Challenges in the introduction of Band to Band tunneling in semi-classical models for Tunnel-FETs

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Outline

- Context
- Quantum models
- Semiclassical models
  - S/D tunneling
  - BBT Tunneling
- Comparison between BBT models
- Open issues and Conclusions

Context for Tunnel-FET modeling

- A new device concept for ultra-low power electronics.

- Quite different from a conventional MOSFET:
  - Inherently based on a complex Q.M. process: BBT

- Presently most planar Tunnel FETs are long devices but should eventually be short ones:
  - models should be able to properly handle the transport regimes in short devices.

- Many of the state of the art nano-electronics technology boosters (crystal orientation and strain / high-k / heterostructures) will be necessary for performant Tunnel-FETs:
  - models should be able to properly handle these boosters

Modeling of technology boosters

- Huge efforts recently made to incorporate in TCAD the new physics related to these technology boosters.
    - Quantization in inversion layers (bulk/SOI)
    - Band structure modifications due to strain/orientation
    - New scattering mechanisms due to new materials/interfaces
- Modeling frameworks:
    - Extension of the industry standard TCAD (density gradient and moment method-based)
    - Development of self-consistent multi-subband DD or Monte Carlo solvers for transport in inversion layers
    - Quantum transport models

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Full-Quantum approaches

Based on the solution of the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m_0}\nabla^2\Psi+\left(U_A+U_C+U_S\right)\Psi$$

Applied and built-in potential

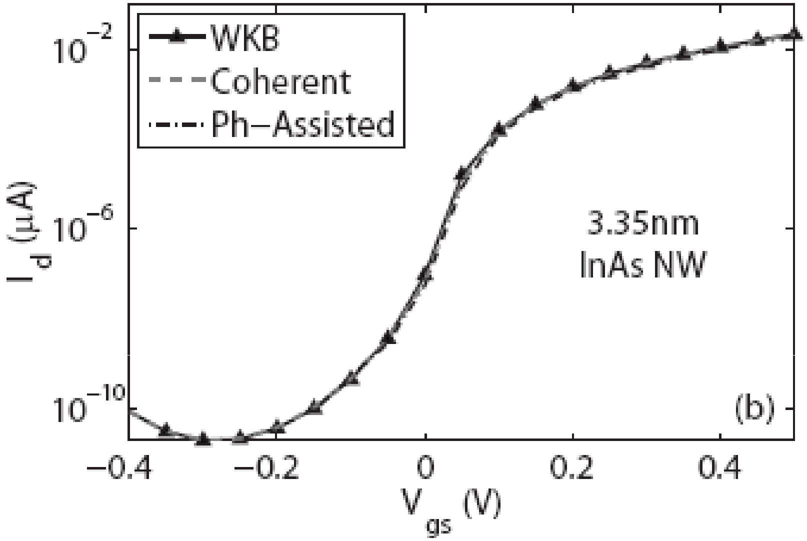
Crystal potential

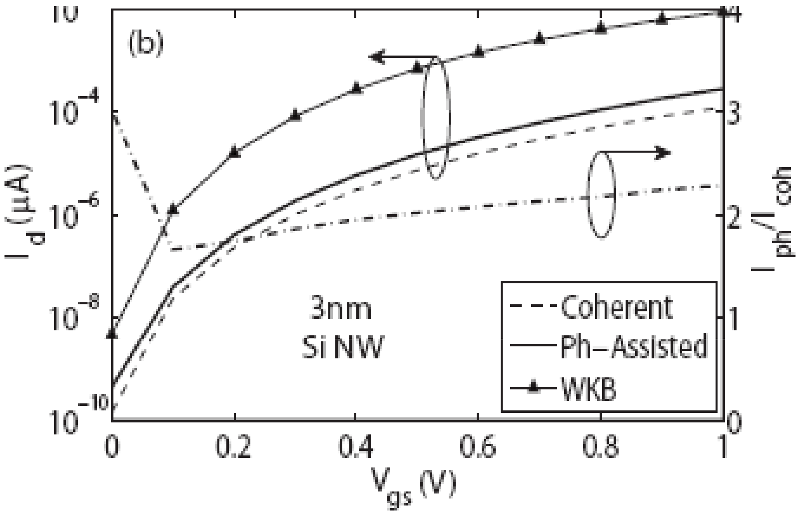
Scattering potential

Application to TFETs:

- Device simulated considering the single atoms under the tight-binding formalism
- Self-consistent Scrödinger (NEGF) + Poisson (3D structures)
- More than 100k atoms are needed !
- It naturally takes into account the effect of size-induced quantization on the E-k relation in the device

Full-Quantum approaches: example





WKB: E-k from tight-binding calculations; same potential profile as in the self-consistent atomistic simulation
Nanowires with L_G = 15nm, no technology boosters

[M.Lousier and G.Klimeck, JAP 2010, p.084507]

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Semi-classical modeling approach

Exact or approximate self-consistent solution of the Poisson and Boltzmann Transport Equations

$$\frac{\partial f}{\partial t}+\vec{v}\cdot\nabla_{\vec{r}} f-\frac{q}{\hbar}\vec{F}\cdot\nabla_{\vec{K}} f=$$

$$\sum_{\vec{K}'} f(\vec{r},\vec{K}',t)\left[1-f(\vec{r},\vec{K},t)\right]S(\vec{K}',\vec{K})-f(\vec{r},\vec{K},t)\left[1-f(\vec{r},\vec{K}',t)\right]S(\vec{K},\vec{K}')$$

$\vec{v}=\nabla_{\vec{K}}E(\vec{K})/\hbar$ Group velocity

$E(\vec{K})$ Band structure

$\left.\right\}$ Mimic the effect of the crystal potential

$S(\vec{K},\vec{K}')$ Scattering rate, computed according to quantum-mechanics (Fermi Golden Rule)

Solved either with the moment’s method or with the Monte Carlo method.

Pros. and Cons. of the semiclassical approach (with Monte Carlo)

- Easy to include complex scattering mechanisms
- Can work in long channel devices (easy calibration)
- Simulation time shorter than full-quantum approaches
- Handles all transport regimes from DD to quasi-ballistic and ballistic
- Quantization in the transverse direction can be included (mode-space; Multi-subband approach)
- Successful inclusion of technology boosters demonstrated for electrons and holes [Lucci, 2005, De Michielis, 2009]

- No quantum effects in the transport direction
- Physical and numerical issues in the simulation of abrupt transitions
- Non obvious implementation of generation/recombination mechanisms

$$E(\vec{R},\vec{K}) = E_r(\vec{R}) + E_k(\vec{K})$$

Semiclassical modeling for Tunnel-FETs

- Challenge: The quantum effect ruling the device operation occurs in the lateral (transport) direction.

