nanoHUB online simulation and more — an NCN project

Full-Band and Atomistic Simulation of Realistic 40nm InAs HEMT

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PURDUE UNIVERSITY

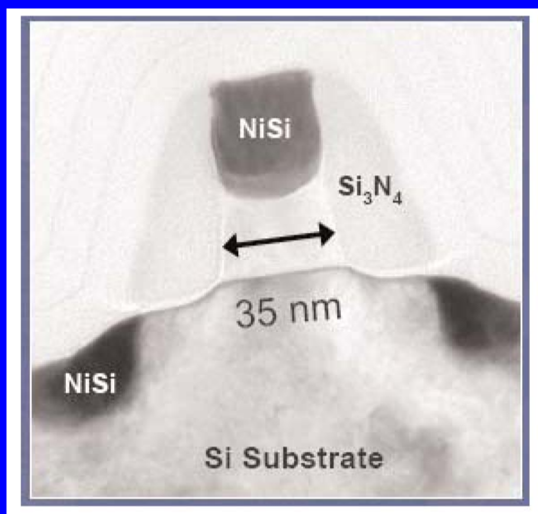
NCN

NSF

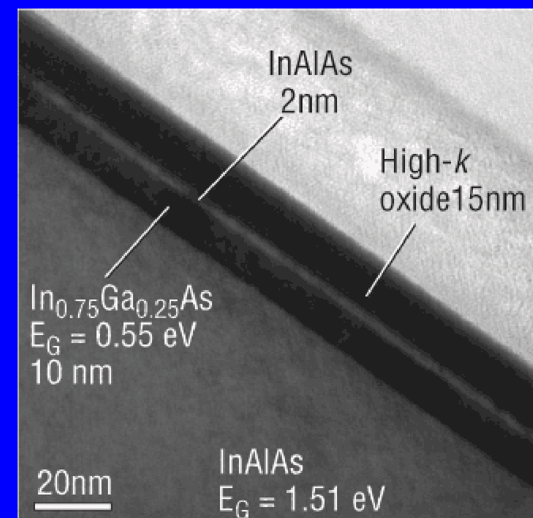
Motivation: Towards III-V MOSFET

Expectation: High Speed (Mobility), Low Power Consumption
On Chip Integration of Electronics and Optics
Challenges : Oxide Layer (high-κ), p-doped Transistors

65nm Node Devices
L_G=35nm



INTEL

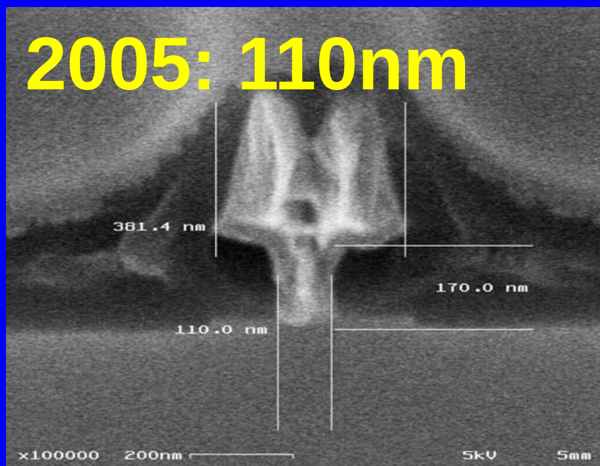


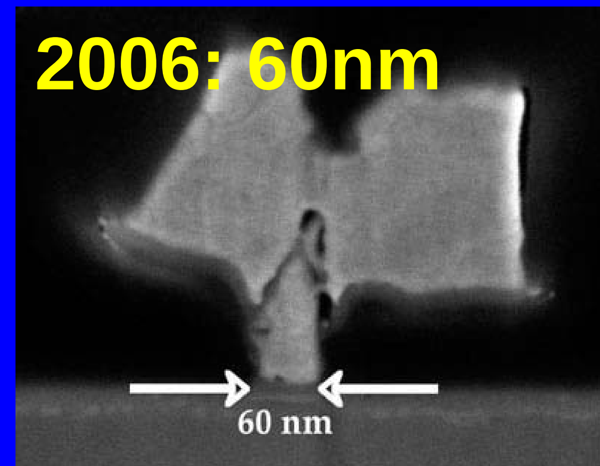
FREESCALE

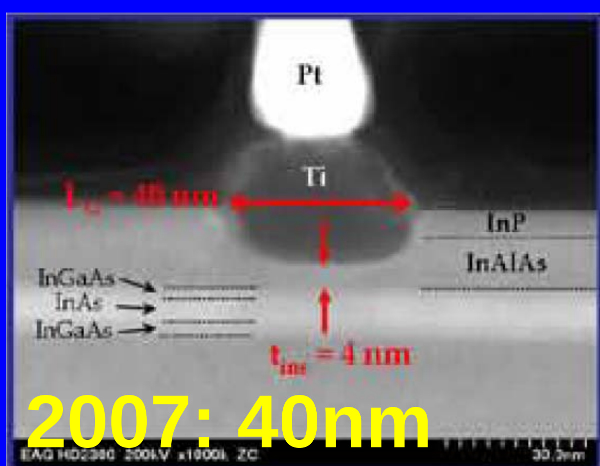
http://download.intel.com/technology/silicon/silicon_paper_06.pdf and
http://www.solid-state.com/display_article/346921/5/none/none/Feat/III-V-MOSFETs-for-future-CMOS-transistor -applications

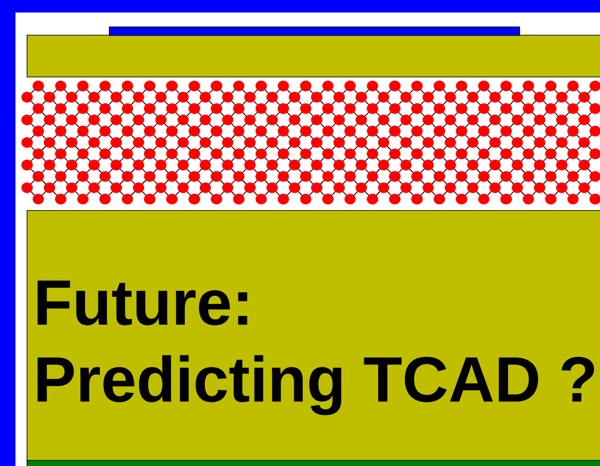
Intermediate Step: III-V HEMTs

Lot of Recent Advancement by del Alamo's Group at MIT
Every Year Devices with a Shorter Gate Length Introduced









Outline

- Motivation
- Simulation Approach
  - Bandstructure and Transport
  - Multi-Scale Domain Decomposition
- Performance Analysis
  - I_d-V_{gs}, I_d-V_{ds}
  - Transconductance
- Challenges and Open Issues
  - Injection Velocity, Leakage Current
- Conclusion and Outlook

