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Departamento de Electrónica y Tecnología
de Computadores

Advanced Simulation of Nanotransistors

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Acknowledgments



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OUTLINE

1. Introduction. Why?
2. Simulation concepts & tools. How?
3. Simulation results. What?
 - A. Carrier mobility (electron & holes): ultrathin FDSOI, DGSOI, strained-Si channels, arbitrary crystallographic orientation
 - B. I-V characteristics of short channel devices. Radiation effects on FinFETs.
 - C. Si nanowires. Transport of 1D electron gases.
 - D. Design of new devices: A-RAM and A2RAM memory cells.



1.- Introduction.

- Why do we do simulation?
 - To have good friends



- To attend conferences and publish papers



- These are good reasons, of course, but there are others

1.- Introduction.

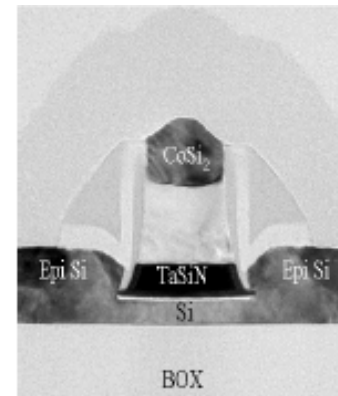
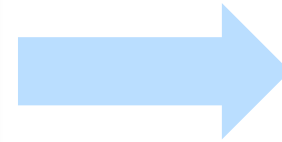
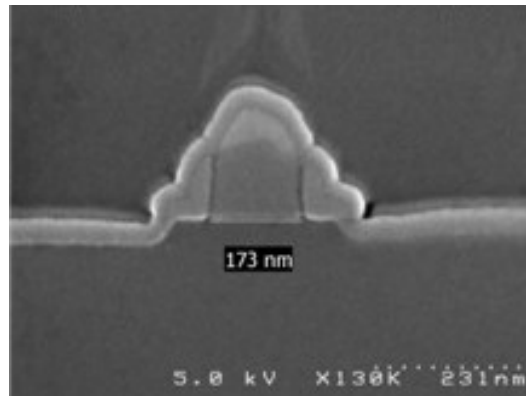
- Why do we do simulation?
 - If we want to use a device in a circuit, you need to understand how the device works !
 - If we want to improve the performance of a given device, you have to know how this device behaves internally!!
 - If you want to propose new devices to overcome the scaling limitations of existing technology, you have to demonstrate that the device works, and you have to optimize it, before fabrication.
 - But this is not easy nor evident with today's devices ! Which are today devices?



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From doping based scaling to thickness based scaling



Following Moore's law: problems with non-trivial solution appear (high dopings, variability issues)

Reconsider the classical concepts

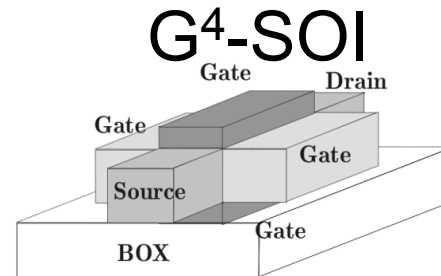
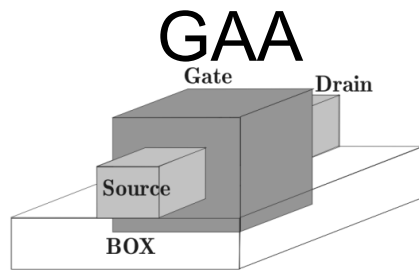
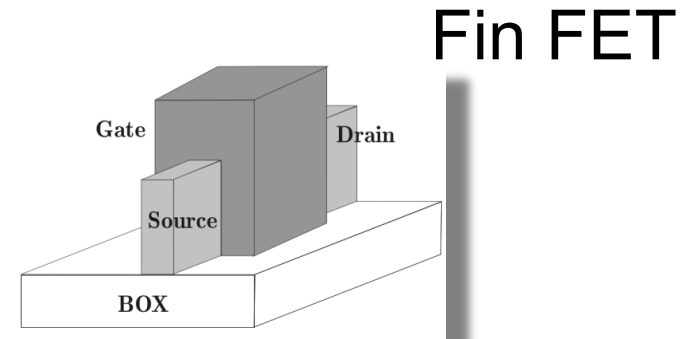
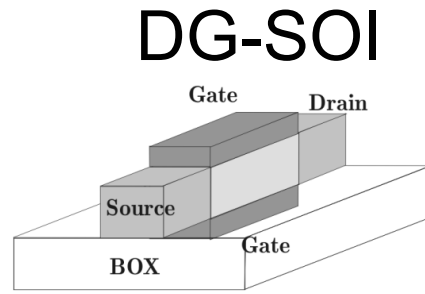
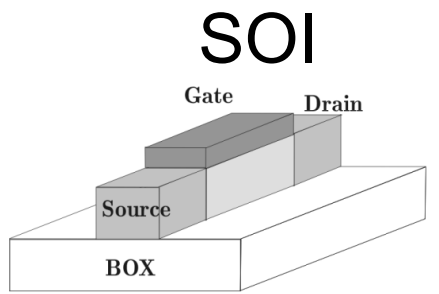


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From doping based scaling to thickness based scaling

If one gate is not enough, why don't we have more than one?



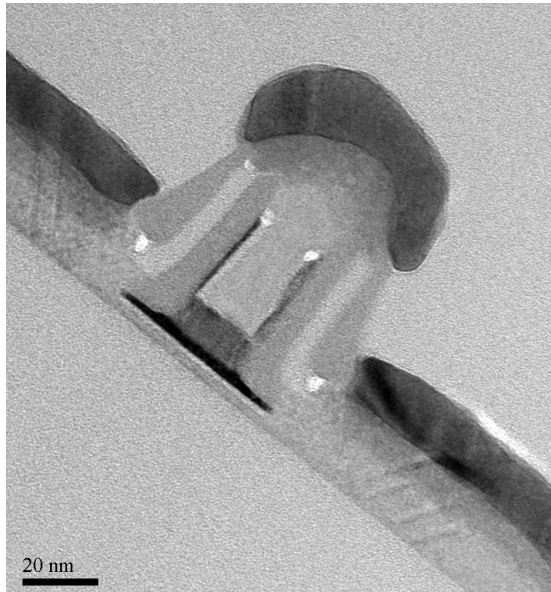
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CMOS Scaling

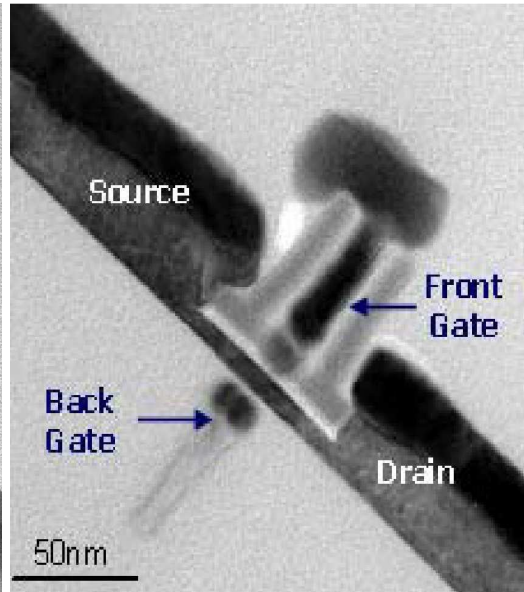
- **SOI: Thickness based & number of gates**

(Courtesy of LETI)



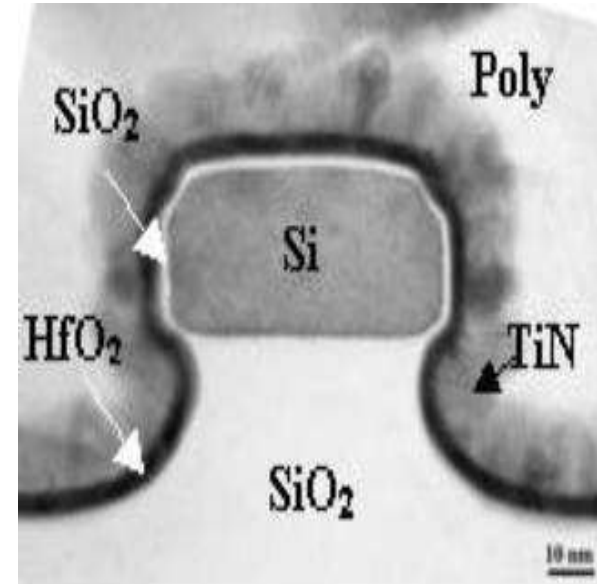
Planar FDSOI

$$T_{Si} \approx L_G / 4$$



Double gate SOI

$$T_{Si} \approx L_G / 2$$



Tri-Gate/FinFET

$$T_{Si} \approx W \approx L_G$$



More Moore

The continuous scaling of CMOS requires significant innovations:

1.- Multi-gate devices. → **better scaling.**

2.- Enhancement of carrier mobility:

a. **Specific doping profiles**

b. **Lightly doped epitaxial layers**

c. **Strained**

d. **Crystal**

Our goal:

Carrier mobility in multigate devices



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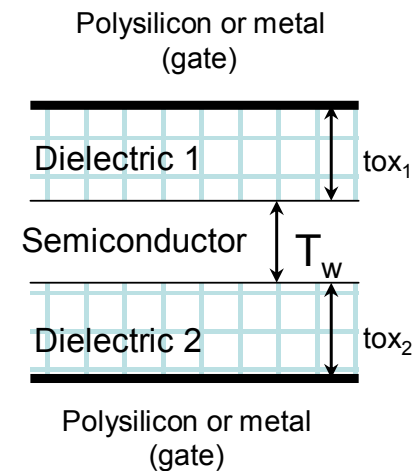
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More Moore

We will consider two kind of devices:

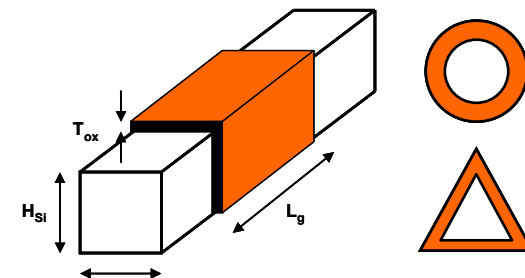
1. Quantum-well devices:

Carriers are confined in one dimension, but can drift in the other two.



2. Quantum-wire devices:

Carriers are confined in two dimensions, and are drifted in the other dimension.



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New simulation challenges

- It is not an easy task !!
- The new device structures require new simulation techniques and tools.
- Conventional tools are not accurate any more.
- Quantum effects become extremely important.
- New procedures are becoming necessary.

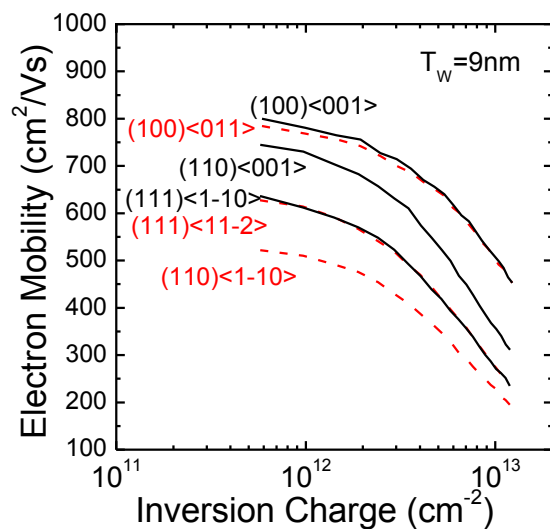


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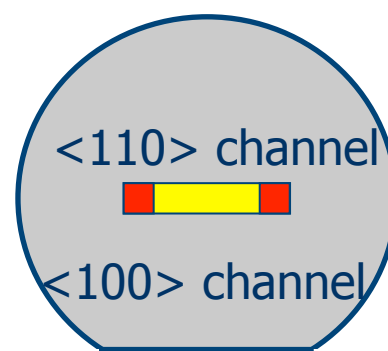
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Simulation examples

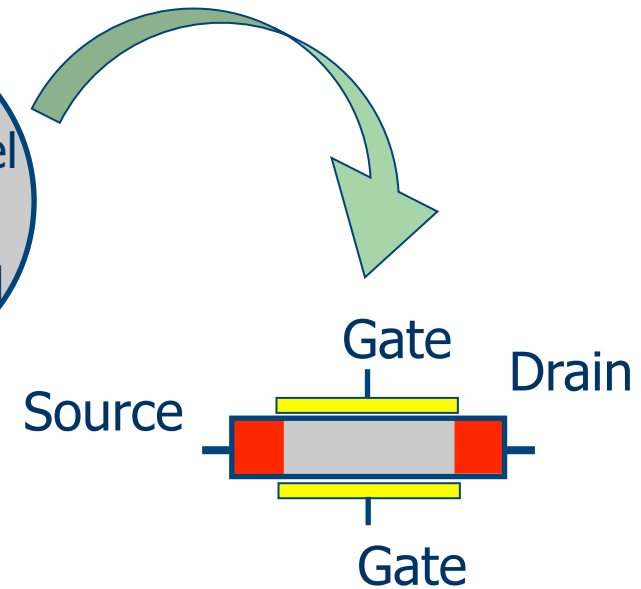
- Simulation of carrier transport in materials and devices.
 - ✓ Goal: simulate the behavior of electron devices, i.e.,
 1. Evaluate the transport properties of charge carriers in materials, or semiconductor structures: carrier mobility, velocity overshoot.



Si-(001)