- Vertical quantization effects may still be relevant

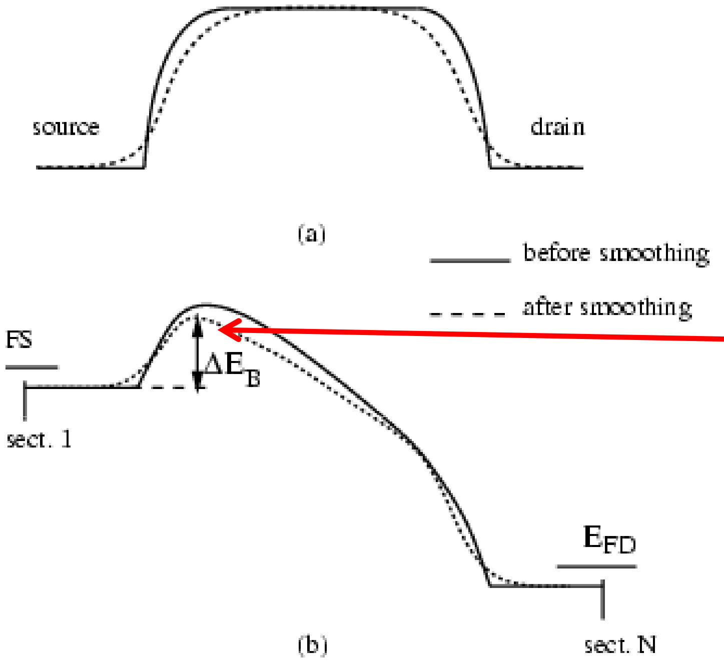
- Examples of lateral QM effects successfully included in semi-classical models:
  - S/D tunneling in short MOSFETs
  - tunneling through SiO2 barriers

S/D tunneling in semiclassical models

- In TCAD → quantum (effective) potentials
- In Monte Carlo → quantum (effective) potentials or real space particle transfer

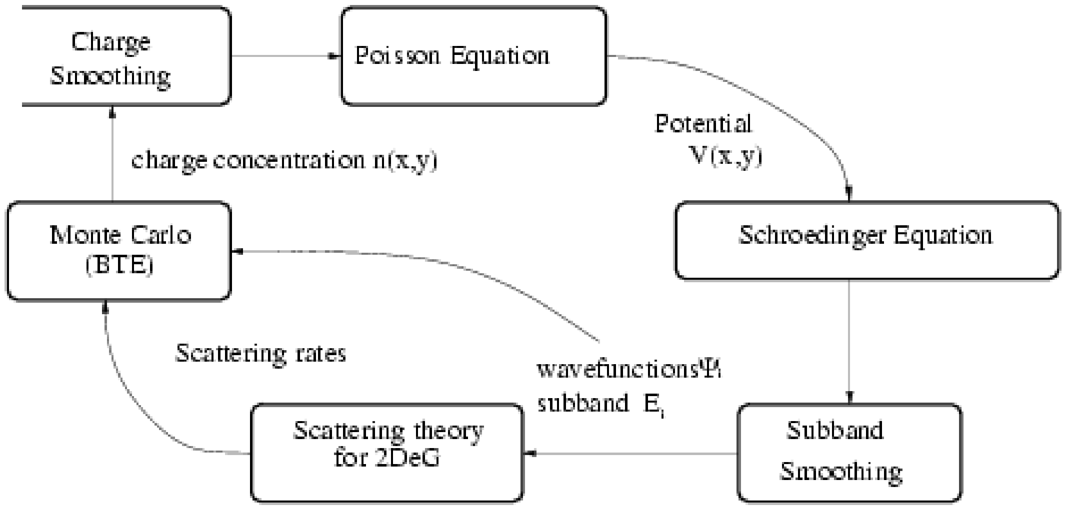
  - A smoothed potential is used (e.g. for the purpose of particle motion) mimiking the fact that a distributed wavepacket feels an average/smooth potential
  - The particles suffering tunneling are those already being simulated (electrons in the conduction band for nMOSFETs)
  - No new particle are generated.

Inclusion of S-D tunneling: Gaussian Smoothening



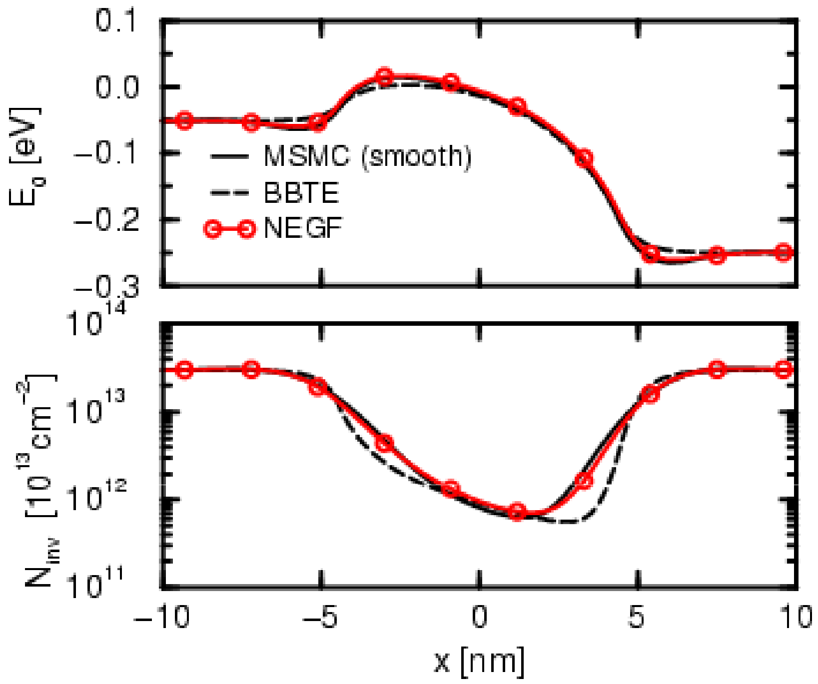
$$E_{Eff}(x) = \int E(x') \frac{1}{\sqrt{2\pi}\sigma_x} \exp\left(-\frac{(x'-x)^2}{2\sigma_x^2} \right) dx'$$