Simulation Approach

Bandstructure Model

Nearest-Neighbor $sp^3d^5s^*$ Tight-Binding Method

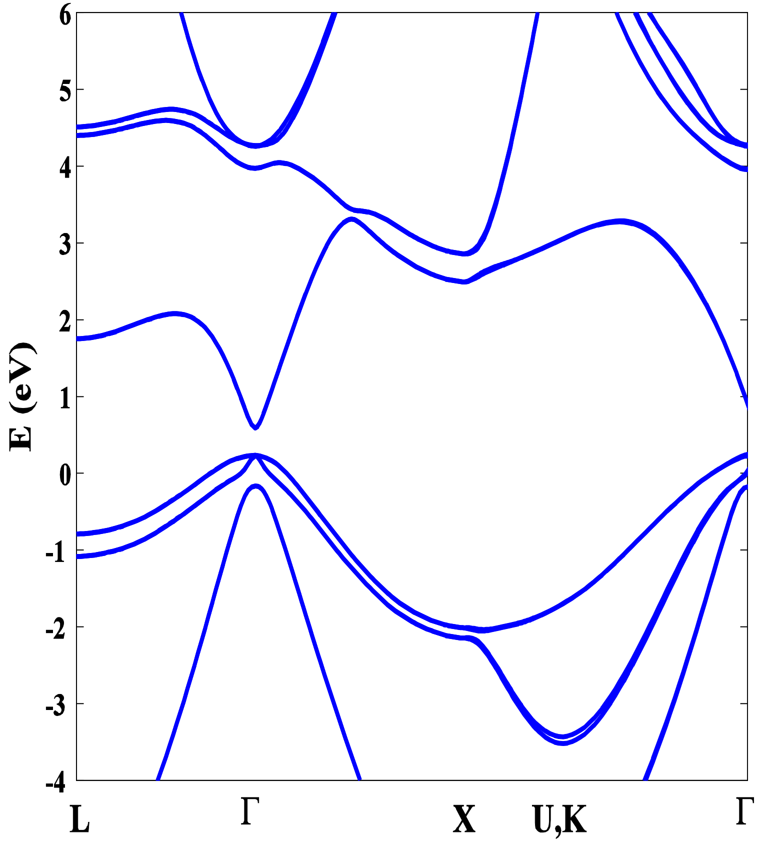
GOOD:

- bulk CB and VB fitted
- extension to nanostructures
- atomistic description
- alloy disorder (InGaAs)
- strain relaxation

BAD:

- high computational effort
- semi-empirical model

InAs Bandstructure

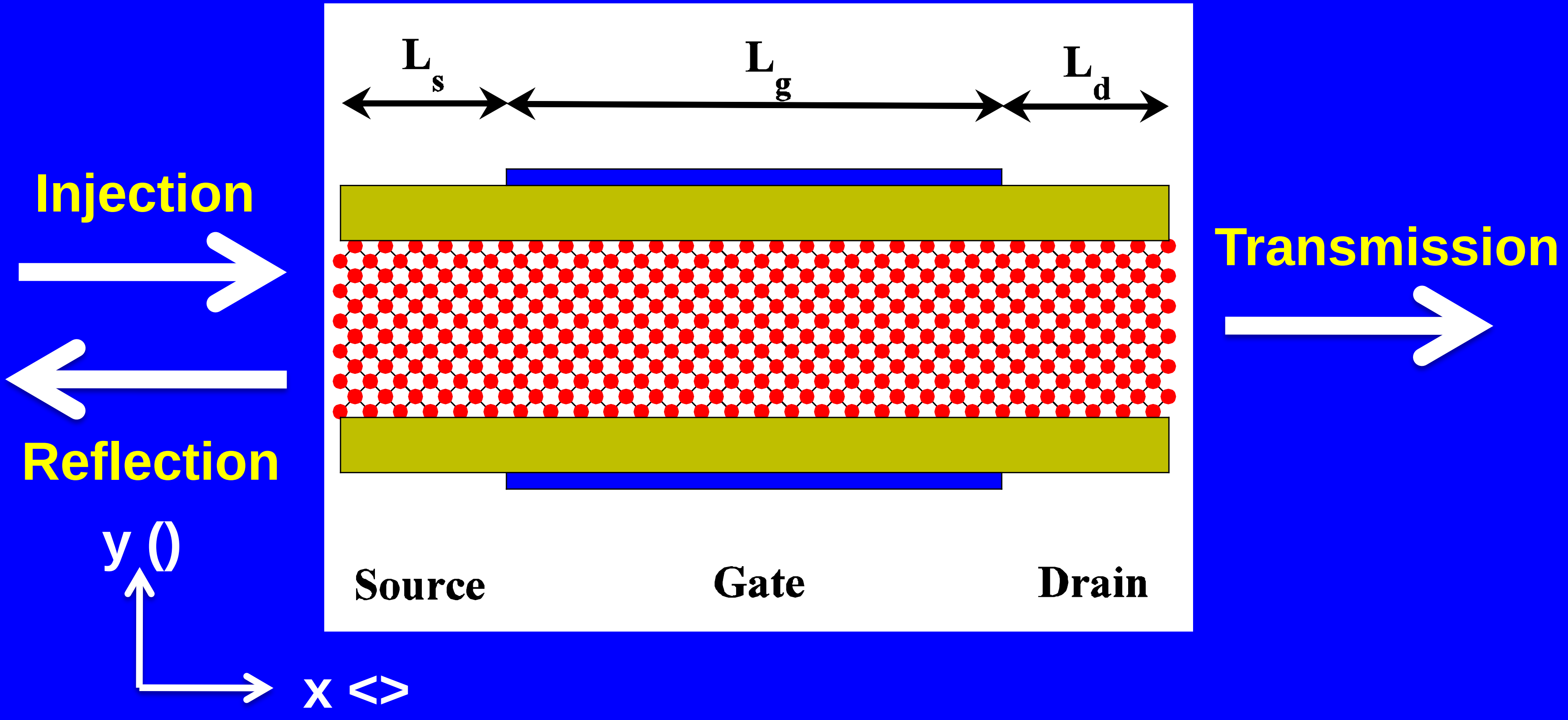


Transport Model (1)

Atomistic and Full-Band Transport: NN $sp^3d^5s^*$ T-B Model

x: transport direction / y: confinement / z: periodic

States Injected at different Energies E and Wavevector k_z



Transport Model (2)

2D Schrödinger Equation

$$H \mid \psi_E > \; = \; E \mid \psi_E >$$

Tight-Binding Ansatz for the Wave Function

$$< r \mid \psi_E > \; = \; \sum_{\sigma,ijk,k_z} C^{\sigma}_{ij}(E,k_z)\Phi_{\sigma}(r - R_{ijk})e^{ik_z z_k}$$

$$(E\text{-}H\text{-}\Sigma)\cdot G^R = I$$

Matrix Inversion

$$(E\text{-}H\text{-}\Sigma)\cdot C = Inj$$

Linear System of Eq.

Transport Model (2)

