ESSDERC 2016 Joint Workshop on:

“III-V compound semiconductor technology and devices for advanced nanoelectronics”

InGaAs Monte Carlo and Drift-Diffusion Models and TCAD simulation: Monte Carlo

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Outline

❖ Introduction

❖ Trap effects on capacitance and mobility in InGaAs

❖ Monte Carlo simulation of InGaAs SOI-FinFETs
  ● Effect of doping profiles
  ● Effect of traps and Fermi-level pinning
  ● Effect of contact resistance and surface roughness

❖ Conclusions
N-type InGaAs devices candidates for coming CMOS technology nodes due to high mobility → new effects to be considered in TCAD simulations:

- Quasi-ballistic effects due to small effective mass pronounced
- Fermi-Dirac statistics relevant
- Quantization requires Schrödinger-Poisson solver due to strong nonparabolicity
- Fermi-level pinning due to border-traps have a strong influence
- Contact resistance is relevant

Explore InGaAs-FinFET performance with Monte Carlo device simulation based on calibrated traps and effective mobilities
Monte Carlo Model

- Band structure: empirical nonlocal pseudopotential table
- Scattering mechanisms
  - Elastic intra- and inelastic inter-valley deformation-potential phonons
  - Polar-optical phonons
  - Ionized impurity scattering according to Brooks-Herring
  - Specular/diffusive surface roughness scattering
- Quantum correction: effective oxide permittivity and workfunctions extracted from 2D Schrödinger-Poisson including wave-function penetration into the oxide
- Fermi-Dirac statistics
- Acceptor-like border traps/donor-like interface traps and contact resistance
Figures taken from F.M. Bufler et al., “Theoretical and Experimental Analysis of Capacitance and Mobility in InGaAs” – Proc. 74th Annu. Device Res. Conf. (DRC), pp. 139-140, Newark, DE, USA, June 2016.
Effective Mobility Calibration

Figures taken from F.M. Bufler et al., “Theoretical and Experimental Analysis of Capacitance and Mobility in InGaAs” – Proc. 74th Annu. Device Res. Conf. (DRC), pp. 139-140, Newark, DE, USA, June 2016.
• Si-like doping: Extension doping and p-type channel doping (only difference to silicon: maximum S/D doping $3 \times 10^{19}$ cm$^{-3}$ instead of $2 \times 10^{20}$ cm$^{-3}$)
• III-V doping: constant n+ S/D doping on lowly doped n-type channel layer, raised source/drain
• Smaller effective gate length leads to higher off-current
• III-V doping involves resistor-like behavior with reduced gate control
• Trap-induced Fermi-level pinning, contact resistance (3125 Ω) and increased surface roughness decreases drain currents further
Performance Comparison

- Only ideal InGaAs with Si-like doping outperforms silicon
- Good agreement with measurements (V. Djara et al., “CMOS-Compatible Replacement Metal Gate InGaAs-OI FinFET With $I_{ON} = 156 \mu A/\mu m$ at $V_{DD}=0.5$ V and $I_{OFF}=100$ nA/\mu m” – IEEE Electron Device Lett. 37 (2), 169 (2016)) without short-channel calibration and geometry matching
Monte Carlo CPU performance

- 20-core Intel(R) Xeon(R) CPU E5-2690 v2 @ 3.00GHz machine
- On-state bias point (Idsat, Idlin) in around 10 minutes on one 20-core machine
- Combining IdVg (~below above VT) with off-state bias point simulation allows overnight complete IdVg curve on two 20-core machines