Lowering of the effective barrier at the source

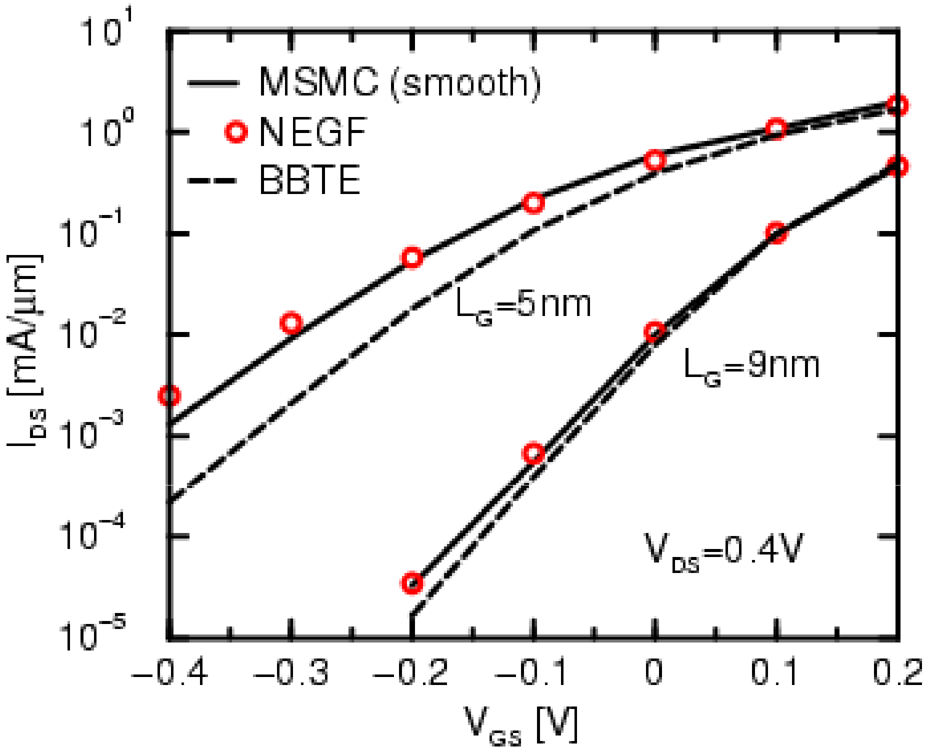


[Palestri,Semic.Sci.Tech., v.25, p.055011, 2010]

Examples



Tsi=3nm, Lg=9nm, Vds=0.2V

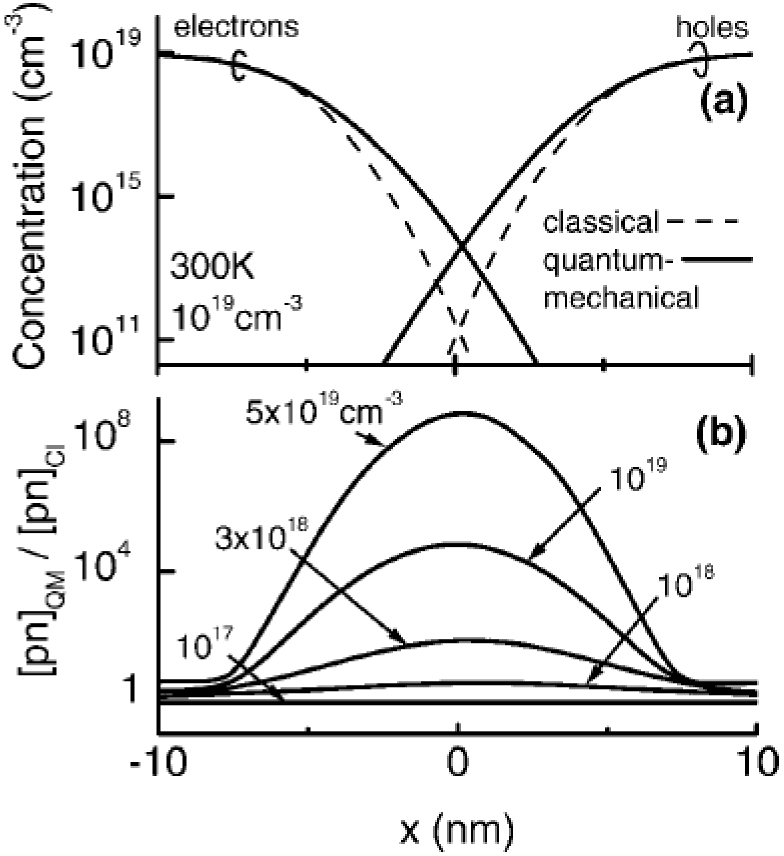


Accurate evaluation of lateral quantum effects in semi-classical models is possible.

Can results of similar quality be achieved for BBT ?

Q.M.effects in heavily doped junctions

- The tunnel junction is a heavily doped one
- The shape of the potential barrier and the width of the depletion region are affected by q.m. effects in the transport direction
- Lateral quantization should remain as part of the picture



[Hurkx, PRB 2006]

BBT in semi-classical MC models

- Objective: Calculate $\langle c, \nu, \mathbf{r}_{\mathrm{out}} | v, \mu, \mathbf{r}_{\mathrm{in}} \rangle$
  - Prepare a wave-packet in state $| v, \mu, \mathbf{r}_{\mathrm{in}} \rangle$
  - Solve the time-dependent Schrödinger Eq.
  - Follow wave-packet evolution in the gap under the action of the field
- Valence band electrons are not simulated
- Treat BBT as a generation mechanism and compute the generation rate

BBT local model (Kane and Hurkx)

- The simplest one is the Kane model in the uniform electric-field limit:

$$G_{B2BT} = A \cdot F^{P} \cdot \exp\left(-\frac{B}{F}\right)$$

with A, P, and B numerical parameters from e.g. [J. J. Liou, Solid-State Elect., v. 33, p. 971, 1990].

- A more elaborate model was proposed in [Hurkx, TED, 1992]

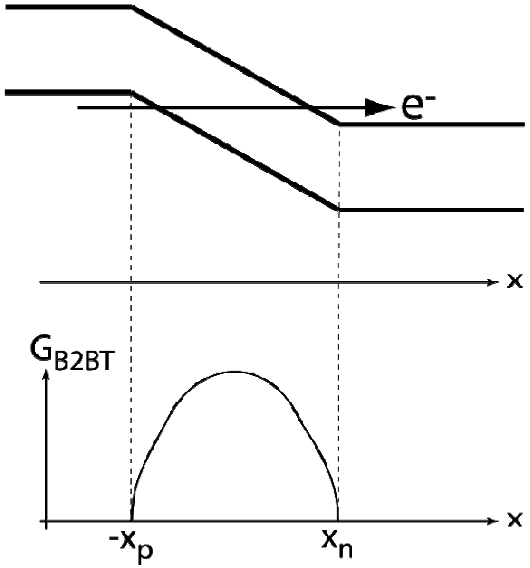
$$G_{B2B} = A \cdot D \cdot \left(\frac{F}{1\,V/cm}\right)^{P} exp\left[\frac{B \cdot E_G \cdot T^{3/2}}{E_G \cdot (300K)^{3/2} \cdot F}\right]$$

