QUASANOVA

QUAntum Simulations and Assessment of NanOdeVice Architectures

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AGENCE NATIONALE DE LA RECHERCHE ANR

Context and highlights

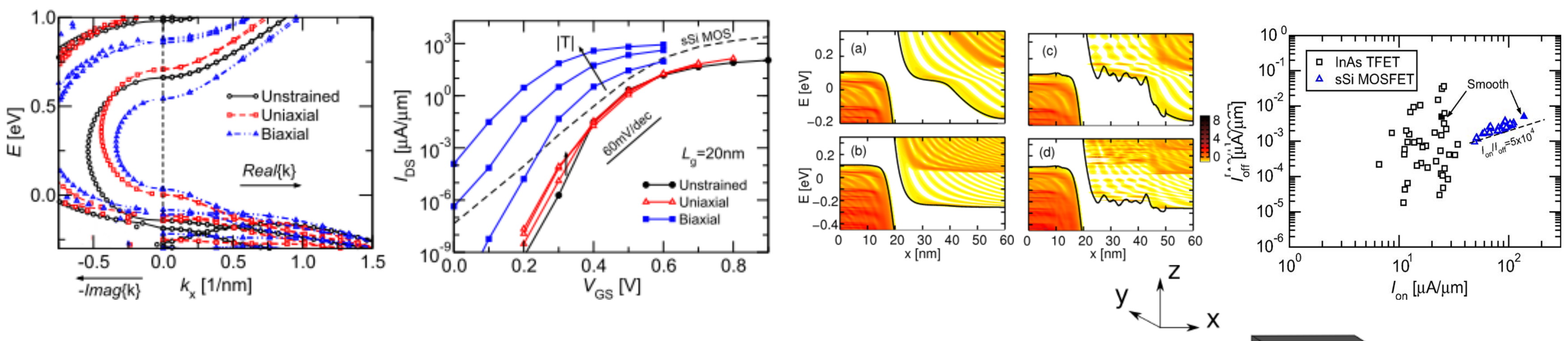
◆ **Objectives:** *development of a new generation of quantum transport simulation tools tackling with atomic scale issues → predictive simulations*

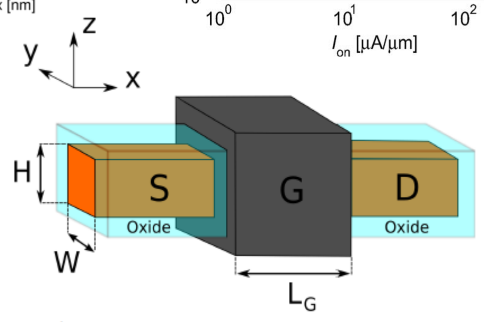
◆ **Approach:** *Basis of a common Green's function formalism conjugaled with molecular dynamics and TCAD*

◆ **Strategy:** *complementary expertises of partners: from ab initio to tight-binding, effective mass and TCAD validated by experimental data.*

◆ **Application to semi-conductor devices:** *comparison of the FD-SOI and nanowire architectures.*

InAs nanowire Tunnel FETs (VB + CB) with phonon scattering, strain and roughness





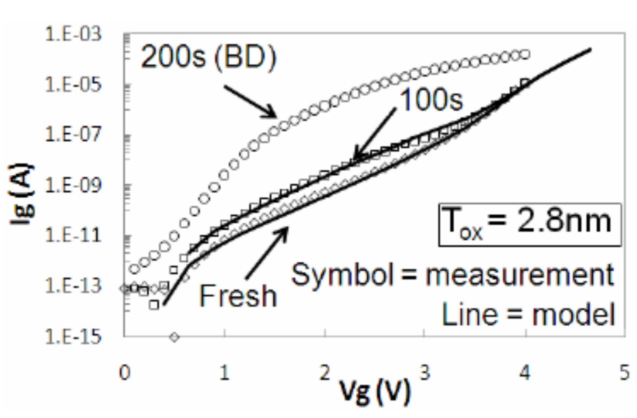
- 8 band k.p Hamiltonian for III-V compounds able to describe transport.
- Increase of ON current due to biaxial strain.
- Enhanced I_{on} and I_{off} variability w.r.t. SiMOSFETs.