-Linear System of Eq. Ax=b

- Size of A: number of atoms times number of orbitals per atom

- ~1000 Energies, 15-30 Momentum

- Parallel Approach

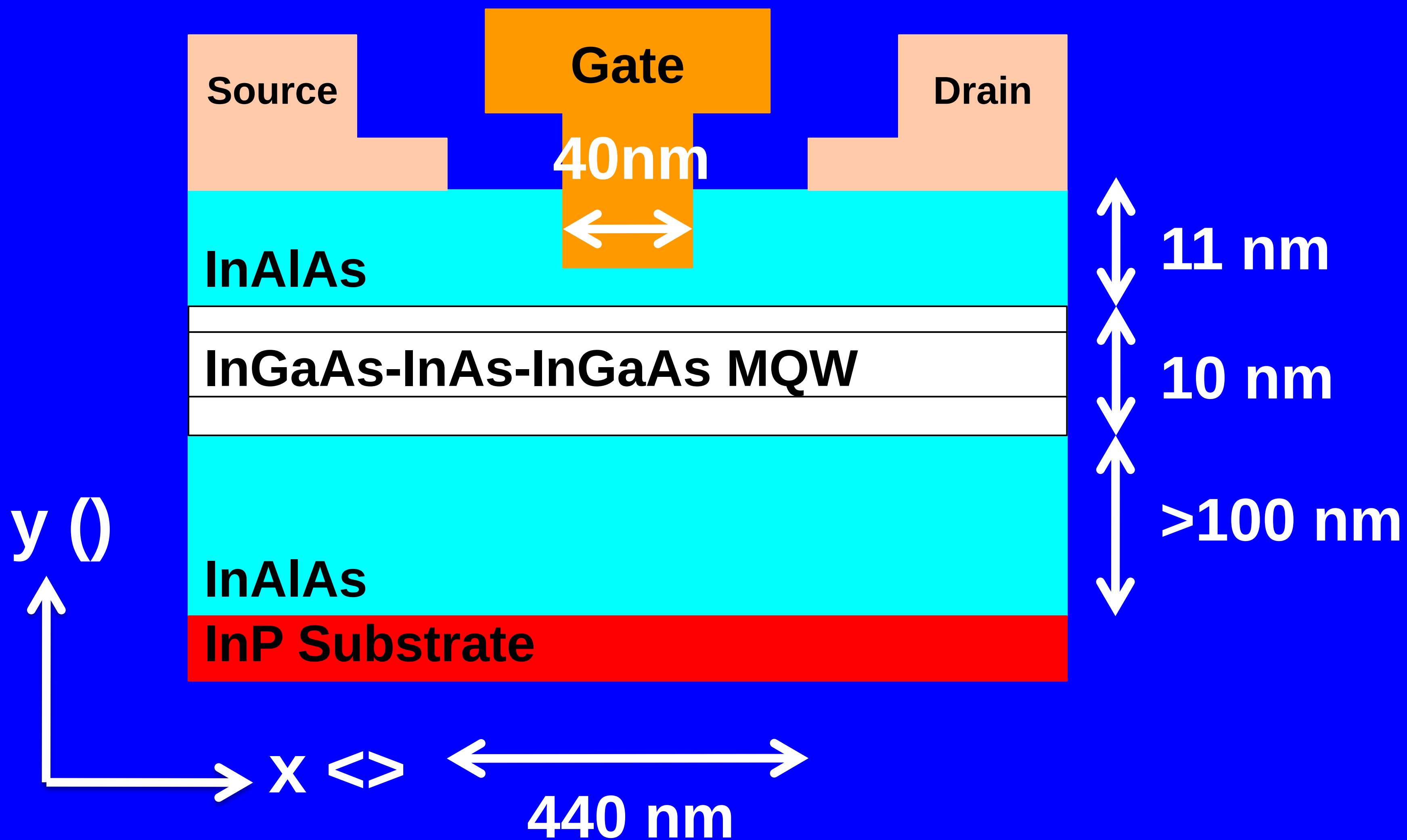
- 2D Domain limited to 15x200 nm2

- Multi Scale Decomposition

Matrix inversion   Linear System of Eq.

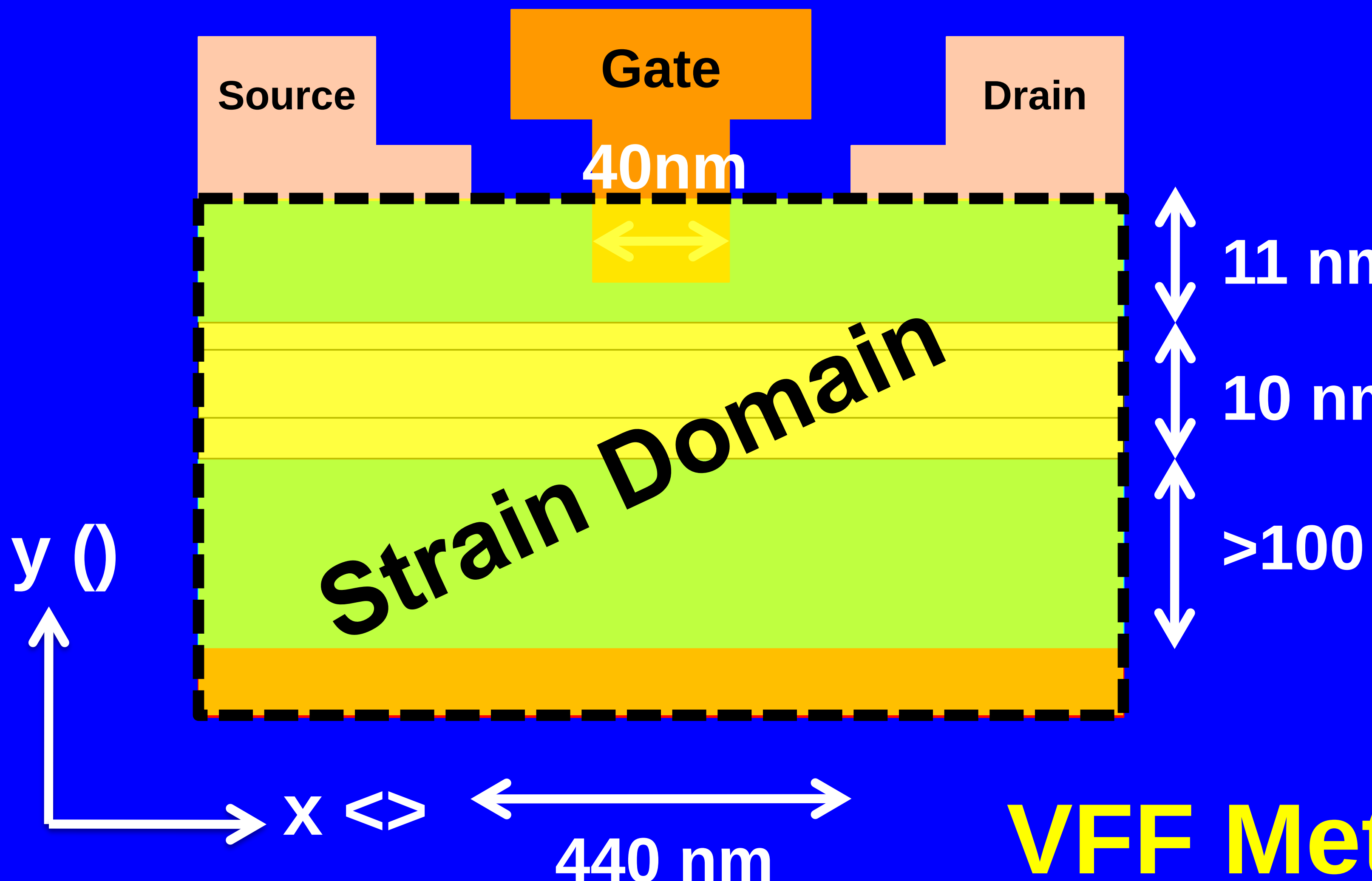
Multi-Scale Domain Decomposition (1)

Device Structure: Transport, Poisson, Strain



Multi-Scale Domain Decomposition (2)