With: $D = \frac{np - n_{i,eff}{}^2}{(n+n_{i,eff})(p+n_{i,eff})}(1 - |\alpha|) + \alpha$

where α=0 for the original Hurkx model [1]

Weaknesses of local models

- tunneling is a non-local phenomena depending on the potential profile
- require calibration for any new structure/material
- may predict a nonzero generation rate even at equilibrium
- same generation rate for electrons and holes
- weak link to material parameters



Non-local models

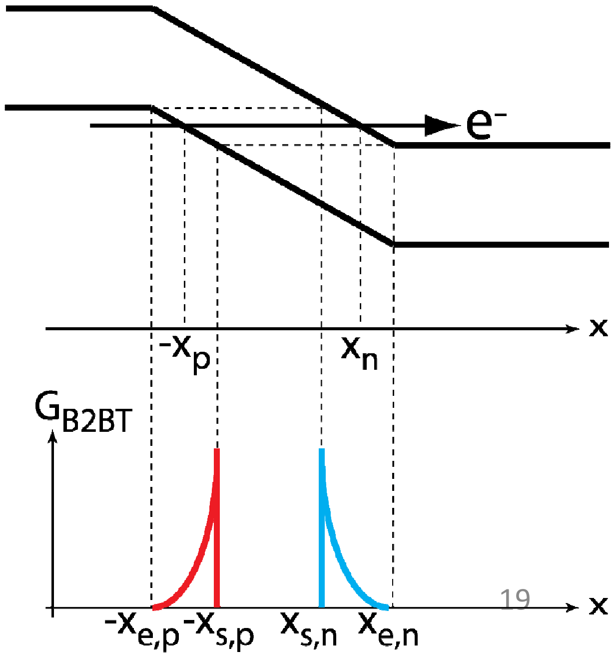
- non-local generation of electron and holes caused by phonon-assisted band-to-band tunneling process.

- The hole generation rate is:

$$G_{B2BT,holes}\left(-x_p\right)=\left|\nabla E_V\left(-x_p\right)\right|C_P\exp\left(-2\int_{-x_p}^{x_0}\kappa_V\,dx-2\int_{x0}^{x_n}\kappa_C\,dx\right)\left\{\left[\exp\left(\frac{\varepsilon-E_{F,n}(x_n)}{KT}\right)+1\right]^{-1}-\left[\exp\left(\frac{\varepsilon-E_{F,p}(-x_p)}{KT}\right)+1\right]^{-1}\right\}$$

- Similar formula for electron generation at x_n

Main model ingredients
- CB and VB profiles
- E-k inside the gap
- tunneling path



Other models

- Follow the classical path (minimum action) and integrate the equations of motion in the gap (imaginary K)

$$\frac{d\mathbf{r}}{dt} = \mathbf{v}\left[\mathbf{k}(t)\right] \qquad \frac{d\mathbf{k}}{dt} = -\frac{e}{\hbar}\mathbf{F}\left[\mathbf{r}(t)\right].$$

- Once the tunneling path is found, evaluate

$$G_{vc}^{(h)}(\mathbf{r}) = G_{vc}^{(e)}(\mathbf{r}_t^{vc}) = \frac{N_v}{\tau_{vc}} \exp\left\{-2\int_{\mathbf{r}}^{\mathbf{r}_t^{vc}} ds\, k_{\mathrm{path}}(s)\right\}$$

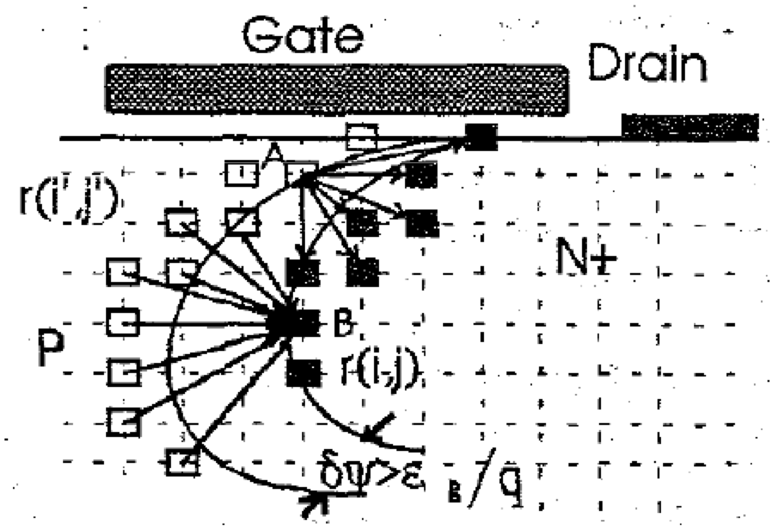
$$G_{vc}^{(h)}(\mathbf{r}) = \sum_{\eta\pm} G_{vc}^{(e)}\left(\mathbf{r}_t^{vc\eta\pm}\right) \sum_{\eta\pm} \frac{N_v}{\tau_{vc\eta\pm}} \times \exp\left\{-2\int_{\mathbf{r}}^{\mathbf{r}_t^{vc\eta\pm}} ds\, k_{\mathrm{path}}(s)\right\}$$

For direct and indirect tunneling respectively

[Fischetti 2007]

Choice of the tunneling path

- Compute the BBT rate over all tunneling paths that fulfill the condition $\Delta V > E_G / q$ [Peng]



- Not clear if it is more or less accurate
- Could be relevant in 2D potential distributions

Other issues with BBT models

- Self-consistency vs. post-processing
- Integration method
- Tunneling probability: WKB, Transfer matrix, etc…
- Multiple branches of the valence band
- Temperature dependence
- Geometry of the tunneling path (1D, 2D, etc…)
- Defects, Traps, …