*F. Conzatti et al. TED **59**, 2085 (2012)*
*F. Conzatti et al. EDL **33**, 806 (2012)*

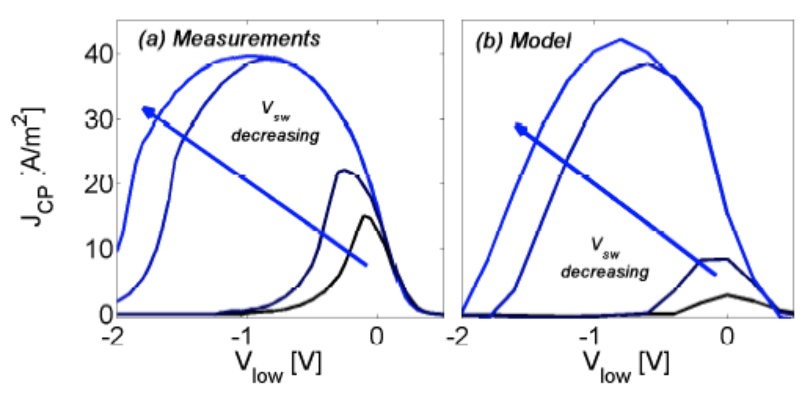
Carrier capture and emission at interfacial oxide defects

Multi-phonon model for capture and emission at Si-SiO_2 interface:

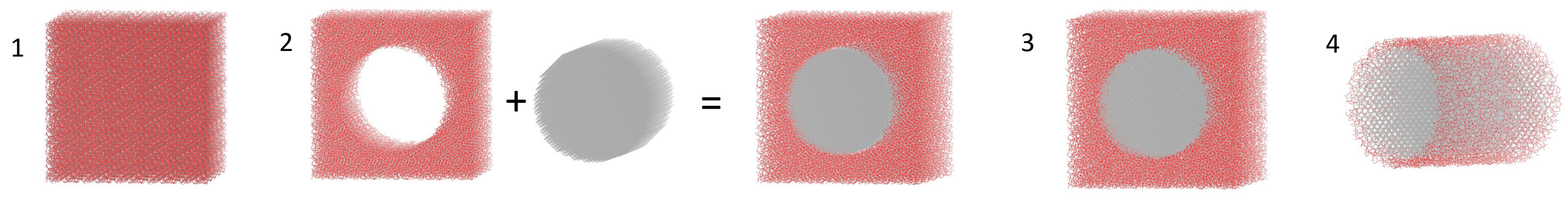
SILC simulations



Charge pumping simulations

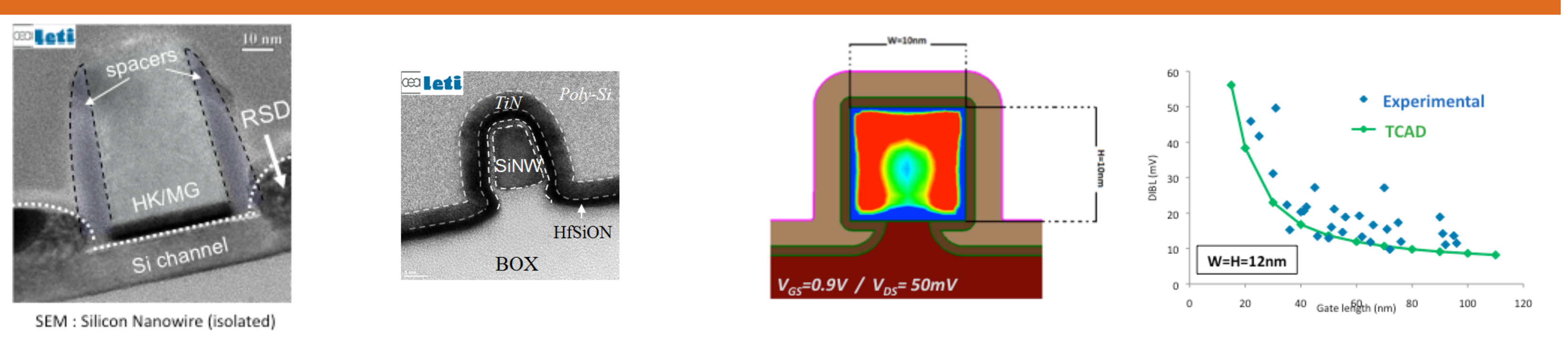


Atomistic model of oxidized nanowires



1. Construction of a silice block.
2. Cutting of 8nm cylinder and insertion of a Si nanowire of the same diameter.
3. Formation of the interface.
4. Cutting of a silice shell.

Simulation of Tri-gate / Omega Gate MOS transistor on SOI substrate for 10 nm technology node