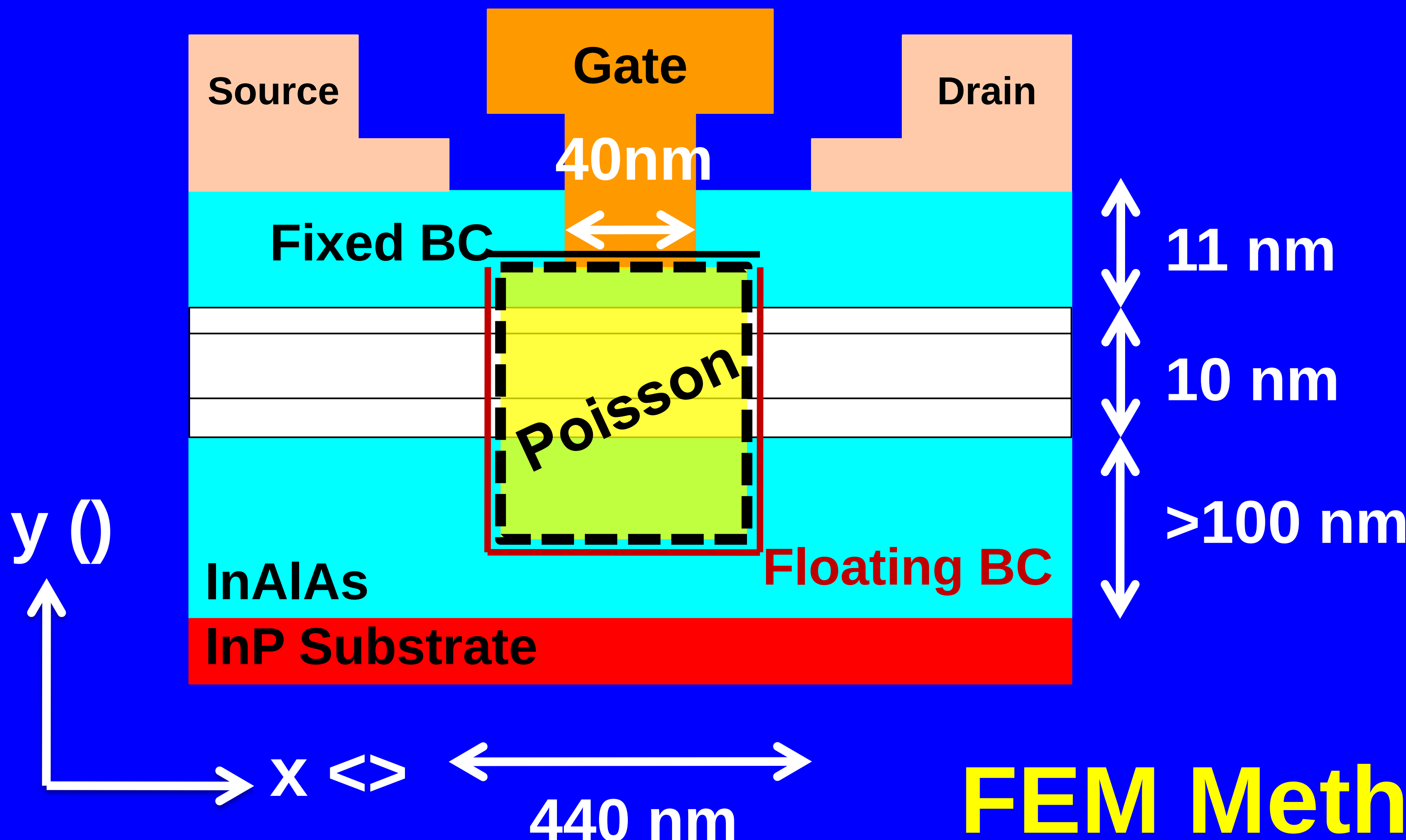
Strain: Long Range Effect down to InP (1.4M Atoms)



VFF Method

Multi-Scale Domain Decomposition (3)

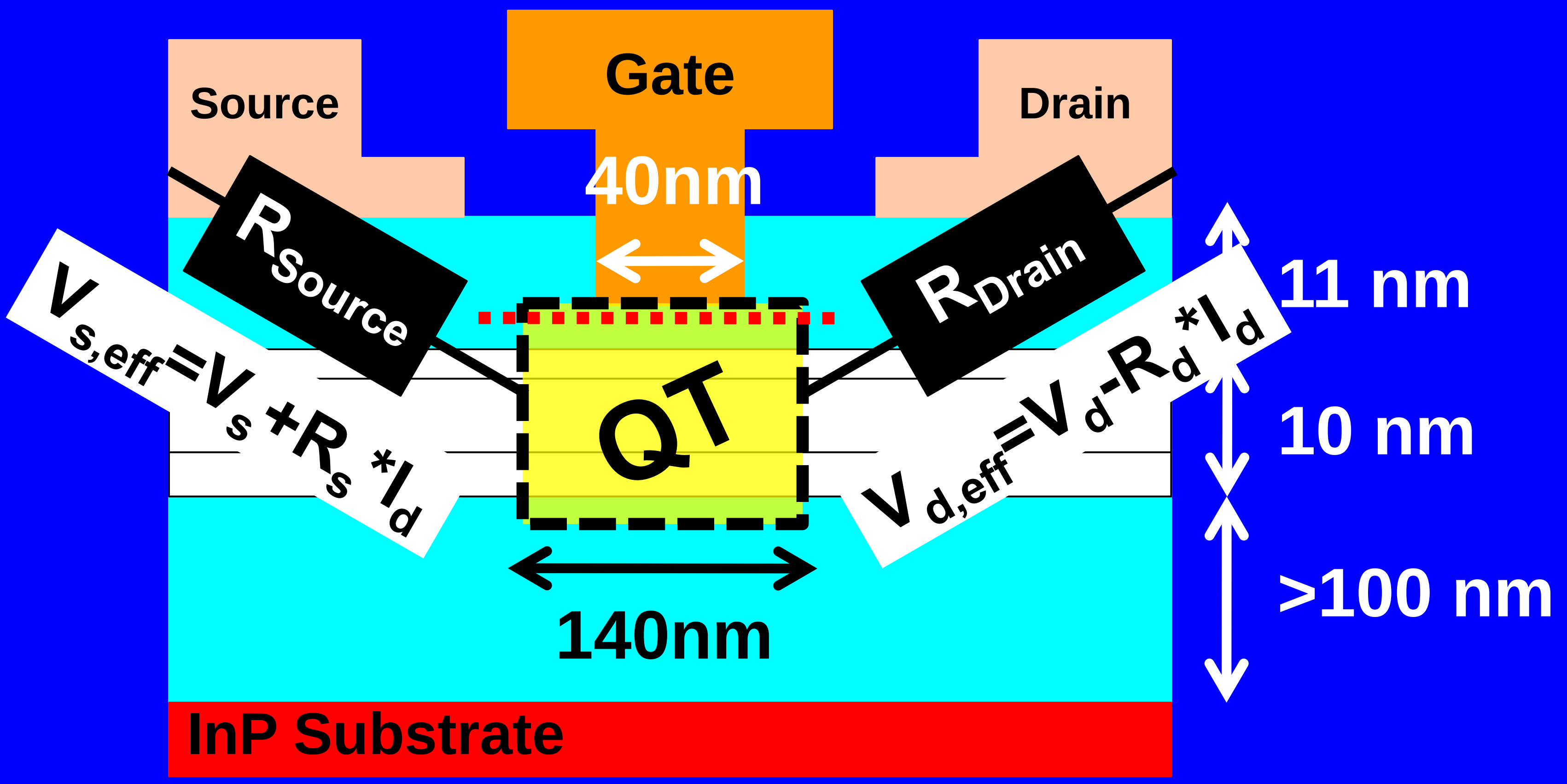
Electrostatic Potential (Poisson): Fields in InAlAs



FEM Method

Multi-Scale Domain Decomposition (4)

Quantum Transport: 140x14 nm^2 area (38,556 Atoms)