$\langle 110 \rangle$

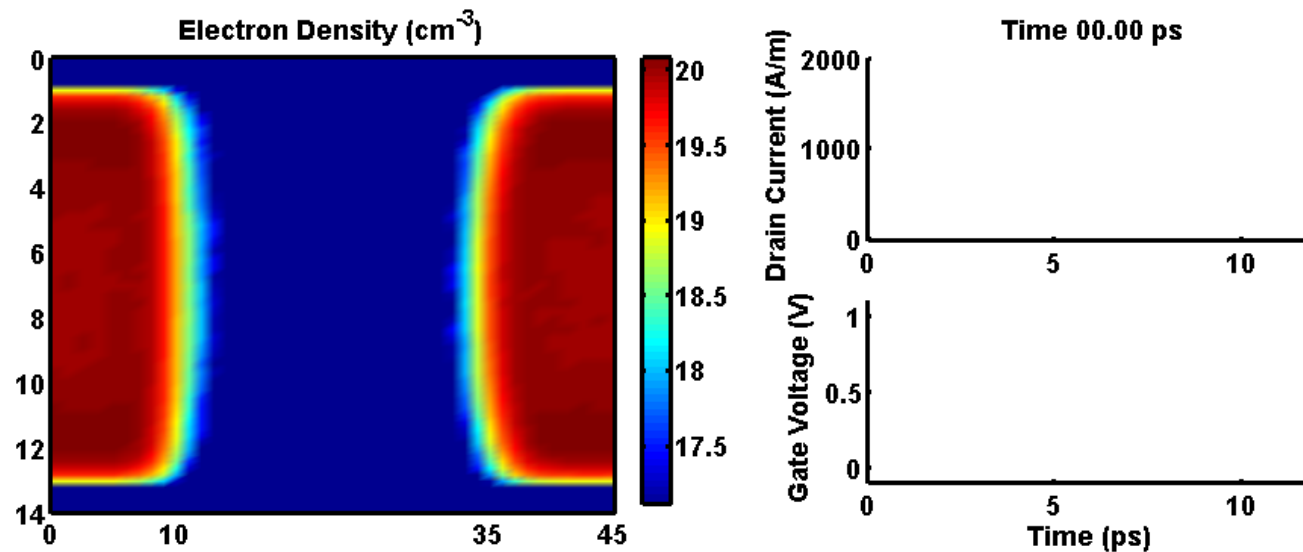


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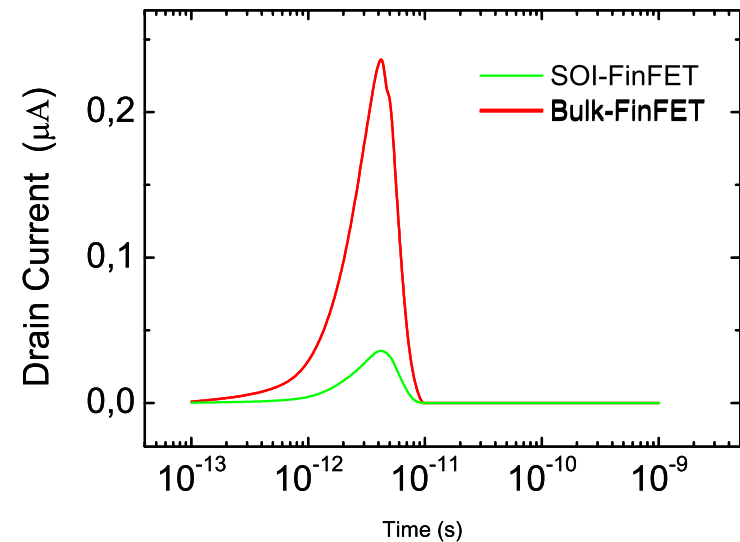
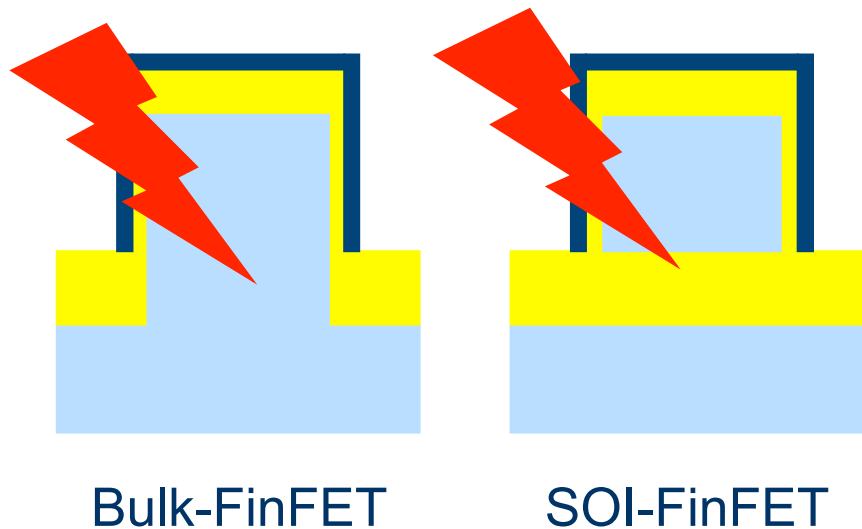
Simulation examples

- Simulation of carrier transport in materials and devices.
 - ✓ Goal: simulate the behavior of electron devices, i.e.,
 1. Calculate the carrier density in a device, knowing the bias applied to them.
 2. Calculate the current at the terminals of a device, knowing the bias applied to them.



Simulation examples

- Simulation of carrier transport in materials and devices.
 - ✓ Goal: simulate the behavior of electron devices, i.e.,
 1. Understand device behavior under physical phenomena:
 2. Understand device behavior under physical phenomena:
 3. Understand device behavior under physical phenomena:
FinFET on Bulk vs FinFET on SOI: radiation effects

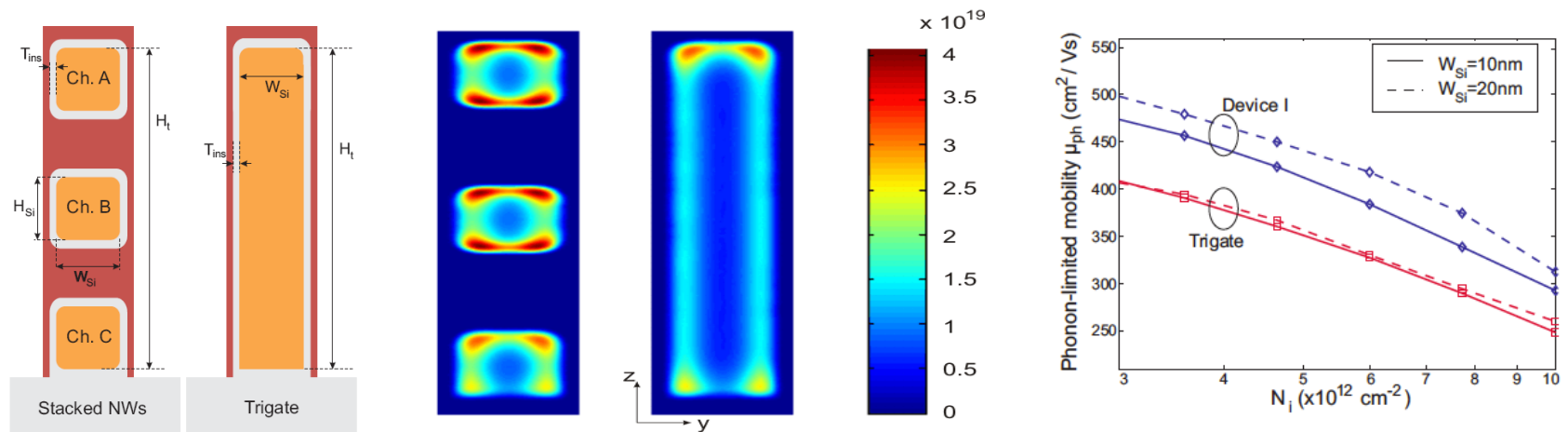


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Simulation examples

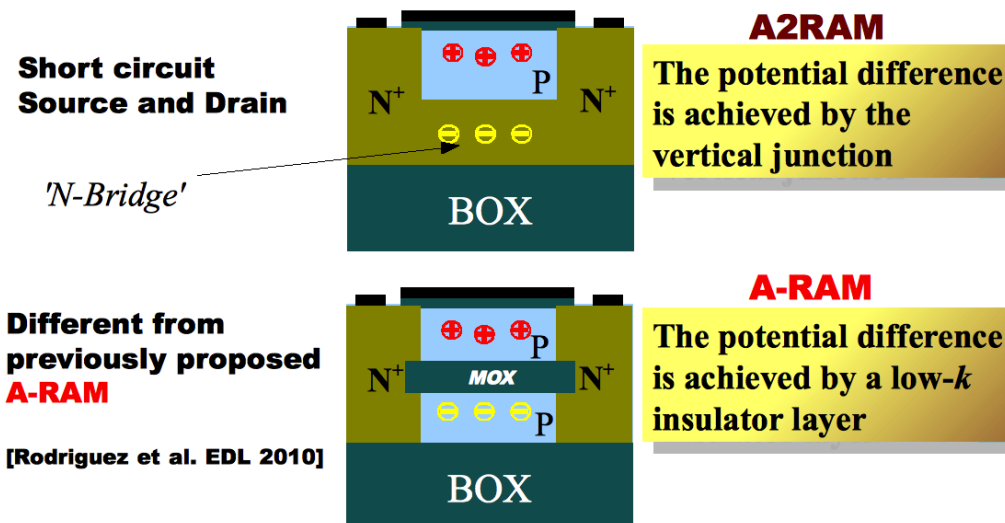
- Simulation of carrier transport in materials and devices.
 - ✓ Goal: simulate the behavior of electron devices, i.e.,
 4. Simulation of Si-nanowires (too many unknowns)
 - ✓ Multigate devices → CMOS scaling
 - ✓ Different design alternatives: FinFETs, MC MOSFETs, GAAs, etc.



Simulation examples

- Simulation of carrier transport in materials and devices.
 - ✓ Goal: simulate the behavior of electron devices, i.e.,
 5. Design new devices: e.g. A-RAM and A2RAM memory cells

The Dual-Body concept



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1. Introduction. Why ?
2. **Simulation concepts and tools. How?**
 1. Simulation of carrier transport.
 2. Electrostatics and Transport.
 3. Band structure. Electrons and holes.
 4. Transport properties. Scattering events. Carrier mobility. Mobility boosters.
 5. Device simulation.
3. Simulation results. What?



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Simulation concepts

- An electron device is a system of many electrically charged particles that interact with an externally applied electric and magnetic fields and with each other.
- Particles are distributed both in geometrical and momentum space, following the particle distribution function:

$$f = f(r, k, t)$$

- The evolution of the particle distribution function is governed by the Boltzmann transport equation, BTE (semiclassical approximation):

$$\frac{\partial f}{\partial t} = -v \cdot \nabla f - \frac{1}{\hbar} \frac{\partial p}{\partial t} \cdot \nabla_k f + \left. \frac{\partial f}{\partial t} \right|_{coll}$$



Simulation concepts

- A closer look to BTE:

$$\frac{\partial f}{\partial t} = -v \cdot \nabla f - \frac{1}{\hbar} \frac{\partial p}{\partial t} \cdot \nabla_k f + \left. \frac{\partial f}{\partial t} \right|_{coll}$$

the group velocity of the carriers, $v = (1/\hbar)\nabla_k E(k)$,
E(k) being the dispersion relation, which takes into account
the periodic potential of the crystal.