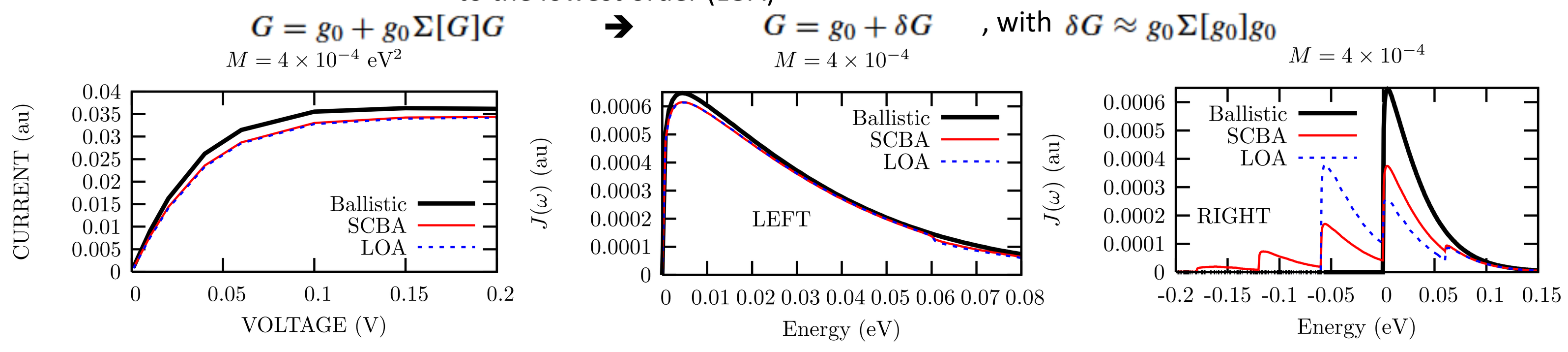
- Fabrication of silicon nanowire MOSFETs at LETI.
- TCAD simulations including quantum corrections (Density Gradient).
- First comparisons with experimental data.

R. Coquand, S. Barraud et al, 2012 13th International Conference on, (pp. 37 - 40), 6-7 March 2012.

Inelastic scattering: One-shot current-conserving lowest-order approximation

to the lowest order (LOA)

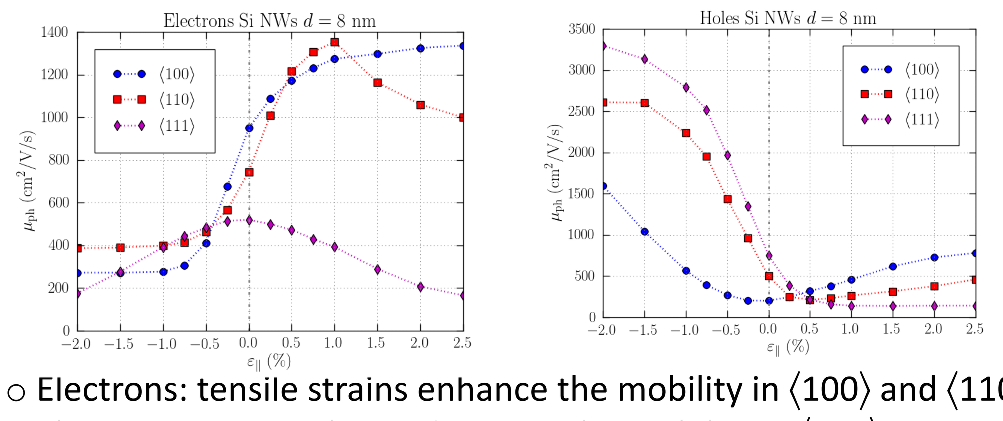
$G = g_0 + g_0\Sigma[G]G$ → $G = g_0 + \delta G$, with $\delta G \approx g_0\Sigma[g_0]g_0$



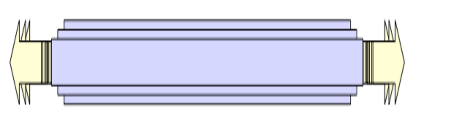
- Self-consistency is sufficient but not necessary to get the current conserved.
- LOA is current-conserving but can lead to spectral instabilities.
- LOA is able to account for current degradations of up to "10%" per phonon mode.

*H. Mera, M. Lannoo, C. Li, N. Cavassilas, and M. Bescond, Phys. Rev. B (R), **86** 161404 (2012)*

Atomistic simulations of stretched nanowires



*Y.M. Niquet, C. Delerue and C. Krzeminski, Nanolett. **12** 3545 (2012)*



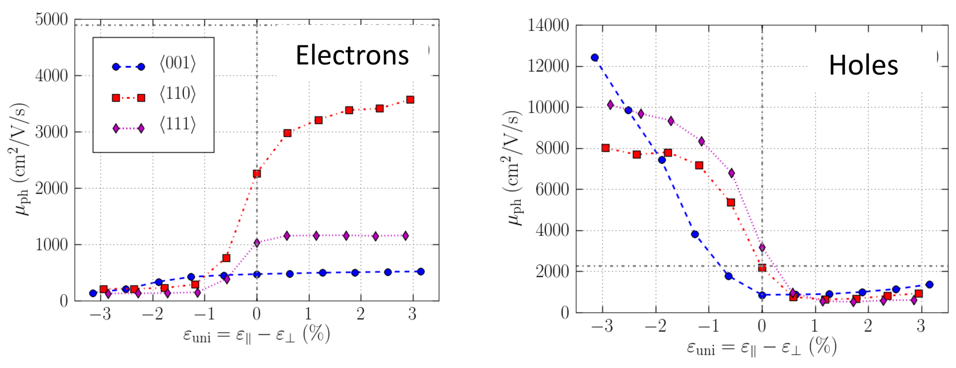
Let us stretch the nanowires by an amount $\varepsilon_{\|}$ along their axis…