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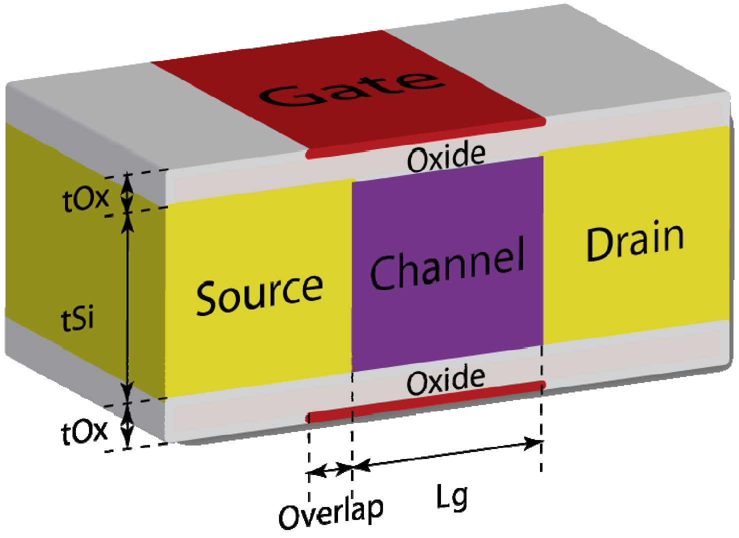
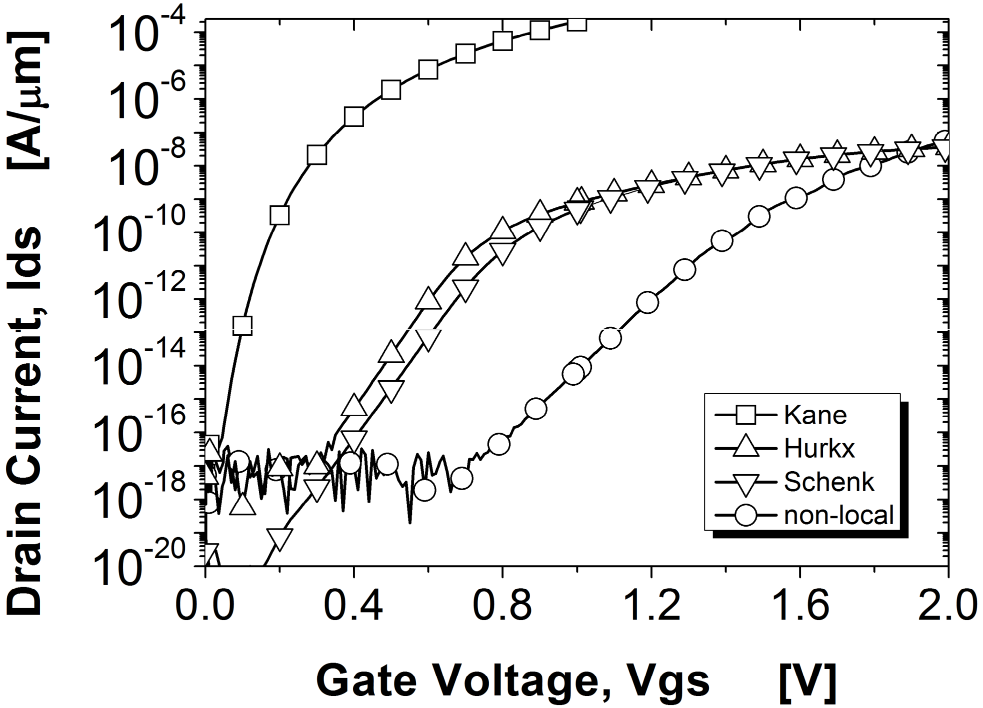
Mutual comparison between models: template device

Lg=10nm+5nm overlap,
tSi=10nm,
tox=3nm (HfO2, eps_ox=25)
Gate Contact: Gold (WF=5.1eV)
Na,source=3e20cm-3
Nd,drain=5e18cm-3
Decay ~4nm/dec

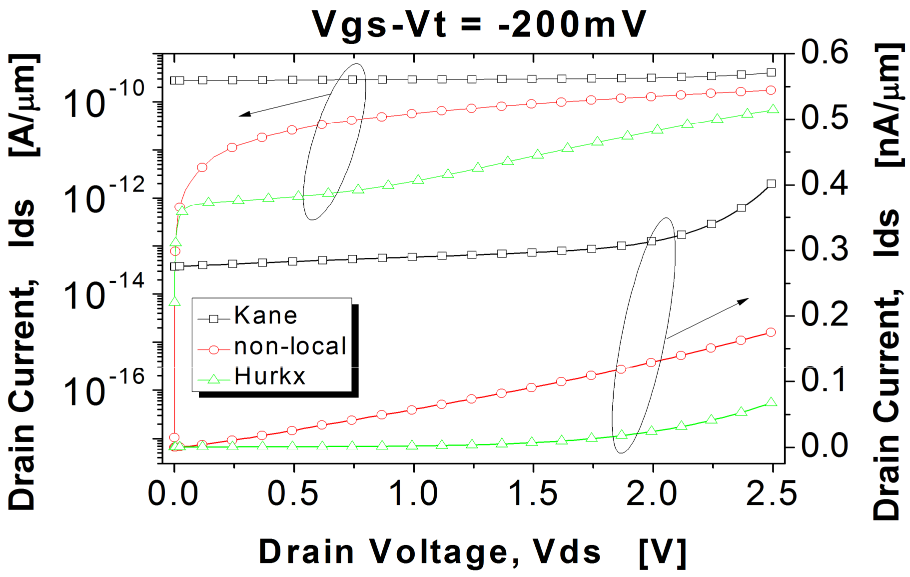


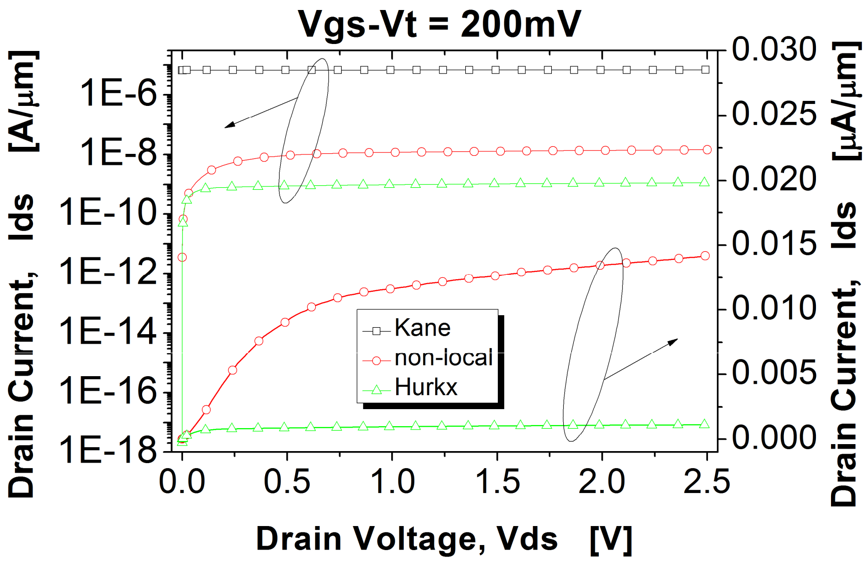
Mutual comparison between models: Ids-Vgs @Vds=200mV