Simulation concepts

- A closer look to BTE:

$$\frac{\partial f}{\partial t} = -v \cdot \nabla f - \frac{1}{\hbar} \frac{\partial p}{\partial t} \cdot \nabla_k f + \left. \frac{\partial f}{\partial t} \right|_{coll}$$

the second term represents the acceleration driven by the Lorentz force:

$$\frac{\partial \vec{p}}{\partial t} = e(\vec{F} + \vec{v} \times \vec{B})$$

the third term represents the changes because of scattering:

$$\left. \frac{\partial f}{\partial t} \right|_{coll} = \sum_{k'} [f(r, k', t)W(k', k) - f(r, k, t)W(k, k')]$$



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Simulation concepts

- To solve Boltzmann Transport Equation we need:
 1. Band structure of the device (not of the material)
 2. Electric and magnetic fields that carriers “see”
 3. Scattering mechanisms:
 1. Phonon scattering
 2. Surface roughness scattering
 3. Coulomb scattering



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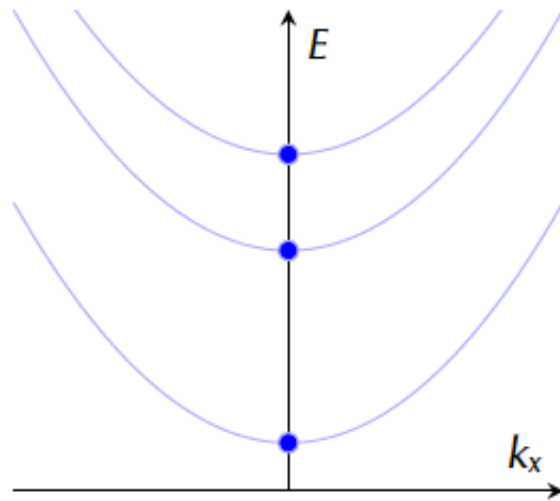
Simulation concepts

- Bandstructure of the device:
 1. Analytical description, Effective Mass Approximation
 2. $k \cdot p$ method
 3. Tight Binding
 4. Pseudopotentials
 5. Ab-initio calculations



Simulation concepts

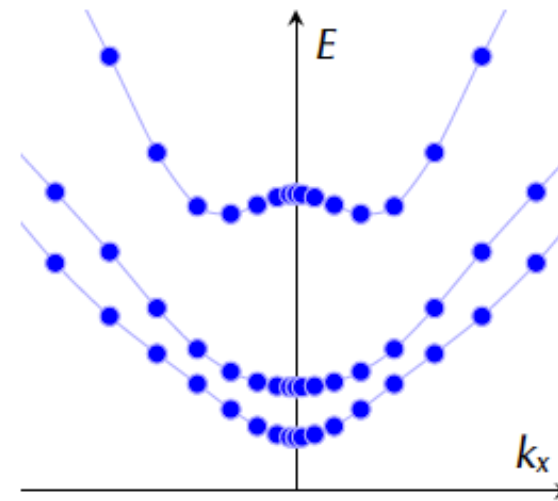
Electrons



$$E = E_i + \frac{\hbar^2 k_x^2}{2m_x}$$

The subband energy is built from the minimum using a parameter

Holes



interpolation: $E = E_i(k_x)$

The energy of the subband has to be calculated for every k_x



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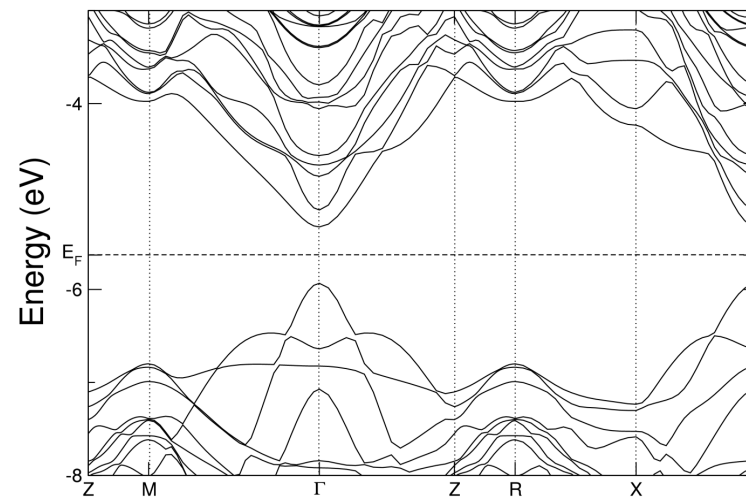
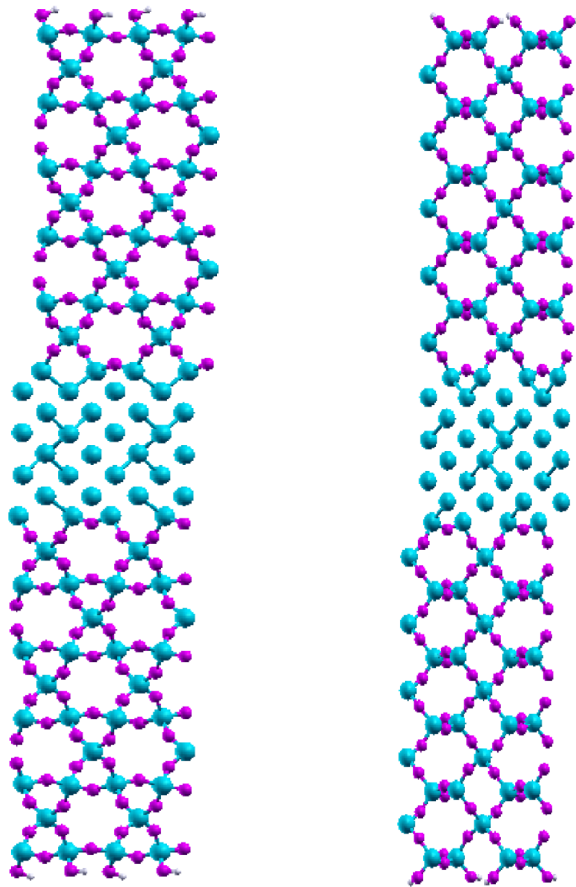
Simulation concepts

- Bandstructure of the device:
 1. Analytical description, Effective Mass Approximation
 2. $k \cdot p$ method
 3. Tight Binding
 4. Pseudopotentials
 5. Ab-initio calculations



Simulation concepts

- Bandstructure of a DGSOI transistor (ab-initio):



Possibility to study atomic-scale phenomena: dopants, dislocations, etc.



Simulation concepts

- A closer look to BTE:

$$\frac{\partial f}{\partial t} = -v \cdot \nabla f - \frac{1}{\hbar} \frac{\partial p}{\partial t} \cdot \nabla_k f + \left. \frac{\partial f}{\partial t} \right|_{coll}$$

From $f(\vec{r}, \vec{k}, t)$ we can evaluate all the variables of interest:

$$n(\vec{r}, t) = \frac{1}{V} \sum_{\vec{k}} f(\vec{r}, \vec{k}, t)$$

$$\vec{J}_n(\vec{r}, t) = \frac{e}{V} \sum_{\vec{k}} \vec{v}(\vec{k}) f(\vec{r}, \vec{k}, t)$$



Simulation concepts

- Our goal is then to solve BTE. However,
- The solution of the BTE for realistic devices is a very difficult task
- Difficulties arise from:
 1. Non homogeneous device structure (doping and topology).
 2. Models for scattering mechanisms.
 3. Complexity of the band structure.
- Most common solutions: statistical methods (Monte Carlo) or drastic approximations (methods of moments: drift-diffusion and hydrodynamic method).
- We have applied the Monte Carlo method to solve the Boltzmann transport equation in advanced devices.