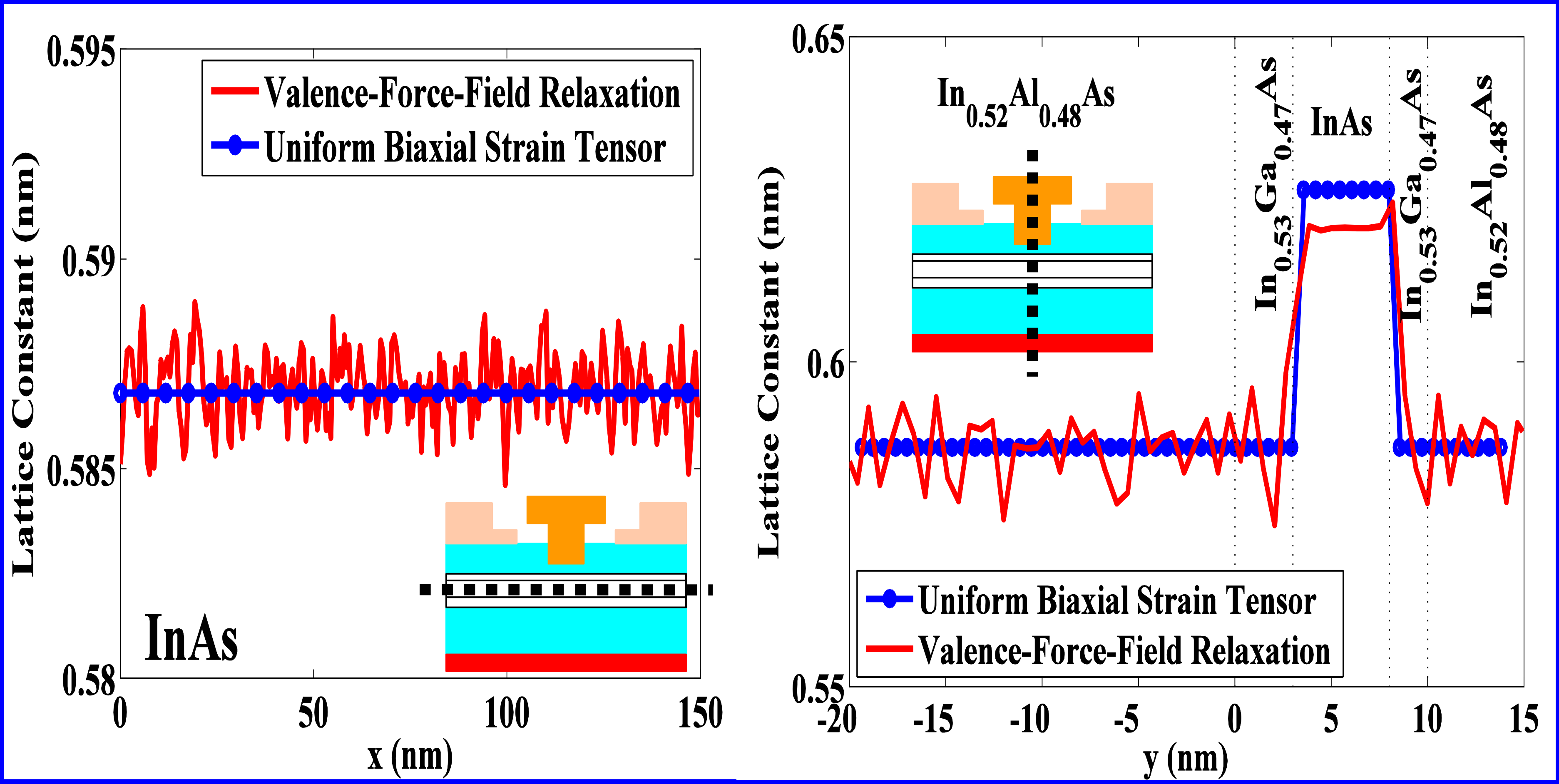
$R_s = R_d = 190\Omega\cdot\mu m$

Tight-Binding

Performance Analysis

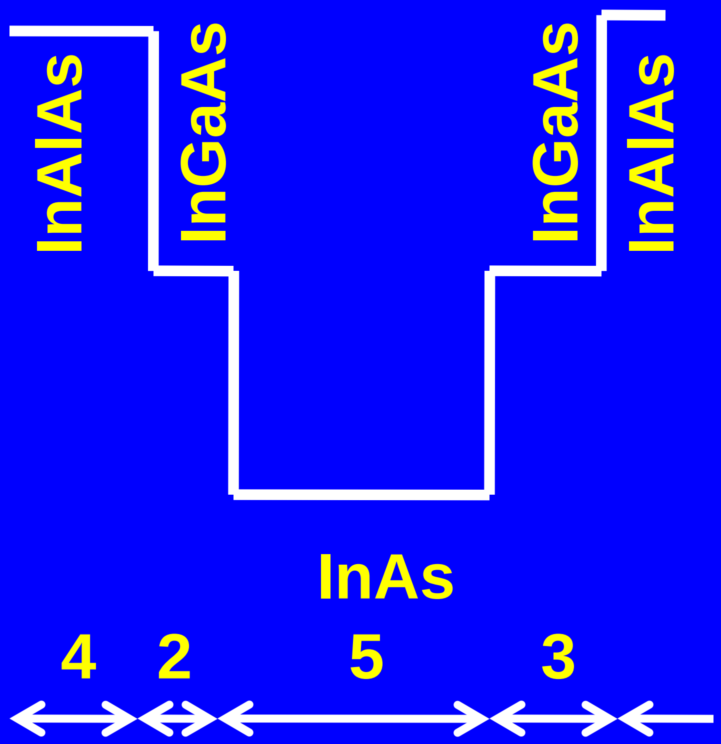
Strain Profile: Alloy Disorder

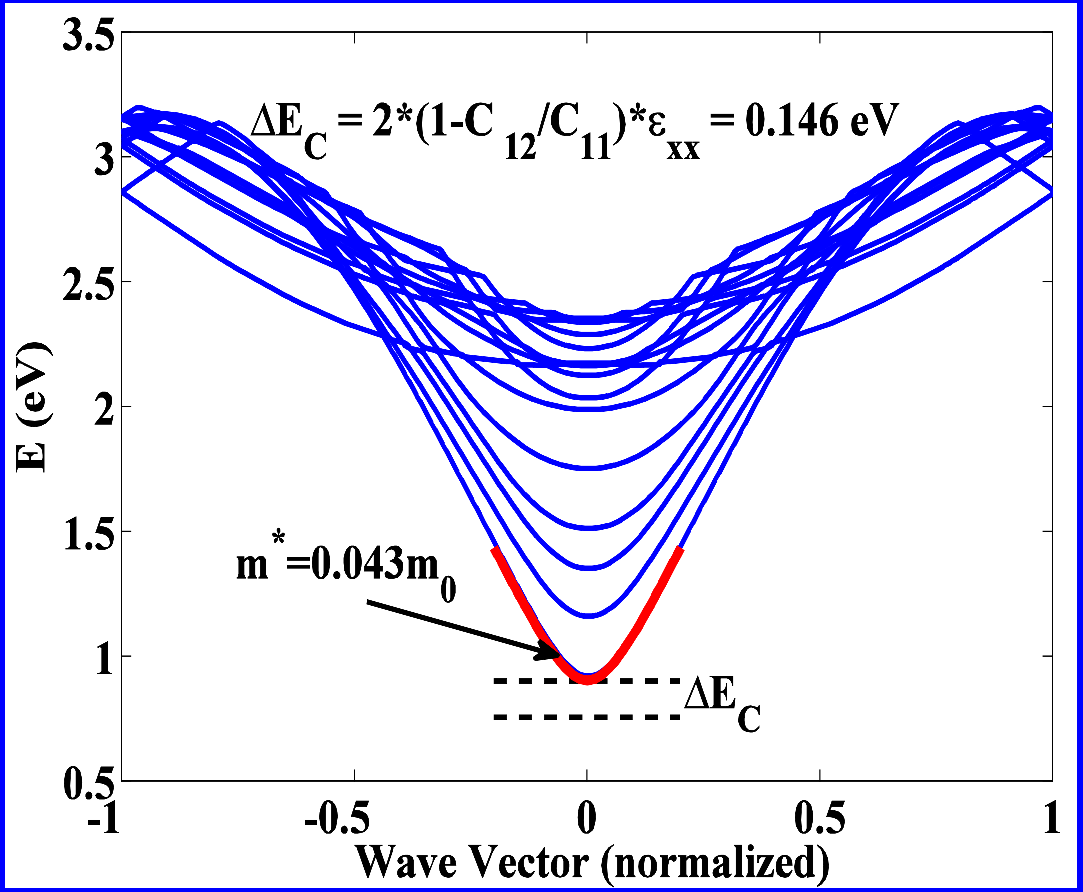
Lattice Constant along (a_x) and across (a_y) the InAs QW
InAs on $In_{0.53}Ga_{0.47}As$ => Biaxial Compression along x and z