Striking difference between the different models in terms of Ion, Vt and SS

Mutual comparison between models: Ids-Vds

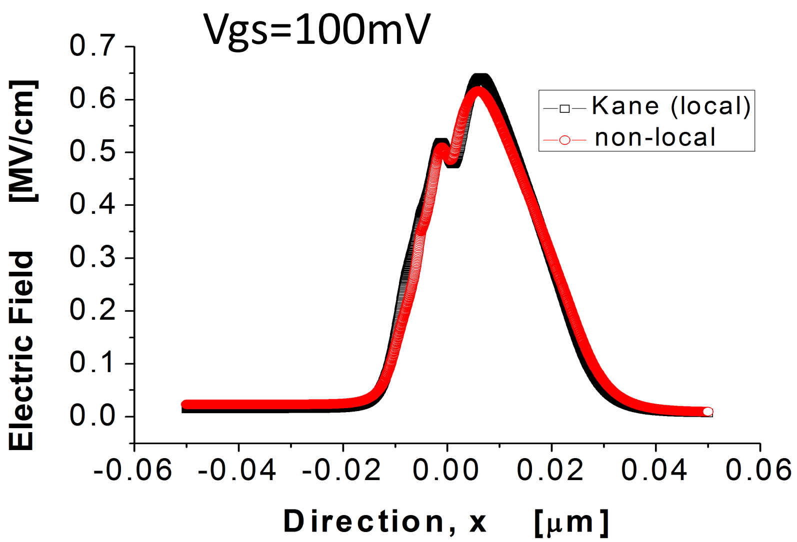


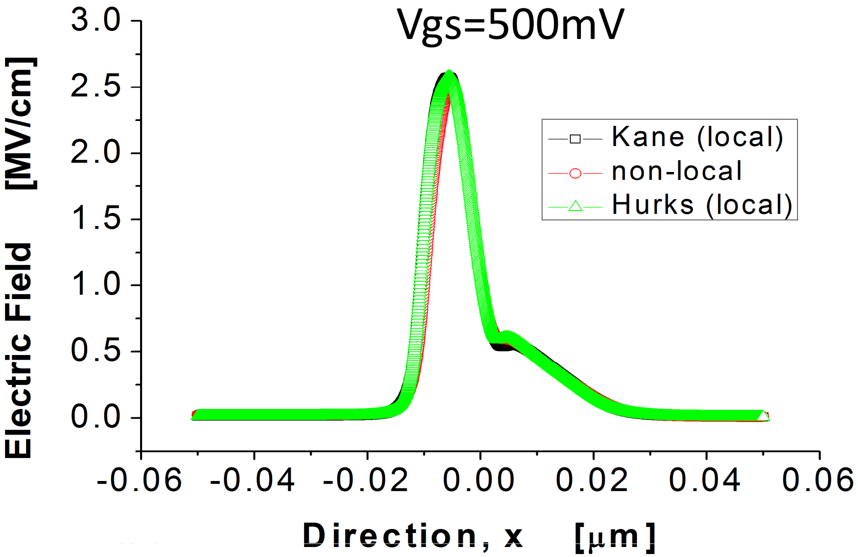


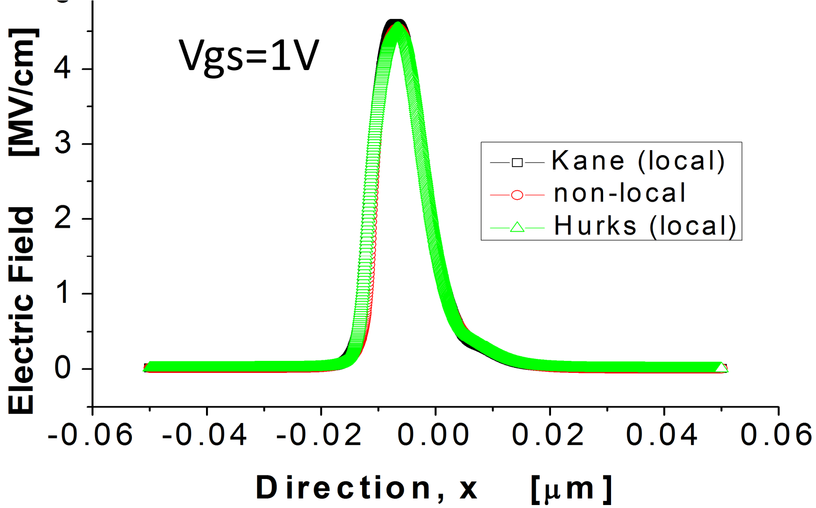
Significant differences are observed also in the output characteristics

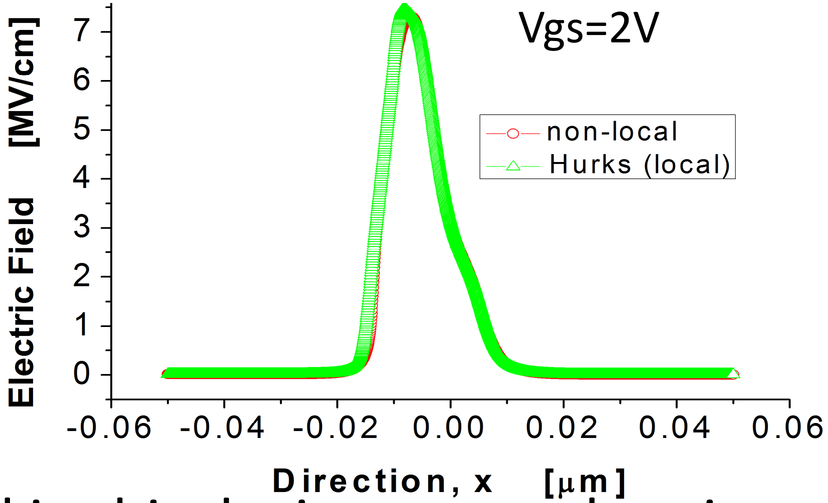
Id≠0 for Vds=0 in the simple Kane model !

Electric Field (weigthed by the electron concentration)