<table>
<thead>
<tr>
<th>Wallclock time</th>
<th>Idsat (2.5% error)</th>
<th>Idlin (2.5% error)</th>
<th>IdVg_sat (~ below above VT)</th>
<th>Ioff_sat (&lt;~10% error)</th>
</tr>
</thead>
<tbody>
<tr>
<td>InGaAs SOI-FinFET</td>
<td>13.5 min</td>
<td>8 min</td>
<td>7 h</td>
<td>15.5 h</td>
</tr>
<tr>
<td>Silicon SOI-FinFET</td>
<td>7.5 min</td>
<td>11.5 min</td>
<td>2.5 h</td>
<td>5.5 h</td>
</tr>
</tbody>
</table>
Efficient 3D Monte Carlo device simulation has been used to analyze InGaAs-FinFET performance:

- Good agreement with measurements achieved
- Only ideal InGaAs-FinFET with Si-like doping outperforms silicon
- Performance improvements should
  - introduce extension doping and p-type channel doping
  - reduce border traps to suppress Fermi-level pinning
  - improve effective channel mobility
- Monte Carlo allows on-state simulation in 10 minutes on one 20-core-machine and complete IdVg curve simulations overnight on two 20-core machines
InGaAs Monte Carlo and Drift-Diffusion Models and TCAD simulation: Drift-Diffusion

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Outline

- Introduction
- TCAD Drift-Diffusion Model Frame
- Contact Resistance Modelling
- Conclusion
Drift-Diffusion Model Frame

- Material parameters for InGaAs extracted from experiment and reference tools
- Calibrated model for low field inversion layer and bulk mobility (University of Bologna, Synopsys)
- Calibrated high field saturation parameters (Synopsys)
- Models and calibrated parameters for ballistic mobility model (University of Bologna, Synopsys: An accurate empirical ballistic mobility model has been implemented and will be presented at ESSDERC 2016 (Session C6L-C – Thursday 15, 2016 @14:55 ) )
- Calibrated parameters for contact resistance (University of Udine, Synopsys)
- Source/drain- and B2B tunneling (ETHZ, Synopsys)
Drift-Diffusion Model Frame: Simulation structures

2D In$_{0.53}$Ga$_{0.47}$As n-FDSOI
Channel direction = <110>
Channel height = 5 nm
Lg = 13.5 – 100 nm

3D In$_{0.53}$Ga$_{0.47}$As n-FinFET
Channel direction = <110>
Fin dimension = 20 nm x 7.62 nm
Lg = 13.5 – 100 nm

Doping Concentration [cm$^{-3}$]
- 3.0E+19
- 4.6E+16
- 7.0E+13
- 2.2E+12
- 1.5E+15
- 1.0E+18
Drift-Diffusion Model Frame: Contact Resistance

TCAD contact resistance models including thermionic and field emission are calibrated to reference data from IUNET-Udine and to experimental data from IBM and IMEC.

The calibrated contact resistance model is implemented in TCAD simulation setups for the simulation of realistic InGaAs channel based devices.
Summary & Conclusion

- Complete Drift-Diffusion Model frame and TCAD simulation setups have been developed and calibrated to Monte Carlo Simulation, to experimental data, and other reference tools from the IIIV-MOS project partners.

- New quasi-ballistic mobility models have been implemented into the TCAD simulation setups.

- Calibrated models for the contact resistance are use in the TCAD simulation setups.
InGaAs Monte Carlo and Drift-Diffusion Models and TCAD simulation

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Outline

- TCAD challenges for emerging III-V technology
- Drift-Diffusion (DD) simulation approach
- Mobility model for InGaAs UTB MOSFETs
  - Role of traps
  - Effect of strain
  - Quasi-ballistic corrections

- Conclusions
TCAD challenges for emerging III-V technology
1. Quantization effects with complex band structures

Ultra-thin $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ on InP

2. Significant interface trap densities & border traps

Figures taken from N.Taoka et al., “Impact of Fermi Level Pinning inside Conduction Band on Electron Mobility of In$_x$Ga$_{1-x}$As MOSFETs and Mobility Enhancement by Pinning Modulation” – IEDM 2011
3. Is strain a booster?