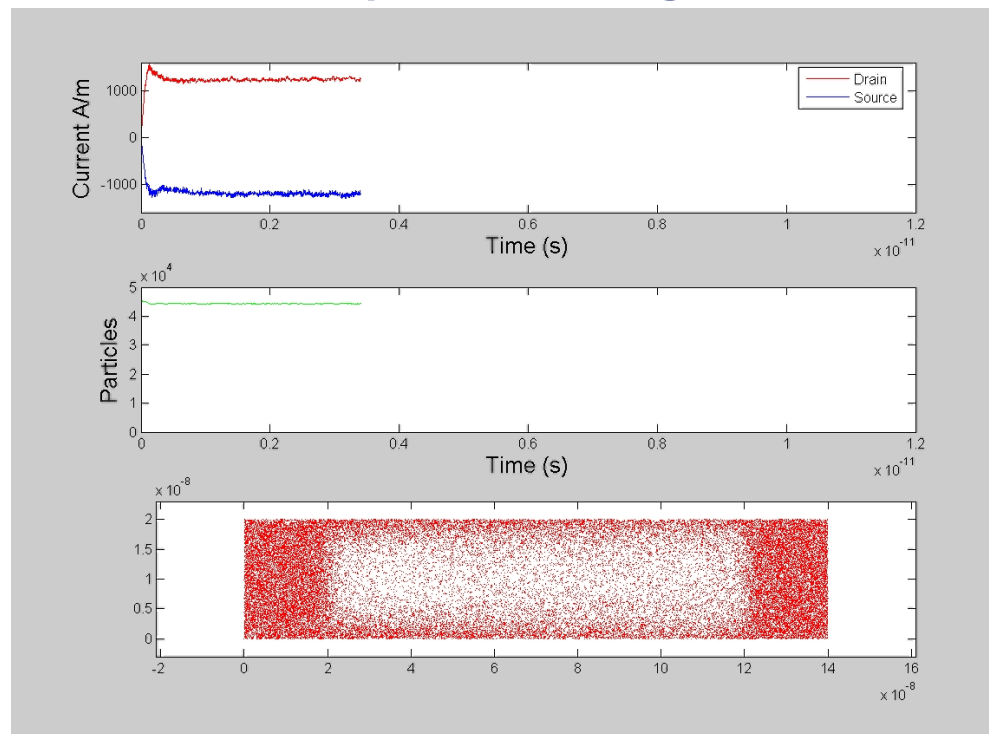


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The Ensemble Monte Carlo method

- We assume that the charged particles move inside the semiconductor structure undergoing a succession of free flights followed by scattering events:



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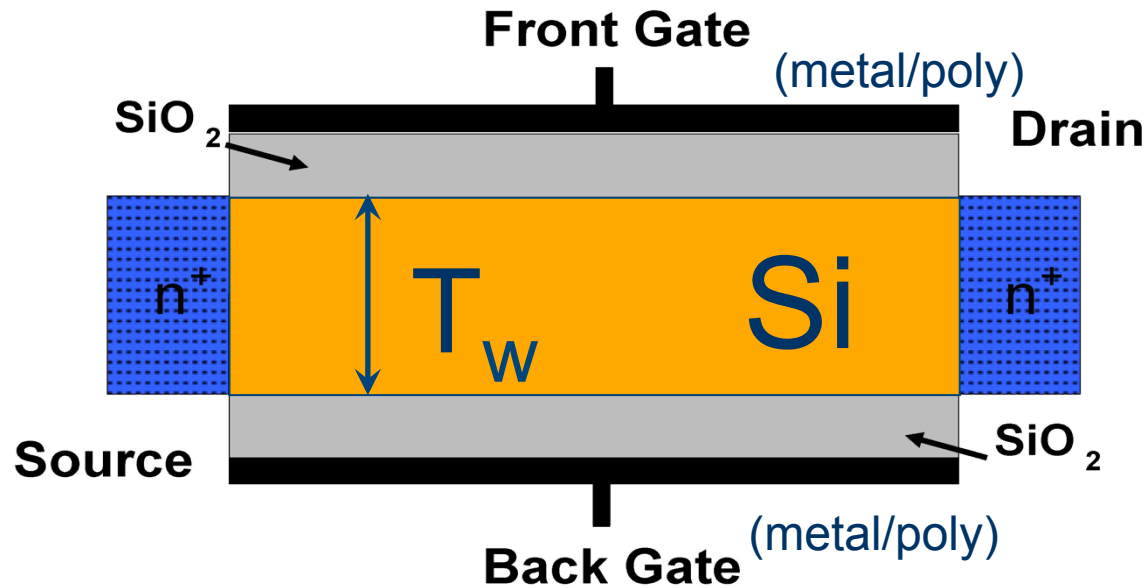
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Double-Gate MOSFETs



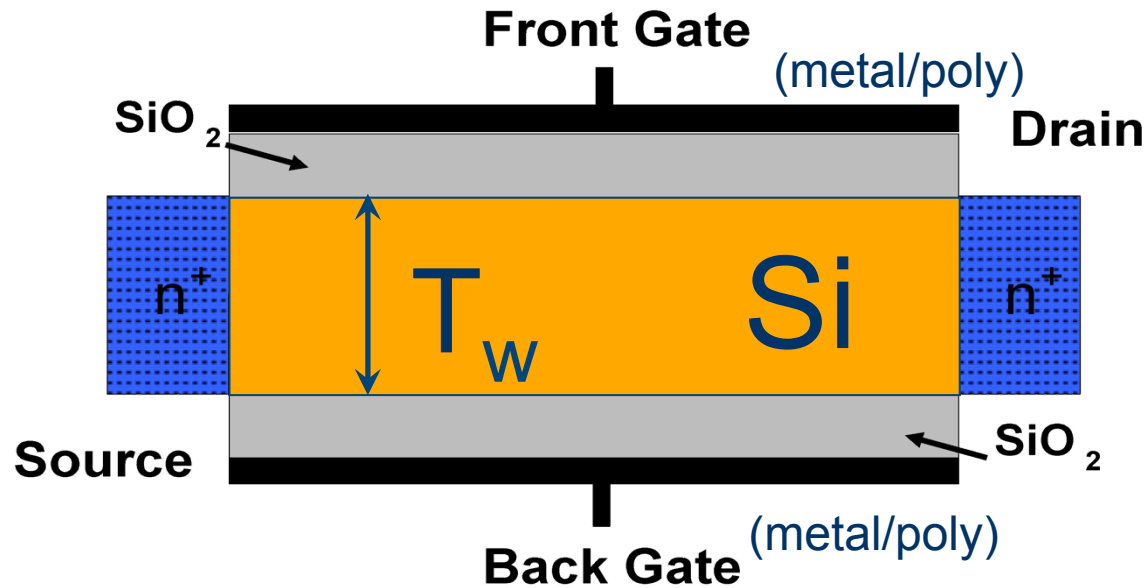
- Gate oxide: SiO_2 or high-k
- T_w : **50 nm to 1.5 nm.**
- Silicon layer undoped.
- N^+ -Poly or midgap metal gates



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Double-Gate MOSFETs



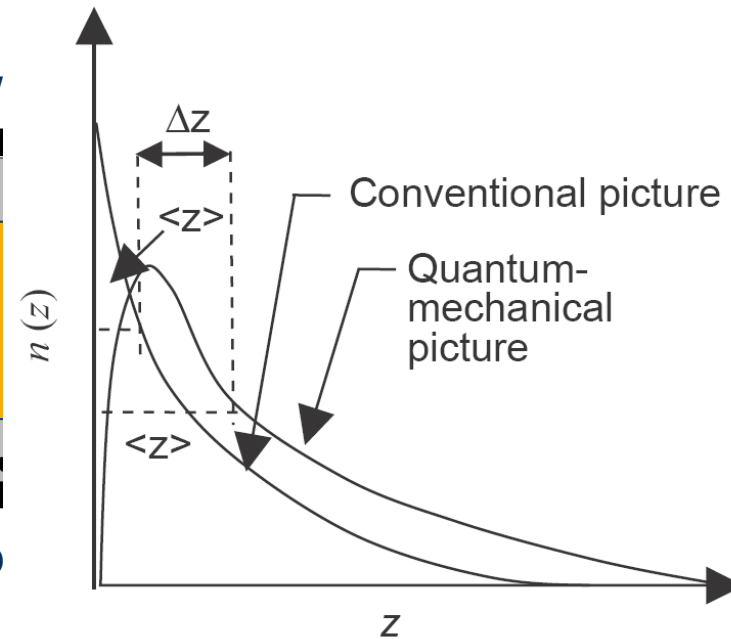
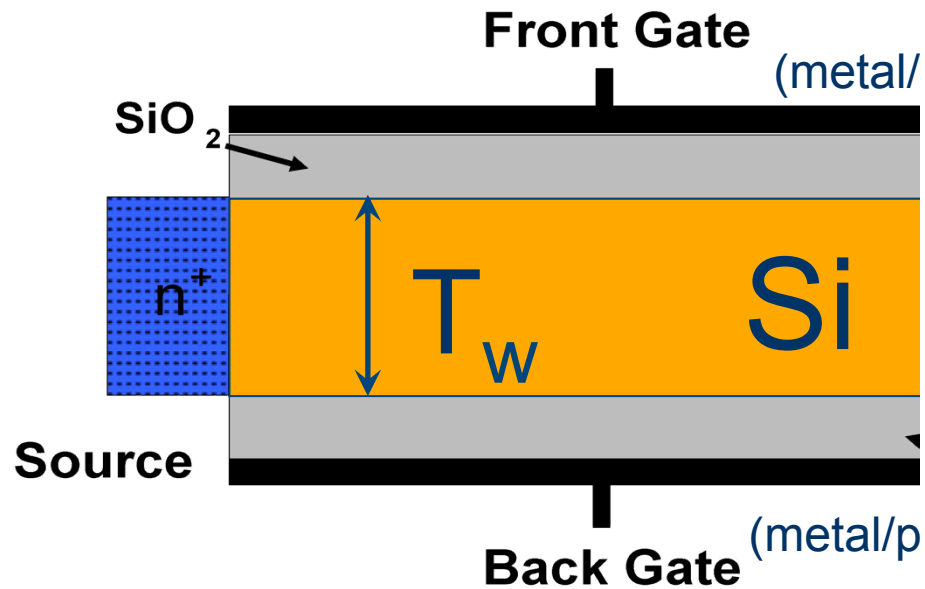
- Silicon thickness becomes comparable to the De Broglie wavelength of carriers: Carriers become quantized in the direction perpendicular to the silicon thickness, T_w