Bandstructure of the MQW Region

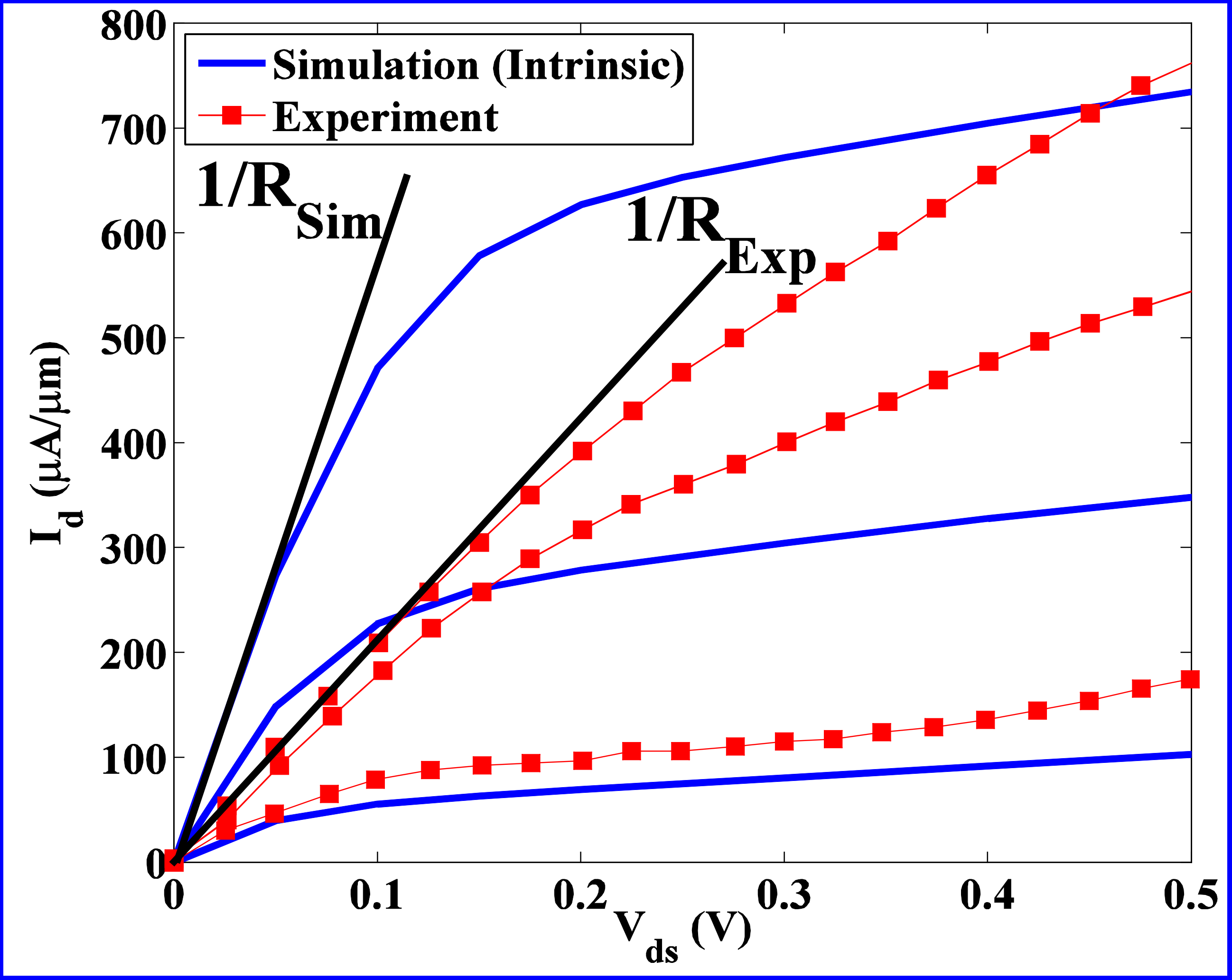
Two Effects: 1) Band Gap Increase (Biaxial Strain)
2) Effective Mass Increase (QW Width)





Intrinsic Output Characteristics

Comparison with Measurement => 2 Discrepancies
(1) Simulated Resistance much too Low, (2) Current too High