S. H. Kim et al., “Strained Extremely-thin Body In0.53Ga0.47As-On-Insulator MOSFETs on Si substrates” – VLSI Symp. 2011

&

Drift-Diffusion (DD) simulation approach
Drift-Diffusion (DD) simulation approach

In semiconductor device modeling, the DD approach has proven to be more efficient, in terms of computational time, with respect to the more rigorous Monte Carlo (MC) approach.

**Key ingredient:**

TCAD mobility model based on physical interpretations, implemented in an accurate Quantum-DD solver, calibrated against experiments.

For short-channel III-V MOSFETs reaching the quasi-ballistic regime: shall we quit DD transport model?
Mobility model for InGaAs UTB MOSFETs
InGaAs UTB MOSFETs

DEVICE UNDER STUDY AND EXPERIMENTAL CHARACTERIZATION:
A. Alian et al., “Impact of the channel thickness on the performance of ultrathin InGaAs channel MOSFET devices” – IEDM 2011

TCAD INVESTIGATION AND LOW-FIELD ELECTRON MOBILITY MODEL:
G. Betti Beneventi et al., “A TCAD low field electron mobility model for thin-body InGaAs on InP MOSFETs calibrated on experimental characteristics” – TED 2015
Role of traps: C-V curves & $D_{it}$

- $T_B$-dependent effective mass & non-parabolicity factor
- A $T_B$-dependent amount of traps is calibrated on the C-V curves

- Schroedinger-Poisson & density-gradient model are in agreement
The low field mobility model – The Matthiessen rule

\[ \mu = \left( \frac{1}{\mu_{PH}} + \frac{1}{\mu_C} + \frac{1}{\mu_{SR}} \right)^{-1} \]

**BULK & SURFACE PHONON MODES**

\[ \mu_{PH} = \left( \frac{1}{\mu_{BPH}} + \frac{1}{\mu_{SPH}} \right)^{-1} \]

\[ \mu_{BPH} = \frac{q \tau_{BPH}}{m^*} \]

\[ \tau_{BPH} = \tau_{BPH0} \frac{1}{m_r} \frac{T_{B,eff,L}}{T_{B0}} \]

\[ \mu_{SPH} = \frac{q \tau_{SPH}}{m^*} \]

\[ \tau_{SPH} = \tau_{SPH0} \exp \left( \frac{\eta T_B}{T_{B0}} \right) \frac{n}{n_0} \]

**Inversion Charge [cm\(^{-2}\)]**

- TOTAL, TB = 5 nm
- Bulk phonon-limited
- Surface phonon-limited

**Mobility \( \mu \) @ max \( n(x) \) [cm\(^2\)/Vs]**
Generalized effective thickness $T_{B,\text{eff}}$

Analytical model fitted against Schroedinger-Poisson data

- Thin-body limit:
  \[ T_T = v T_B + T_{T0} \left( \frac{T_B}{T_{B0}} \right)^\alpha \frac{F_{\text{eff}}}{F_0} \]

- Bulk limit:
  \[ T_E = T_{E0} \left( \frac{F_{\text{eff}}}{F_0} \right)^{-\chi} \]

- Combined effective thickness:
  \[ T_{B,\text{eff}} = \frac{T_T}{\left[ 1 + (T_T/T_E)^\beta \right]^{1/\beta}} \]
**THE MATTHIESSEN RULE**

\[
\mu = \left( \frac{1}{\mu_{PH}} + \frac{1}{\mu_C} + \frac{1}{\mu_{SR}} \right)^{-1}
\]

**COULOMB-LIMITED MOBILITY**

\[
\mu_C = \frac{q\tau_C}{m^*}
\]

\[
\tau_C = \tau_{C0} \left( \frac{n}{n_0} \right)^\gamma
\]

**SURFACE ROUGHNESS**

\[
\tau_{SR} = \tau_{SR0} \frac{1}{m_r} \left( \frac{F}{F_0} \right)^{-\delta}
\]

\[
\mu_{SR} = \frac{q\tau_{SR}}{m^*}
\]