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Double-Gate MOSFETs



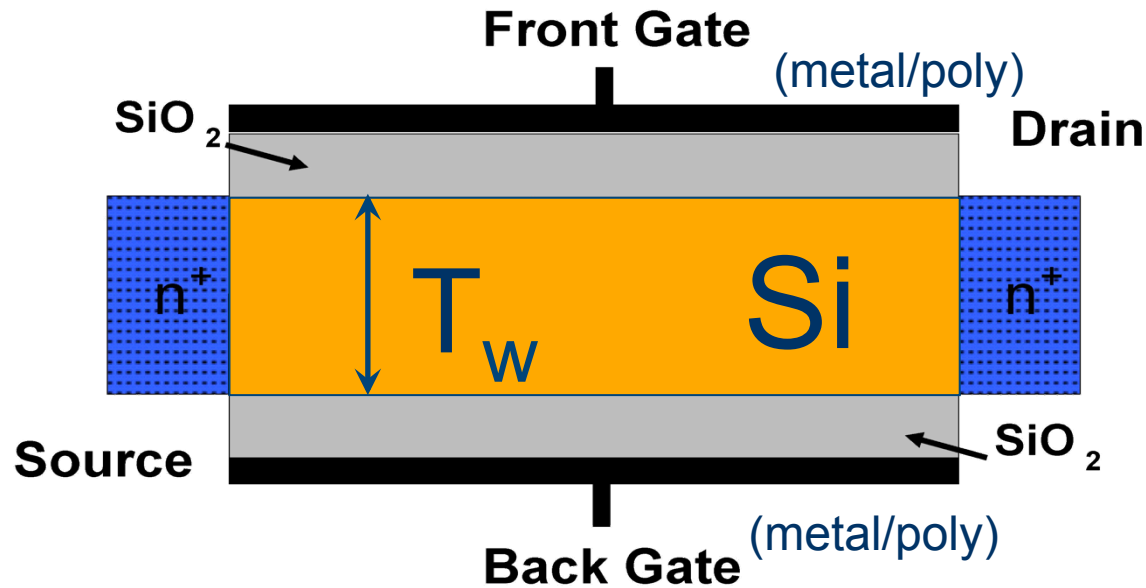
- We have to self-consistently solve the Poisson and Schroedinger equations to calculate the distribution of the carriers in the structure.



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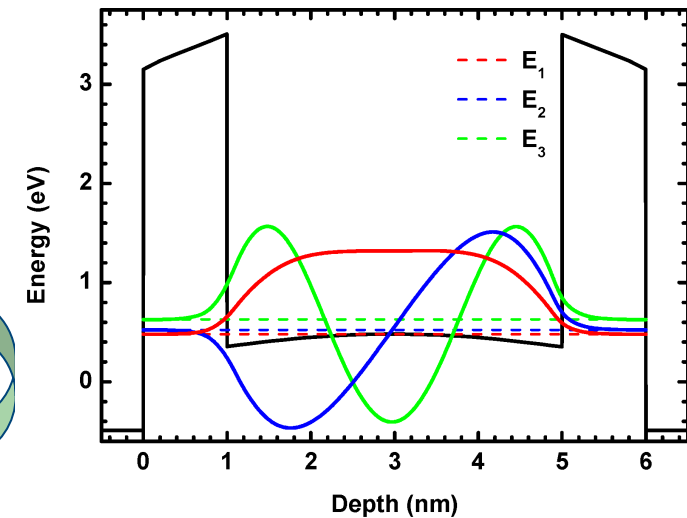
Double-Gate MOSFETs



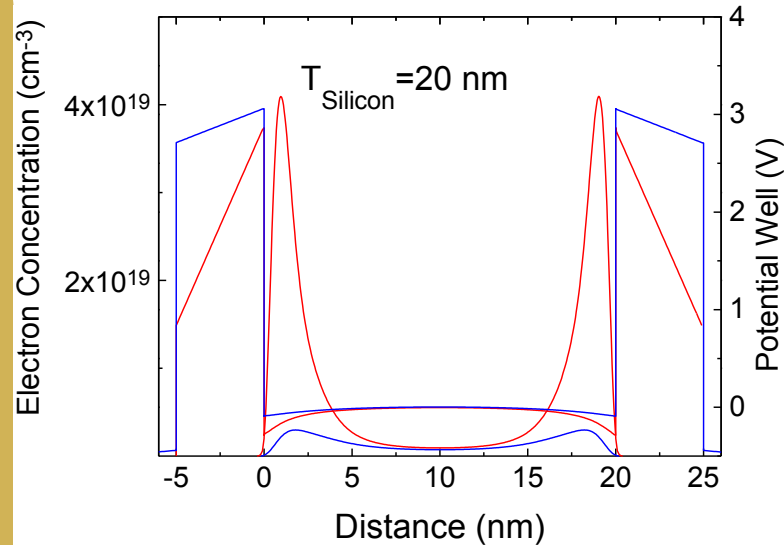
- Under the assumption of very long channel device:

$$-\frac{\hbar^2}{2m_z} \frac{d^2\psi_i}{dz^2} - e\phi(z)\psi = E_i\psi_i$$

$$\frac{d^2\phi}{dz^2} = -\frac{1}{\epsilon_{Si}} \sum_i n_i |\psi_i|^2$$



Double-Gate MOSFETs

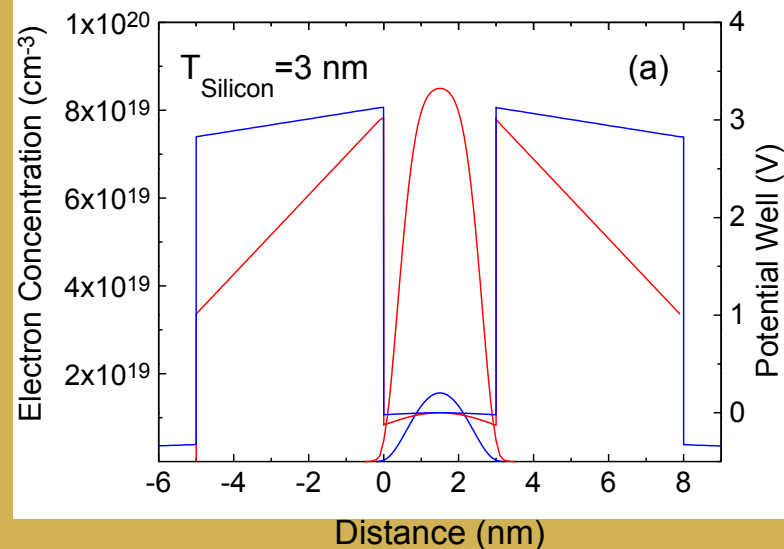


- *Two channels connected in parallel*

- Carriers are confined near each Si/SiO₂ interface.