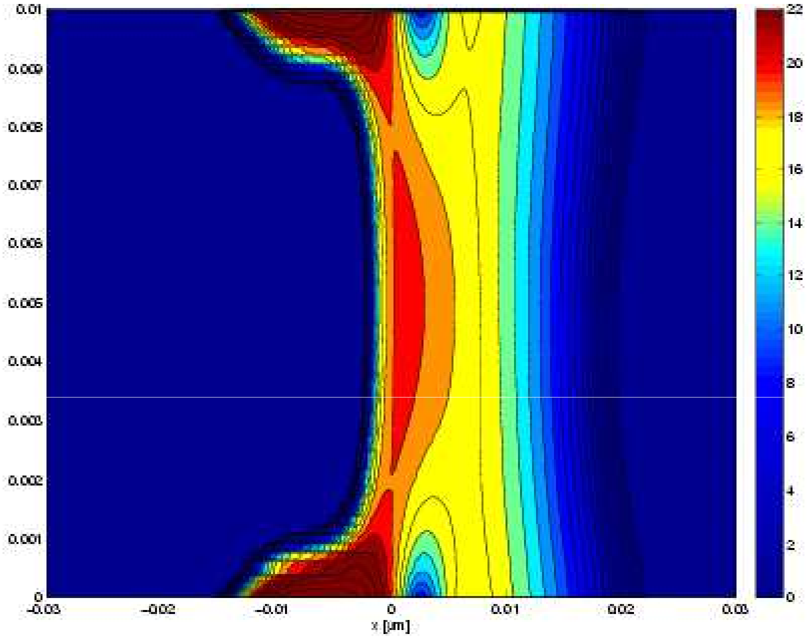




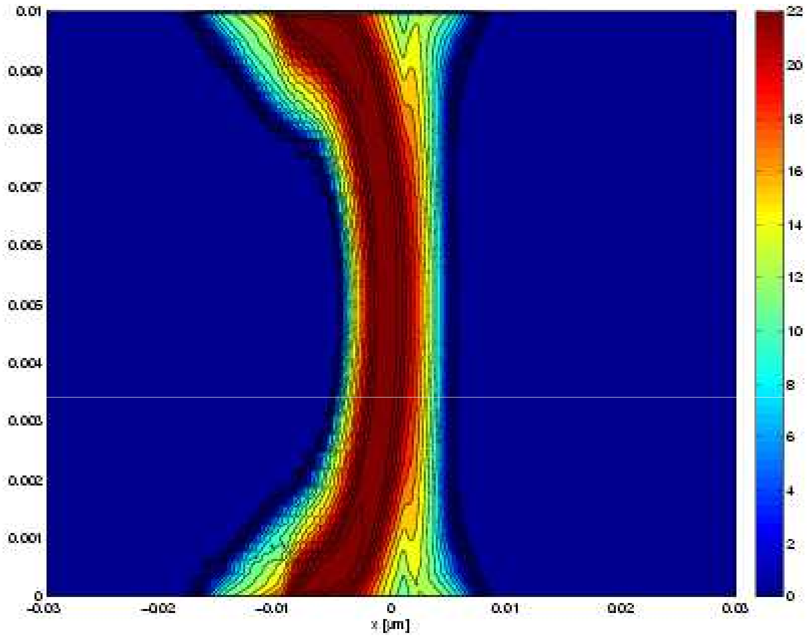
Effect of self-consistency is very small in this device: same electric field profile in the presence of significantly different generation rates

Generation rates from local models

(same color scale in both pictures,
color range from 1^e20 to 1^e23 [cm^-3s^-1], logspaced!)



Kane, Vgs=250mV
Ids=0.35e-8A/um



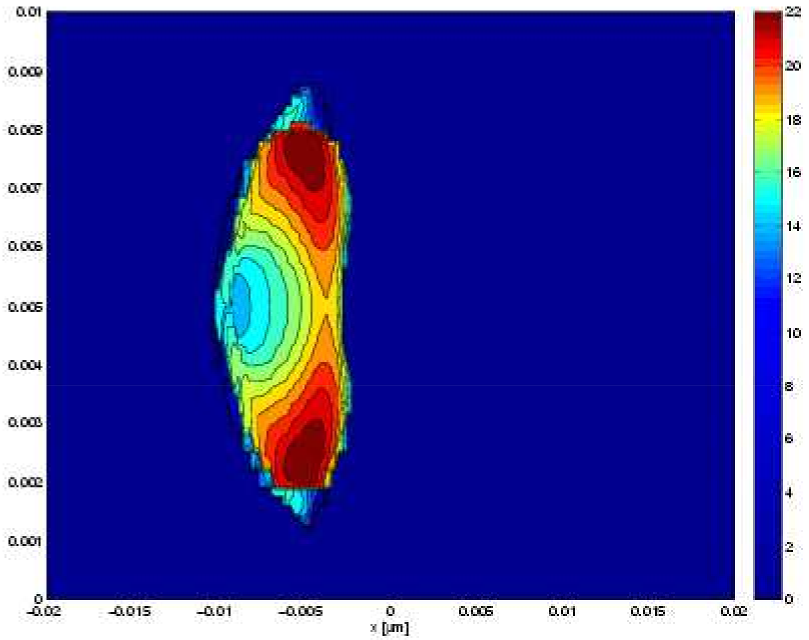
Hurkx, Vgs=1.5V
Ids=1.12e-8A/um

Strong generation at the Si/SiO2 interface in the Kane model

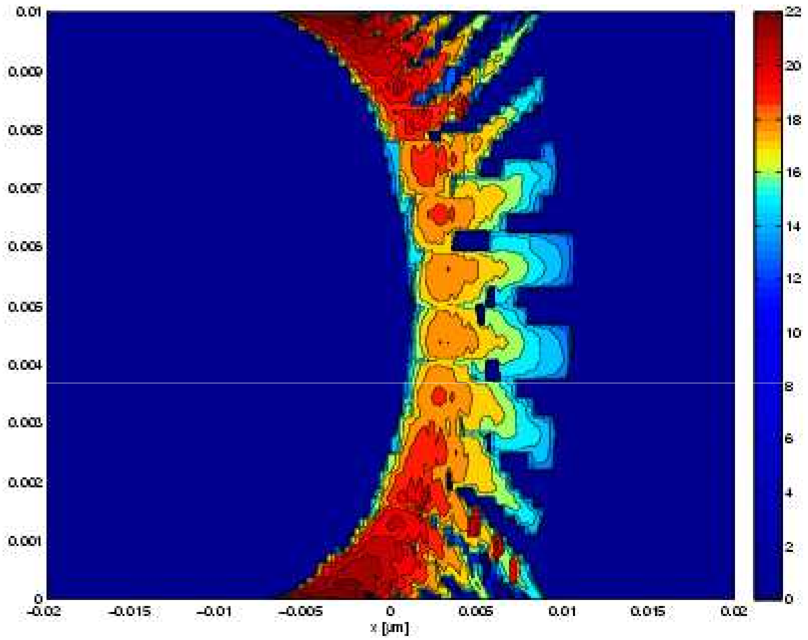
Non-Local Model

(same color scale as prevoius slide)

