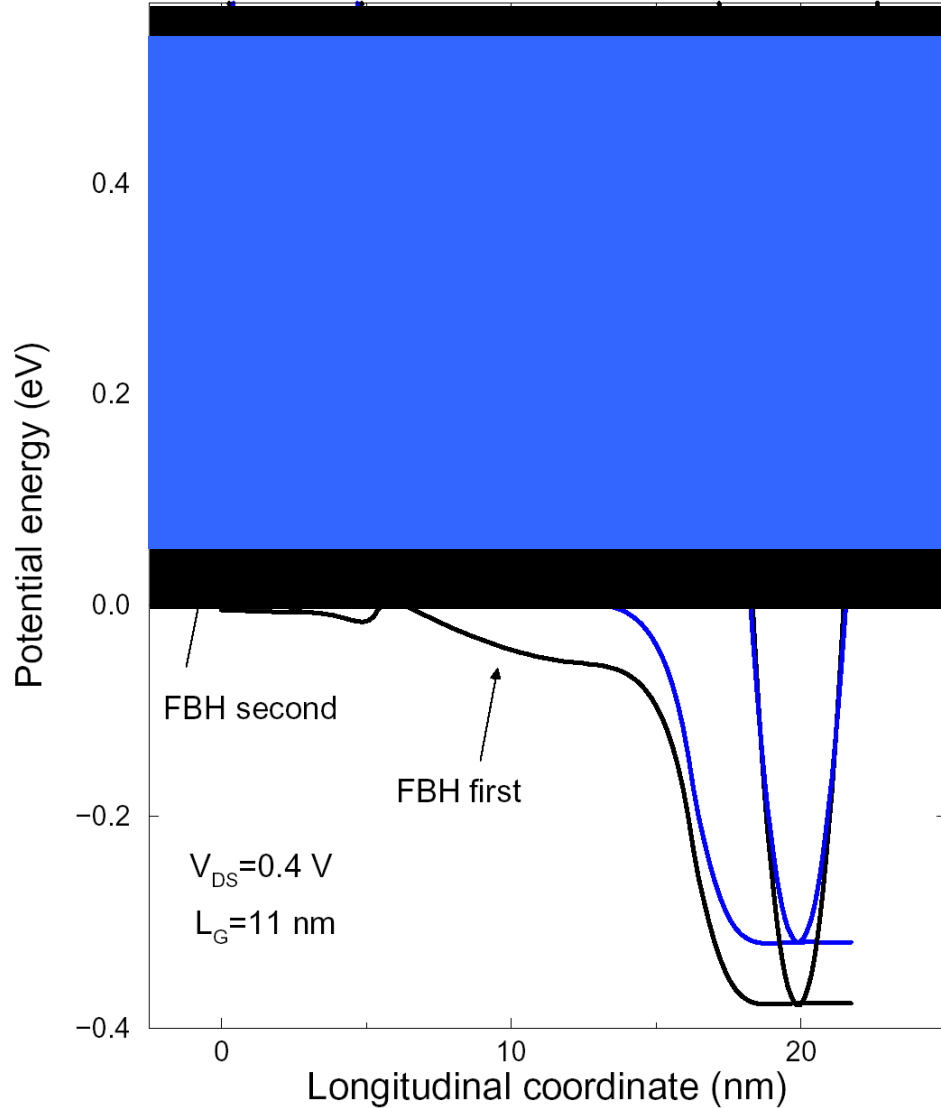
Application to device simulation: flow chart



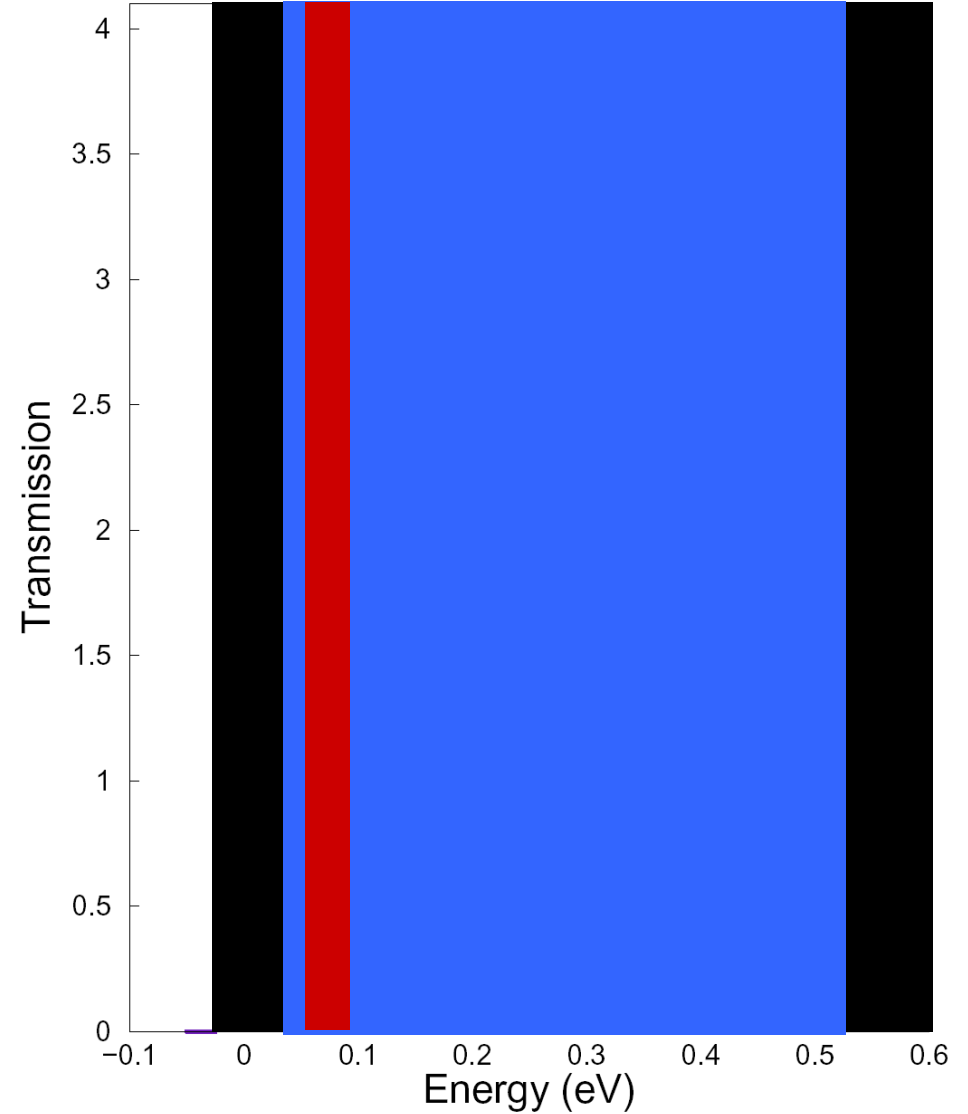
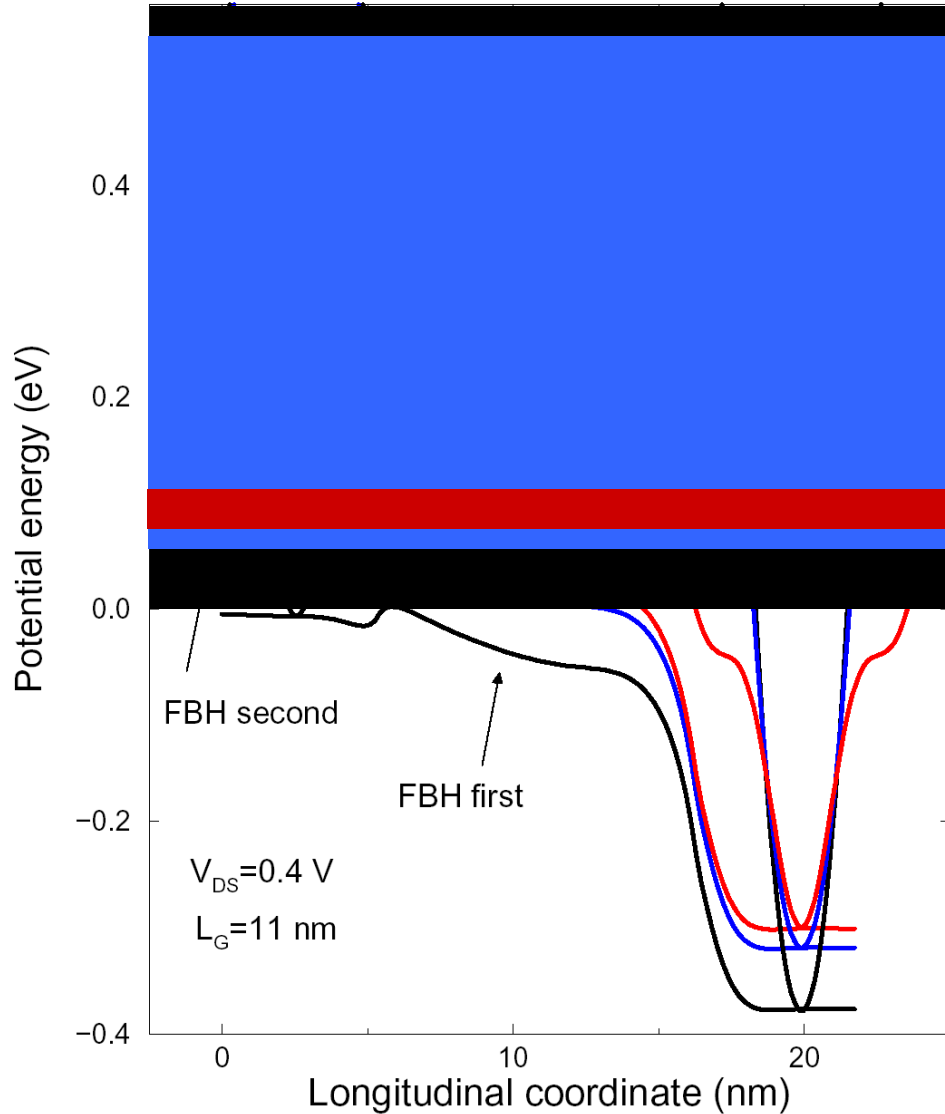