V_{gs}=0.40 V

V_{gs}=0.15 V

V_{gs}=0.20 V

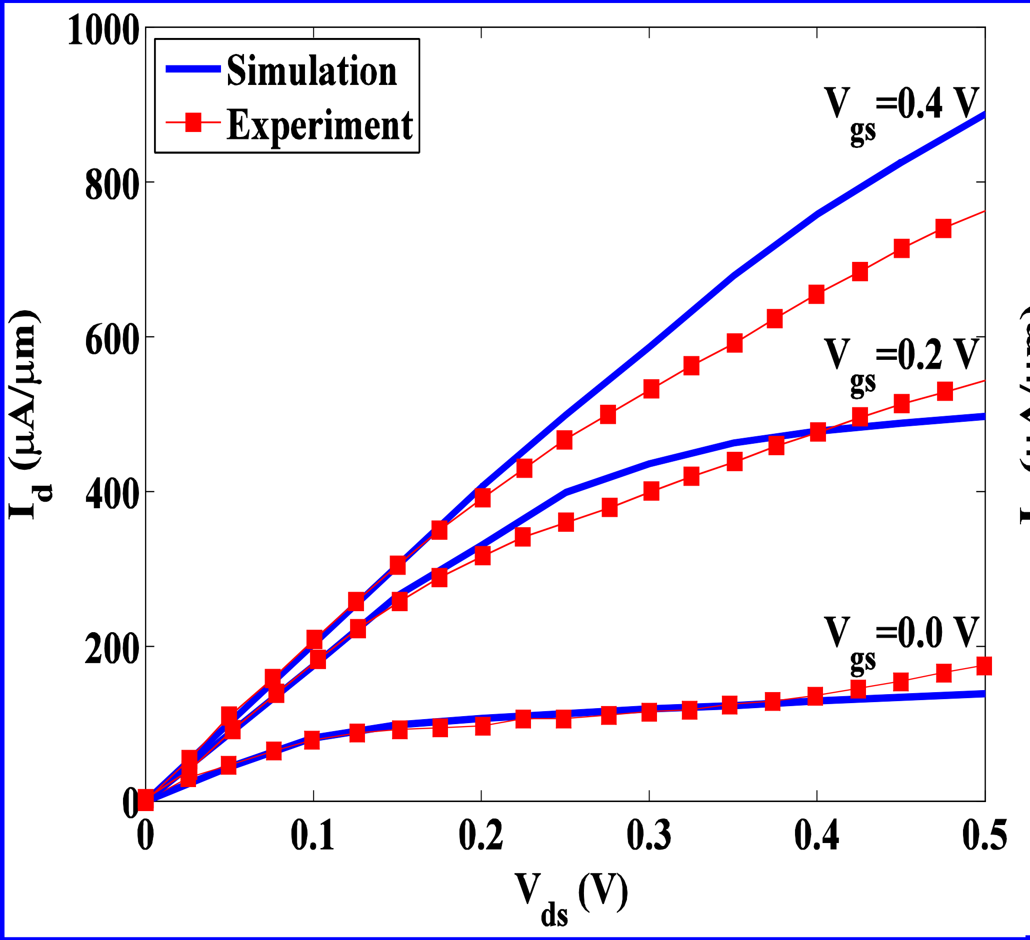
V_{gs}=0.05 V

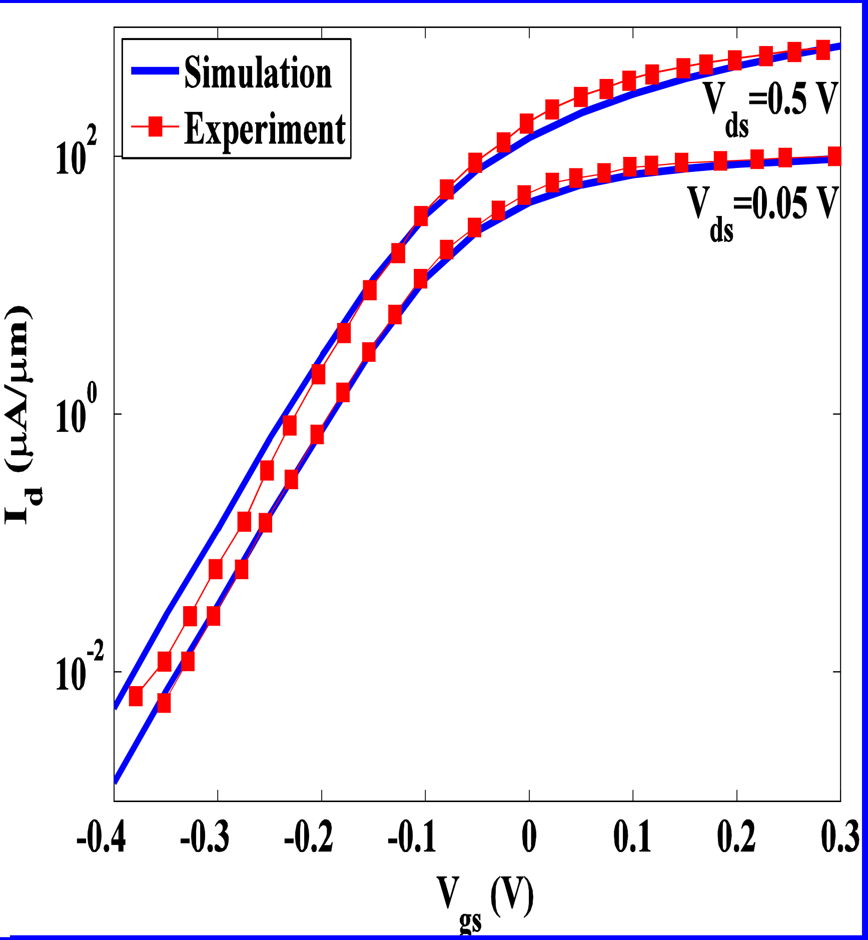
V_{gs}=0.0 V

V_{gs}=-0.05 V

Current Characteristics

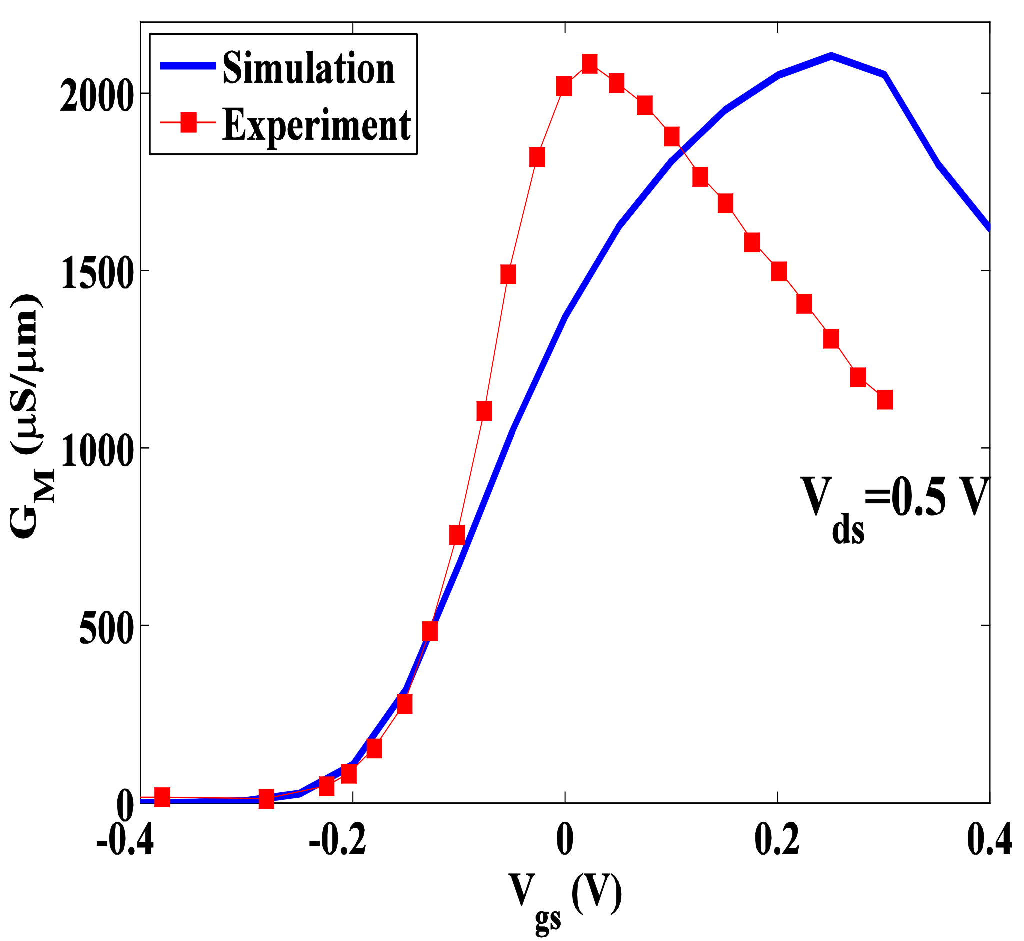
I_d-V_{ds} and I_d-V_{gs} with Source and Drain Resistances
Simulated ON-current still too High: not Completely Ballistic?





Transconductance G_M

Turn-ON and Maximum of G_M Correct, not the Slopes
Decrease of Simulated G_M due to Source Starvation
Source Resistances is not the Limiting Factor of $G_{M,Lim}$



$$G_M = dI_d/dV_{gs}$$

$$= dI_d/dV_{gseff} \times dV_{gseff}/dV_{gs}$$

$$V_{gseff} = V_{gs} - R_s \times I_d$$

$$G_M = \frac{dI_d/dV_{gseff}}{1 + R_S \times dI_d/dV_{gseff}}$$

$$G_{M,Lim} \approx 1/R_s$$
$$\approx 5e3\ \mu S/\mu m$$

Summary of Performances

Transistor Parameters from Simulation and Experiment: ON-Current, Threshold Voltage, Subthreshold Swing, DIBL, Maximum of Transconductance, and Injection Velocity

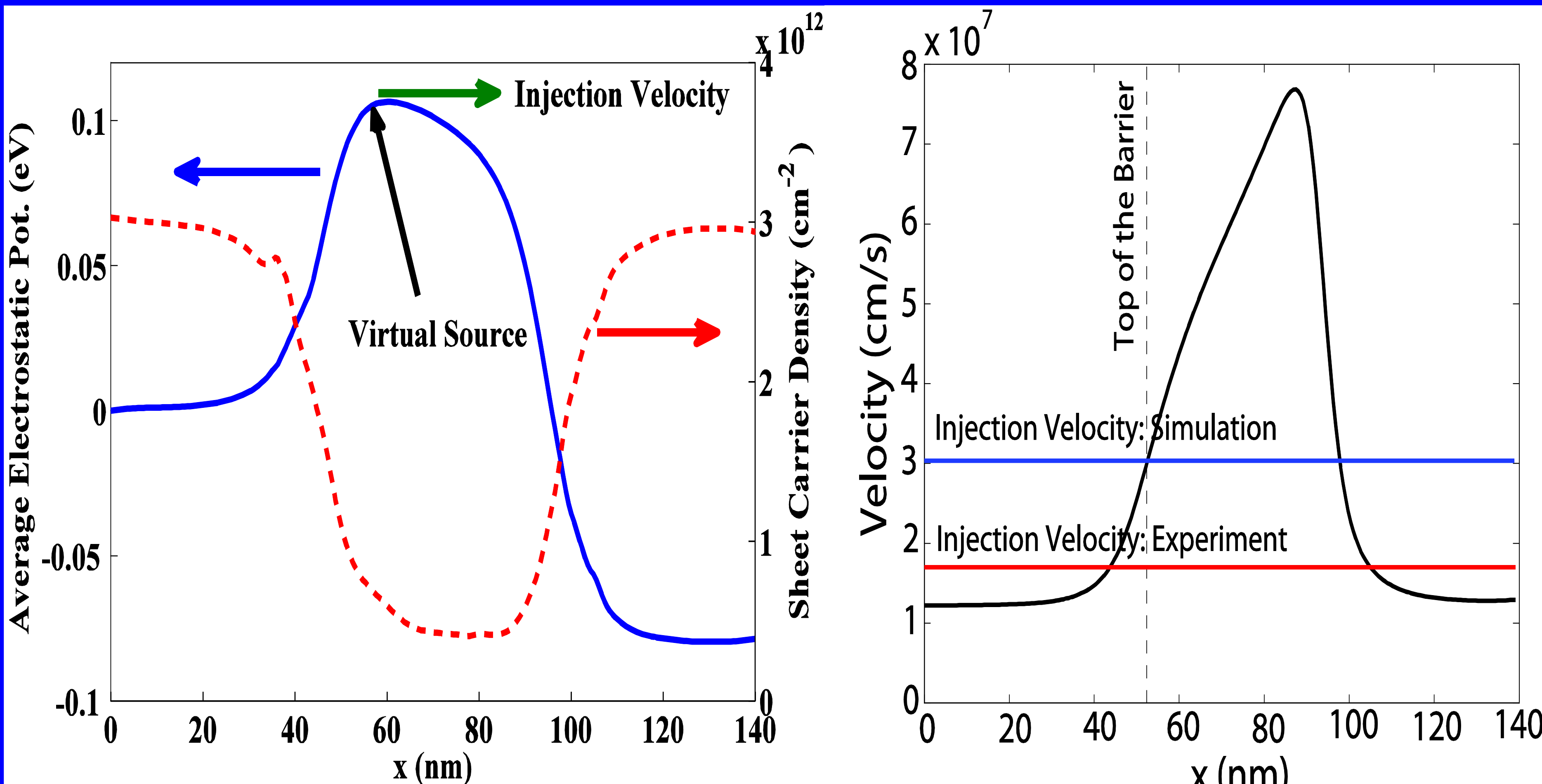
	Experiment	Simulation
V_{CC} (V)	0.5	0.5
I_{ON} at V_{gs}=0.3 V (μA/μm)	656	676
V_{th} (V)	-0.23	-0.23
SS (mV/dec.)	70	72.7
DIBL (mV/V)	80	96
G_{max} (μS/μm)	2083	2105
n_{2D} in Channel (cm^{-2})	2.9e12	2.9e12
Injection Velocity (cm/s)	1.7e7	3.0e7