holes



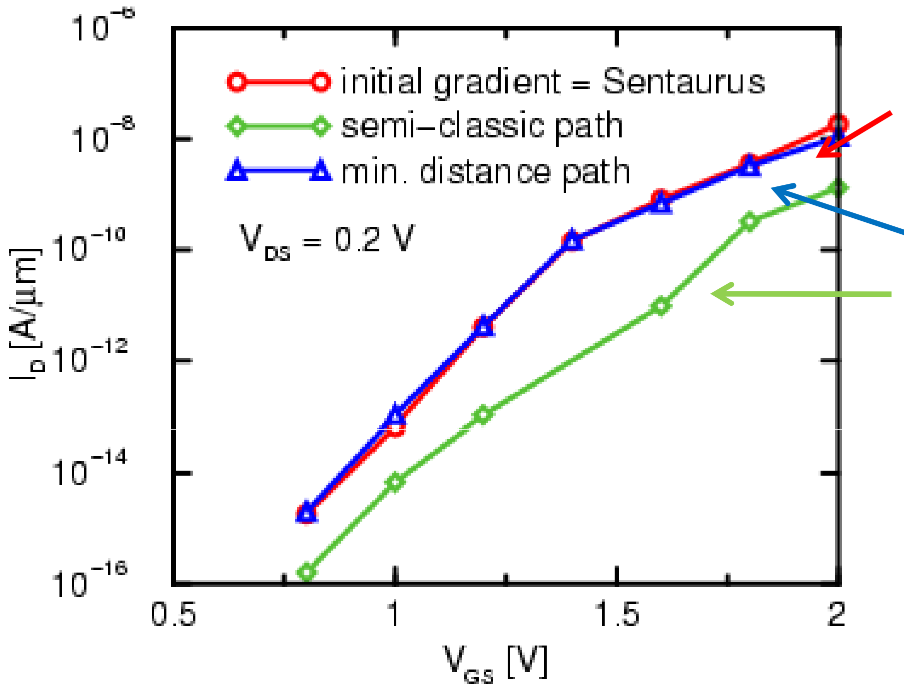
electrons



Vgs=1.8V, Ids=1.13e-8A/um

Different gen.rate profiles for electrons and holes.
Hole gen.rate is null close to the Si/SiO2 interface because the tunneling path would end in the oxide

Non-local model: influence of the tunneling path

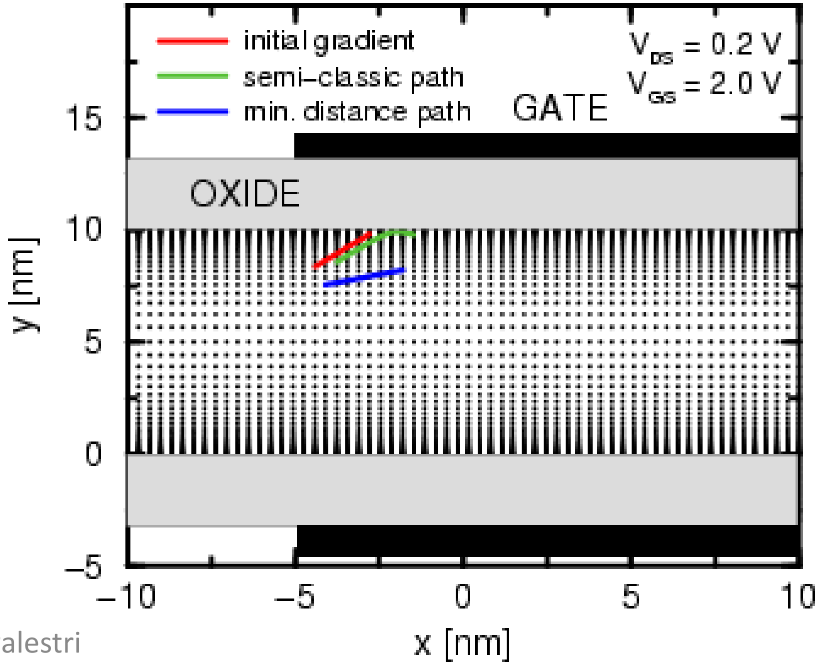


Gradient of the potential at the generation point

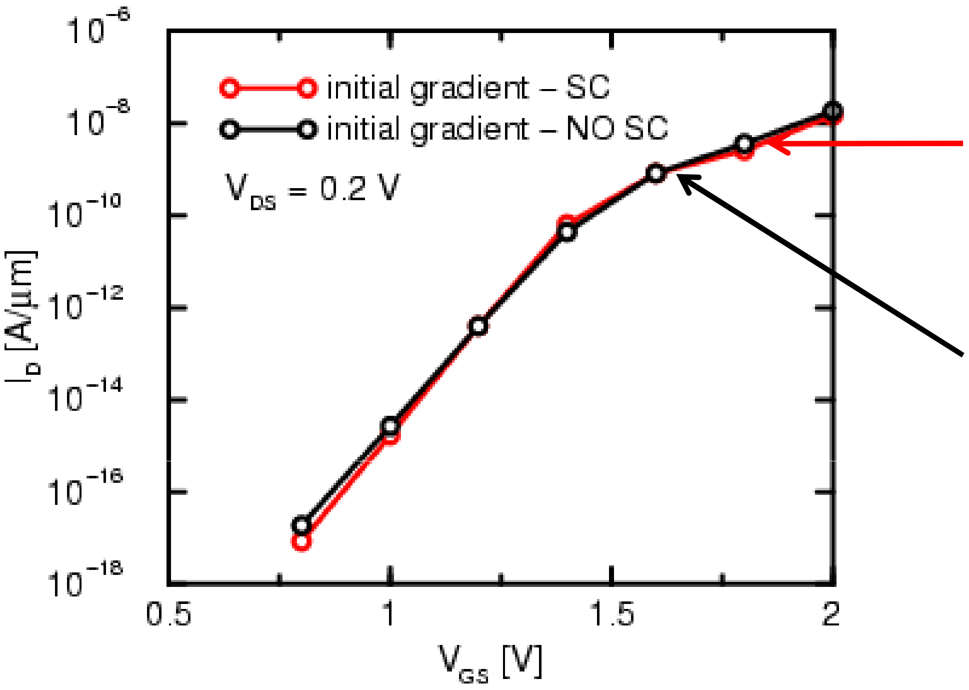
Shortest path between VB and CB

Follows the electric field direction from point to point

Only one path starting from each grid point. It may produce artifacts.



Effect of transport and self-consistency



Self-consistent MC simulation

Integral of the gen.rate computed from the potential profile of a DD simulation

In the considered device the effect of transport and BBT generation on the electrostatics is very small

BBT successfully integrated in a state-of-the art MC simulator; stability issues and statistical enhancement problems have been solved

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Other open issues

- Strain and hetero-junction would result in complex CB and VB profiles and E-k in the gap changing with position
- Care should be taken when using WKB in hetero-structures

  [Majkusiak, *SINANO* book, Schenk 1989]
- How to handle quantization perpendicular to the tunneling path ?

Conclusions

- Semi-classical models are very mature and can handle complex structures with all the relevant technology boosters
- Quantum effects such as vertical quantization and source-to-drain tunneling already successfully included
- BBT can be added as an additional generation term but several critical challenges remain
- Promising initial results
- Subtle physical and numerical issues
- Comparison with experiments is important but not sufficient
- Benchmarking with detailed quantum transport models is necessary for simple devices