- Electrons: tensile strains enhance the mobility in ⟨100⟩ and ⟨110⟩ Si NWs.
- Electrons: Strains always decrease the mobility in ⟨111⟩ Si NWs.
- Holes: compressive strains enhance the mobility in ⟨110⟩ and ⟨111⟩ Si NWs.
- Holes: strains always increase the mobility in ⟨100⟩ Si NWs.

Mobility in (strained) Ge nanowires

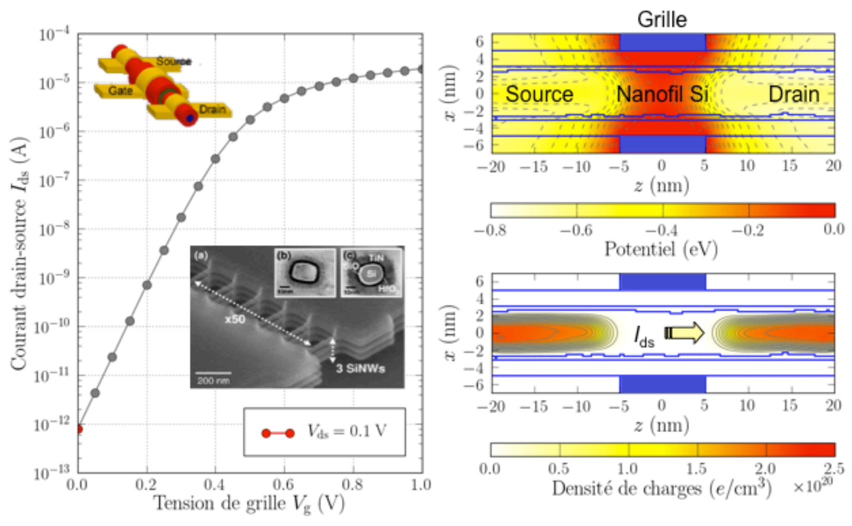
*Y. M. Niquet and C. Delerue, JAP **112**, 084301 (2012)*

Methodology:
1) Electron (hole) states: tight-binding
2) Phonons + relaxation of strains: valence-force field
3) Full resolution of Boltzmann equation



In strained Ge NWs, the mobility can reach >3000 $cm^2/V/s$ for electrons, 12 000 $cm^2/V/s$ for holes → Ge NWs promising for ultimate devices.

Simulations based on GPU calculations



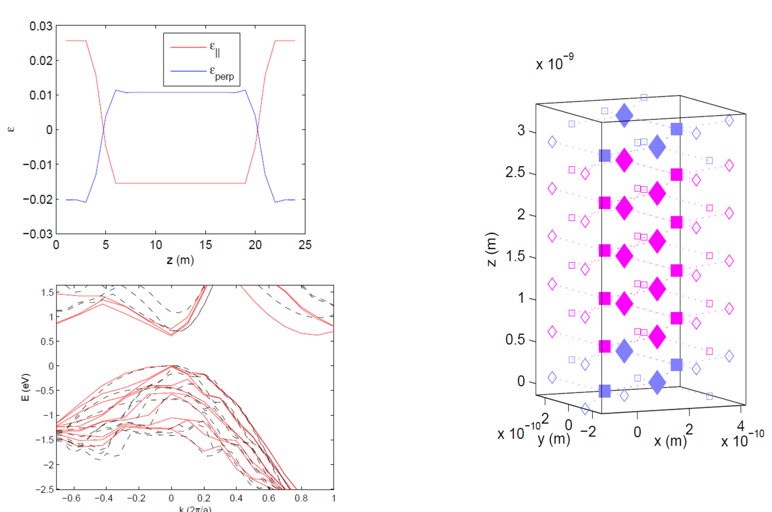
Y.-M. Niquet, F. Triozon and C. Delerue, troisième prix au concours Bull-Fourier (calcul intensif)

- Atomistic simulations of transport in nano-transistors with GPU calculations (code « TB_Sim »).

Atomistic pseudopotential methods

- EPM Hamiltonians built up according to atom positions in a given supercell.
- Atom position computed with an empirical valence force model: **profile of strain level.**
- Comparison between AEPM (red) and tight-binding (black):

Calibration of parameters for k.p Hamiltonians



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