Challenges and Open Issues

Injection Velocity

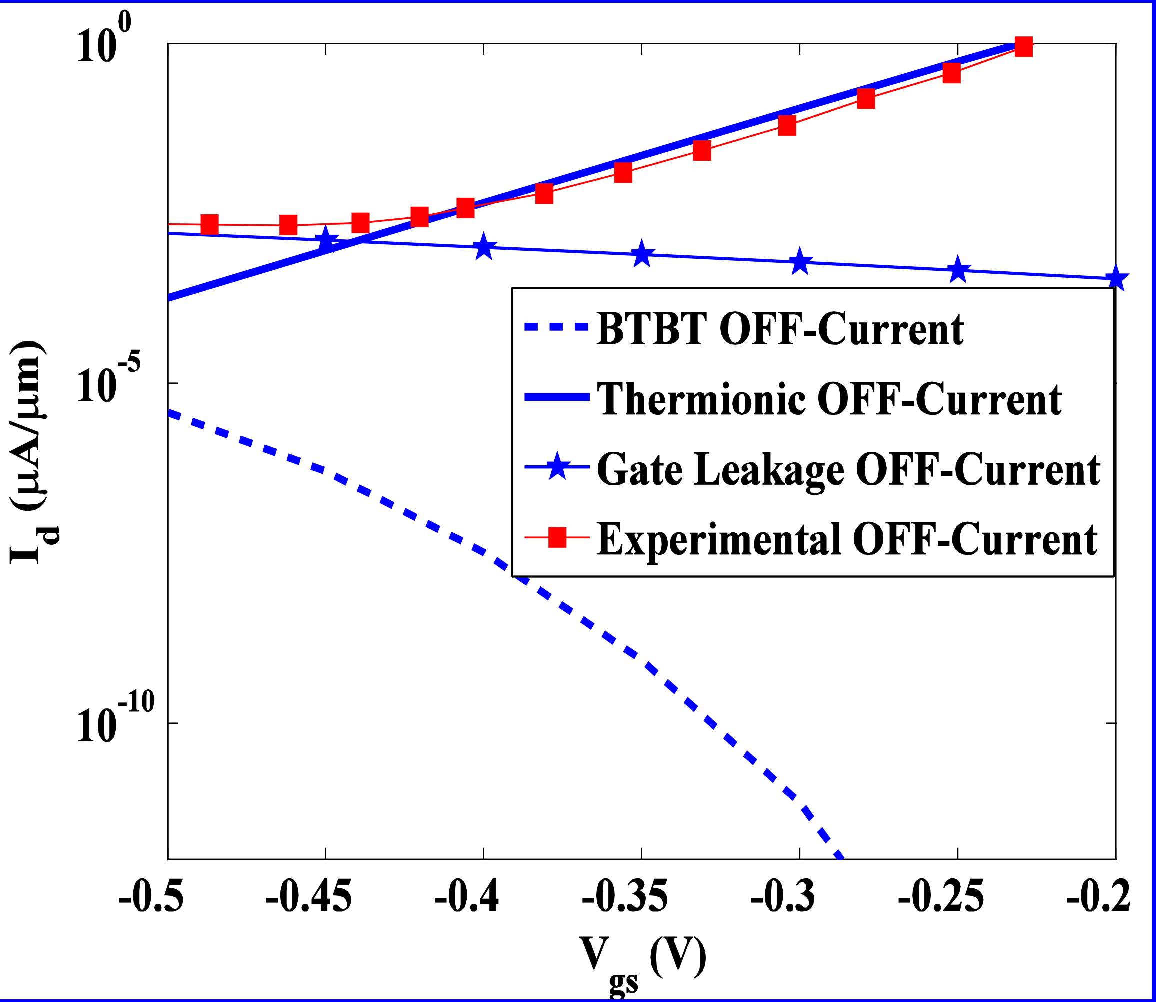
Injection Velocity at Virtual Source: $J = q \times N_{dens} \times v_{inj}$

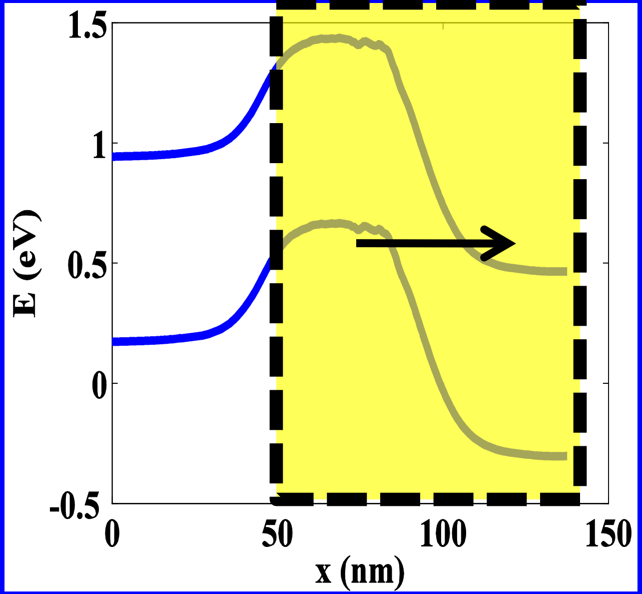
Simulated Velocity Overestimates Measurement by 1.76×



Leakage Currents: BTBT and Gate

BTBT OFF-Current Added as a Post-Processing Simulation
Gate Leakage OFF-Current under Investigation (EM Model)





BTBT Sim. Domain
After SC Calculation
FB Required

Conclusion and Outlook

- **Quantum Transport Simulator**
  - Full-Band and Atomistic
  - III-V HEMTs
- **Performance Analysis**
  - Good Agreement with Experiment
  - Some Open Issues
- **Outlook**
  - Improve Models (Contact)
  - Investigate Scaling of Gate Length
  - Scattering?