Transmission coefficient – 1st subband



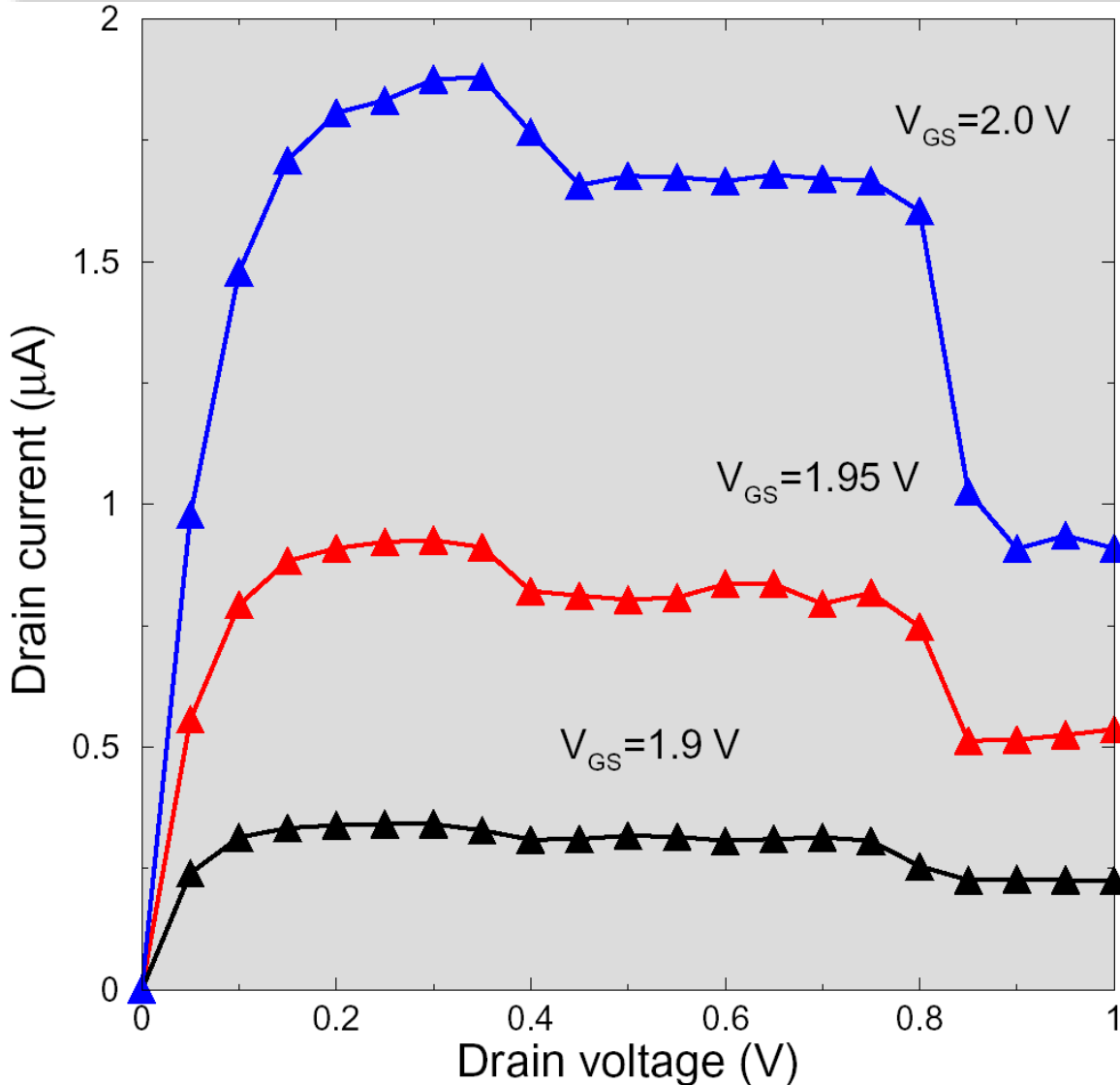
Transmission coefficient – 2nd subband