- *Volume inversion*

- Carriers are no longer confined at one interface but distributed throughout the entire silicon film



$$N_{inv} = 1.3 \times 10^{12} \text{ cm}^{-2} \quad (\text{blue line})$$

$$N_{inv} = 8.5 \times 10^{12} \text{ cm}^{-2} \quad (\text{red line})$$

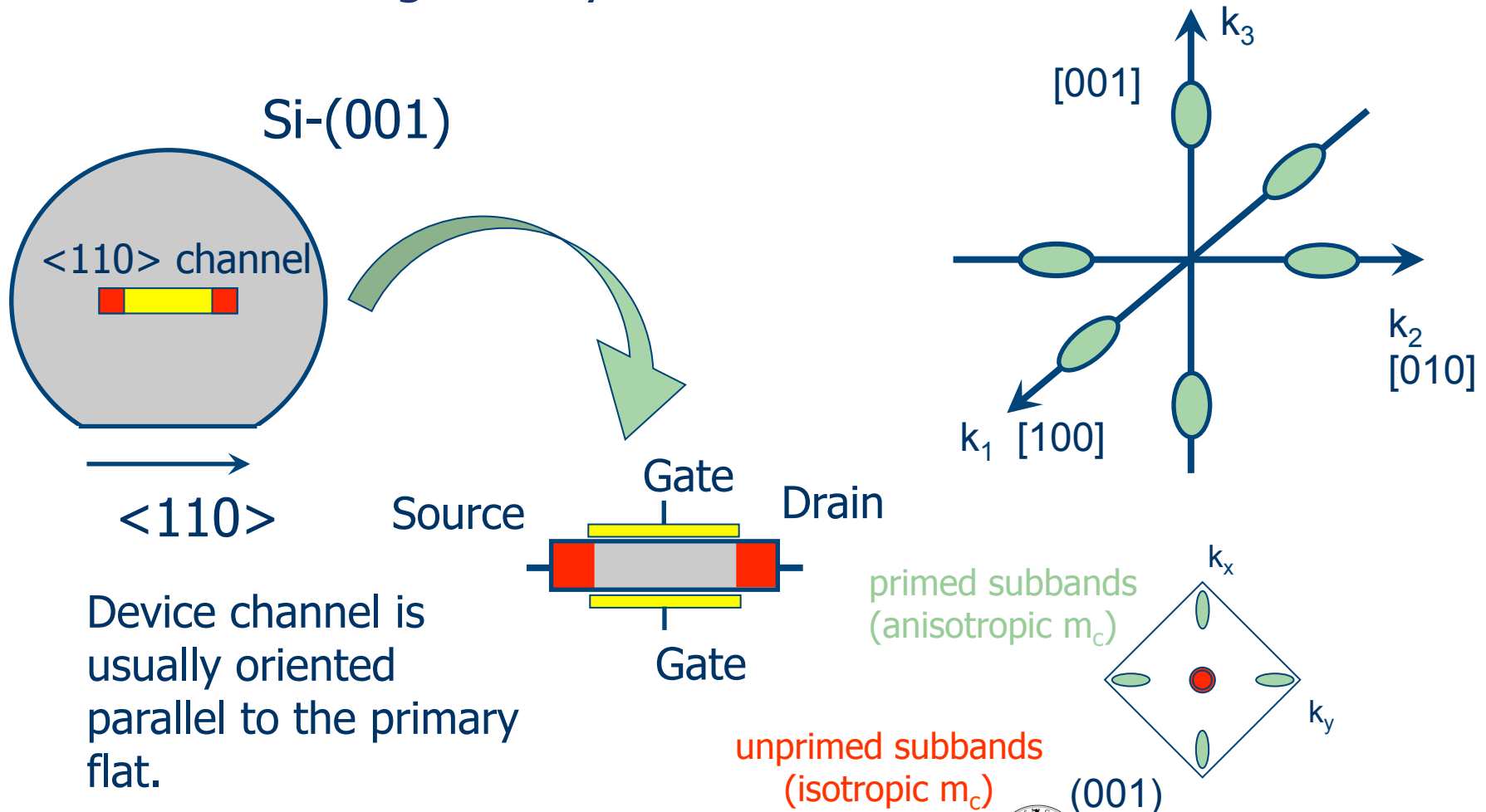


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Double-Gate MOSFETs

- In conventional planar Si technology, (001) crystal orientation is generally used for MOSFETs.



Device channel is usually oriented parallel to the primary flat.



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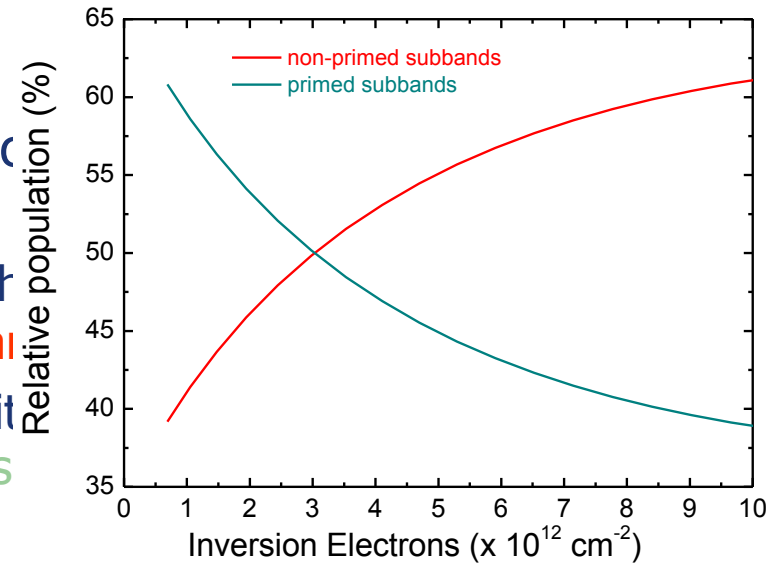
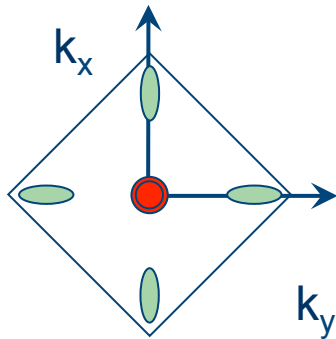
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Double-Gate MOSFETs

- In conventional planar Si technology, (001) crystal orientation is MOSFETs :

Si-(001): Quantization splits Si-c degeneracy:

- Two lower valleys with m_c (unprimed subbands)
- Four higher valleys with m_c (primed subbands)



$$m_{\langle 100 \rangle} = m_t$$

$$m_{\langle 010 \rangle} = m_t$$

$$n_v = 2$$

$$m_{\langle 100 \rangle} = m_l$$

$$m_{\langle 010 \rangle} = m_t$$

$$n_v = 4$$

(001)



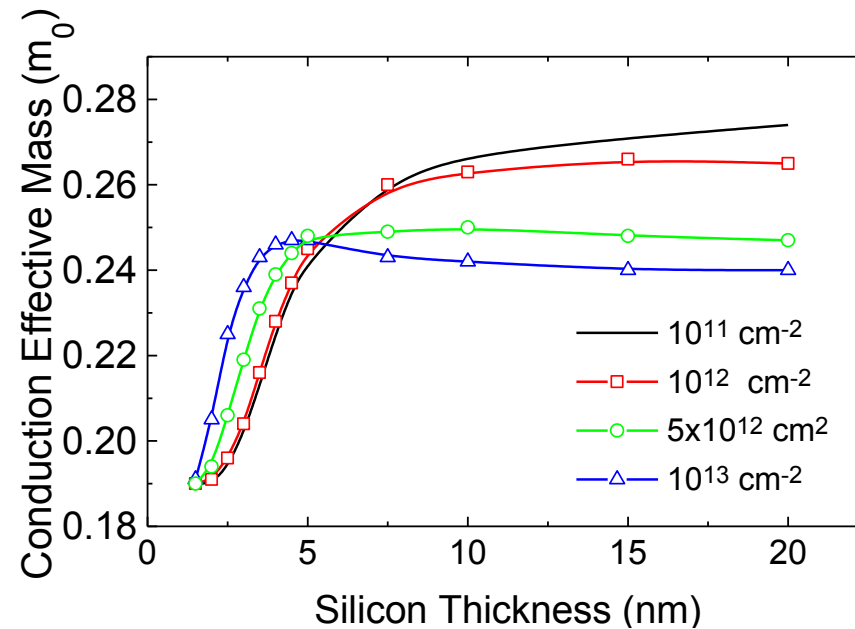
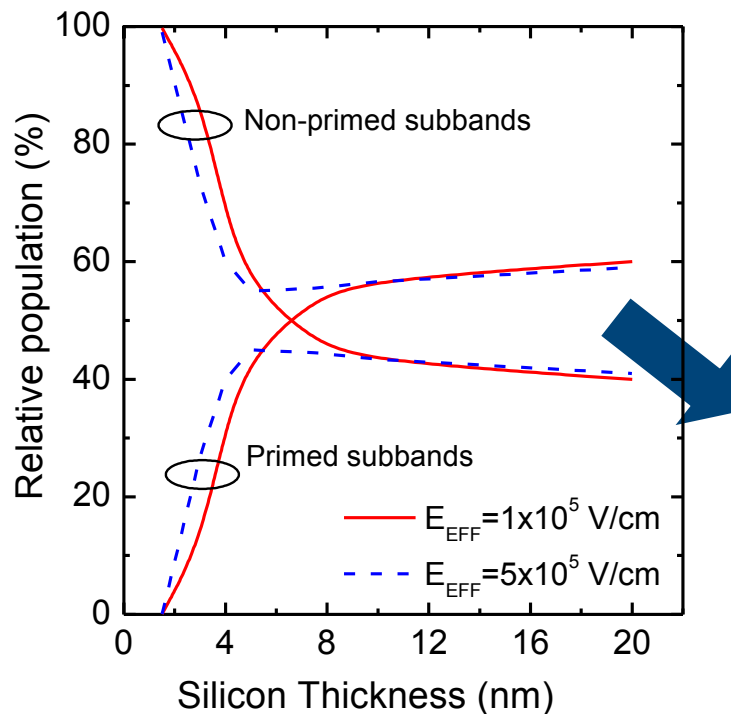
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Volume inversion

