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 conjugated with molecular dynamics and TCAD

Strategy: Complementary expertise 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 kp Hamiltonian for III-V compounds able to describe transport.
- Increase of ON current due to bipolar strain.
- Enhanced \( L_1 \) and \( L_2 \) variability w.r.t. SIMOFETs.
- Fabrication of silicon nanowire MOSFETs at LETI.
- TCAD simulations including quantum corrections (Density Gradient).

Carrier capture and emission at interfacial oxide defects

Multi-phonon model for capture and emission at Si-SiO \(_2\) interface:

\[ \text{SILC simulations} \]

\[ \text{Charge pumping simulations} \]

Atomistic model of oxidized nanowires

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

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

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

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

- 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.

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\(^{-1}\)s\(^{-1}\) for electrons, 12 000 cm\(^2\)V\(^{-1}\)s\(^{-1}\) for holes. Ge NWs promising for ultimate devices.

Simulations based on GPU calculations

- Atomistic simulations of transport in nano-transistors with GPU calculations (code = TB_Sim)

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