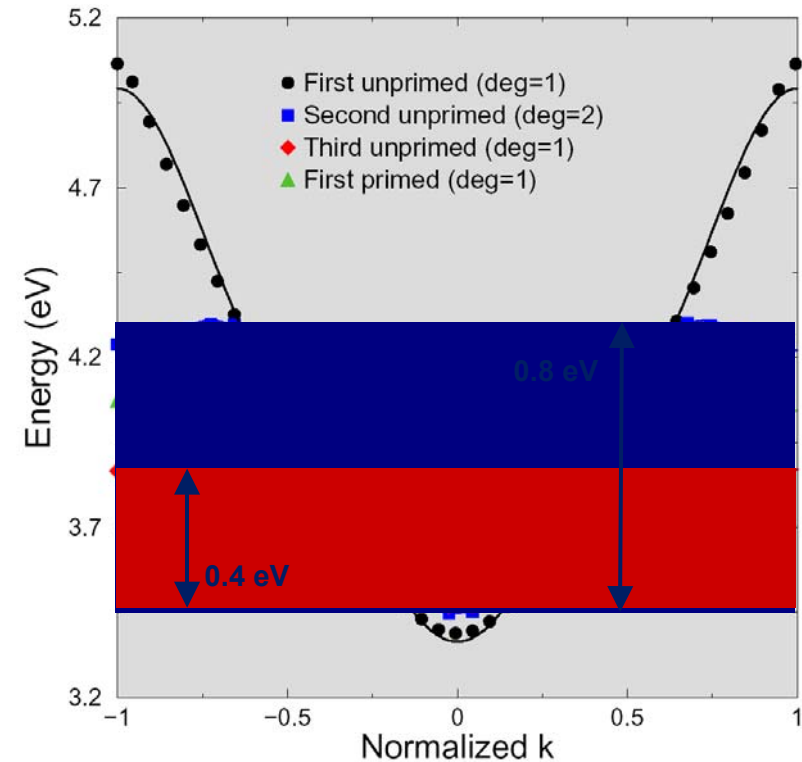
Transmission coefficient – 3rd subband



Output characteristics



- Two negative output conductance intervals are clearly visible.
- The drop at $V_{DS} = 0.8 \text{ V}$ 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 losing 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?