**Coulomb centers and surface roughness**

- **Surface roughness**
- **Coulomb-limited**
- **Phonon-limited**
- **TOTAL, TB = 15 nm**

**Mobility @max n(x)[cm²/Vs]**

- 1,0E+02
- 1,0E+03
- 1,0E+04
- 1,0E+05

**Inversion Charge [cm⁻²]**

- 3E+11
- 3E+12
Validation against experiments

Local mobility model implemented in the DG-DD approach via the TCAD Physical-Model Interface (PMI)

Analytical model fitted against IMEC experiments

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**Effective Mobility [cm²/Vs]**

- EXP, TB = 15 nm
- EXP, TB = 10 nm
- EXP, TB = 5 nm

**Inversion Charge [cm⁻²]**

**Drain Current [µA/µm]**

- EXP, TB = 15 nm
- EXP, TB = 10 nm
- EXP, TB = 5 nm

**VGS [V]**
Effect of strain
The InGaAs heterostructure

DEVICE UNDER STUDY AND EXPERIMENTAL CHARACTERIZATION:


TCAD INVESTIGATION AND ELECTRON MOBILITY MODEL:

The model described so far has been generalized to **biaxial strain**

- $E_C$ shift, effective masses and non-parabolicity factor via the in-house simulator based on a 4-band $k\cdot p$ Hamiltonian [M. Visciarelli et al., EDL 2016];

- $D_{IT}$ fitted against inversion charge vs. $V_{GS}$ obtained from Hall measurements.
The inversion-charge reaches larger values with biaxial tensile strain; it can be nicely reproduced by accounting for the $E_C$ shift (theoretically calculated) and an additional small reduction of $D_{IT}$ (fitted against experiments).
• Tensile-strained effective mobility vs. total charge (free + trapped charge) → 25 – 35% enhancement

• Nicely reproduced by the proposed model by implementing the tensile-strained masses calculated by the $k \cdot p$ model with no additional fitting parameter
Quasi-ballistic regime
The ballistic mobility term

- Reaching the quasi-ballistic regime, DD transport model overestimates current at low fields → Shall we quit DD?

\[
\mu_{\text{eff}} = \frac{1}{\mu_{\text{bal}}} + \frac{1}{\mu_{\text{SC}}}
\]

Electron mobility in a long (collision-dominated) sample

\[
\mu = \mu_{\text{ballistic}} + \mu_{\text{scattering}}
\]

Proposed quasi-ballistic corrections

- The ballistic mobility can be calculated and used to correct the TCAD low-field mobility model.

\[
\frac{1}{\mu_{\text{eff}}} = \frac{1}{\mu_{\text{bal}}} + \frac{L}{L_G} \frac{1}{\mu_{\text{SC}}}
\]

correction factor

electron mobility in a long (collision-dominated) sample

\[
\frac{1}{\mu_{\text{eff}}} = \frac{1}{\mu_{\text{bal}}} + \frac{1}{\mu_{\text{SC}}}
\]

ballistic mobility

Session C6L-C – Thursday 15, 2016 – 14:35
«TCAD low-field mobility model for InGaAs UTB MOSFETs including quasi-ballistic corrections»
Conclusions

An accurate TCAD approach for InGaAs ultra-thin-body MOSFETs has been devised in the frame of the III-V-MOS EU Project:

- The mobility model is physically based, includes quantum confinement, non-parabolicity and interface traps. Experiments are nicely reproduced.

- The model captures the biaxially-strained mobility of a $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ MOSFET without need of ad-hoc fitting parameters.

- A procedure for including quasi ballistic effects in short-channel devices has been implemented and will be presented at ESSDERC 2016 (Session C6L-C – Thursday 15, 2016 @14:35)

A good step towards extending the validity of traditional DD simulation approaches to emerging III-V technologies.