A-1) Subband Modulation Effect

Redistribution of subband population



Reduction of conduction effective mass



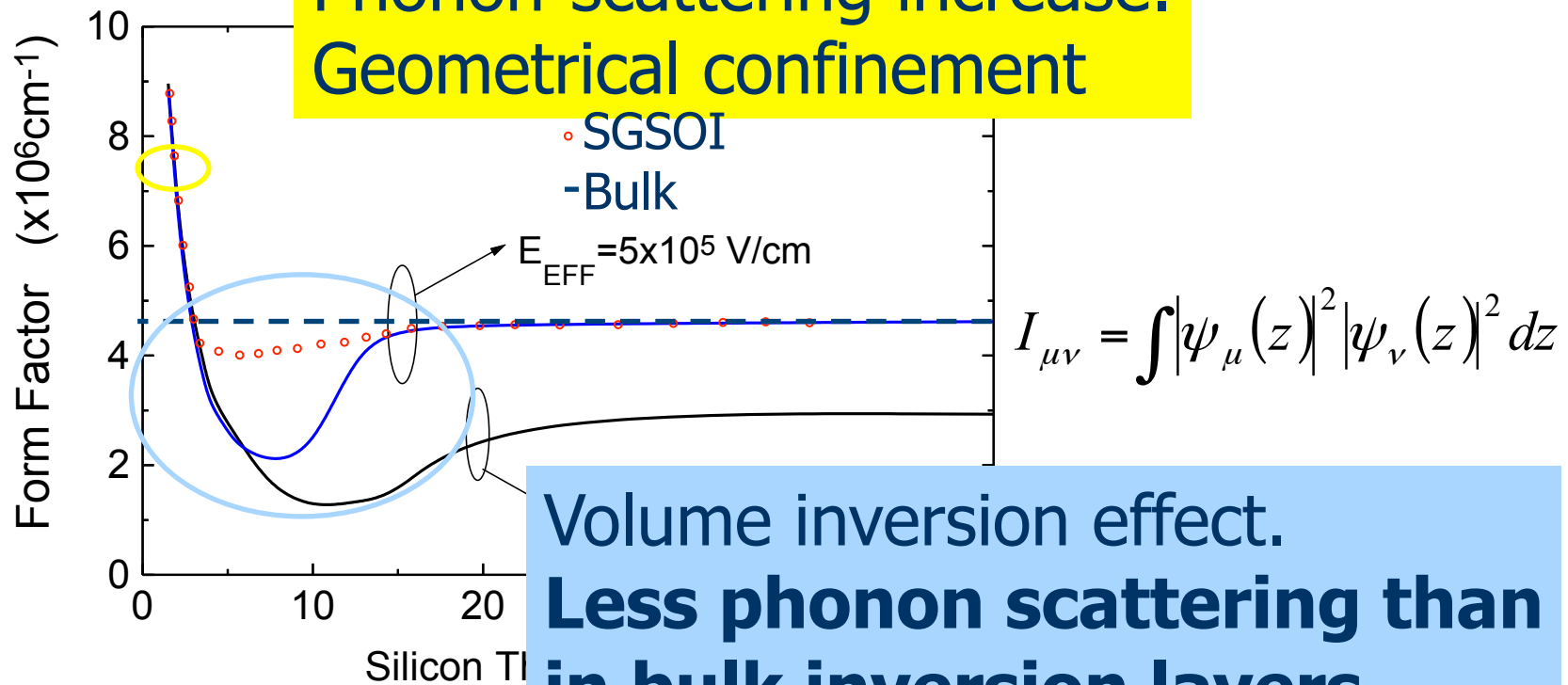
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Volume inversion

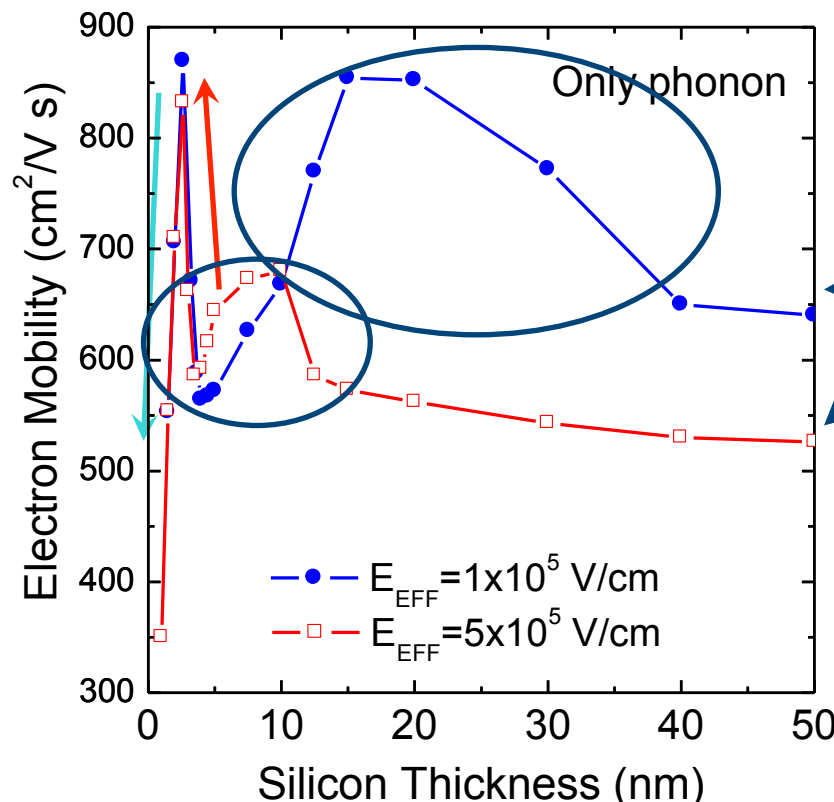
A-2 Phonon scattering limitation

Volume inversion makes that in the range 25-10 nm phonon scattering decreases instead of increasing as expected



Electron Mobility

• PHONON SCATTERING (I)



Volume Inversion

Subband Modulation

Bulk MOSFET

Phonon Increase

Electron mobility is higher than in bulk silicon inversion layers

In addition to a better control of SCE, we have higher μ !!



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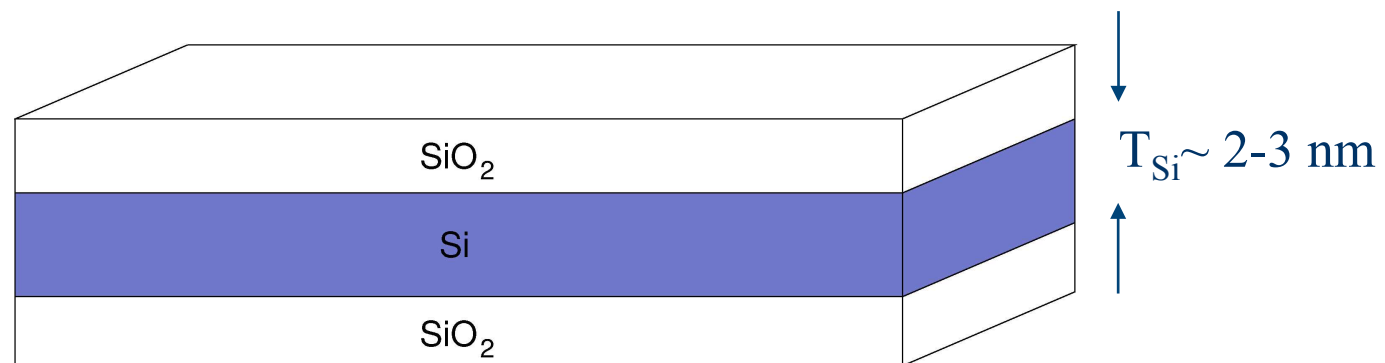
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Electron Mobility

- PHONON SCATTERING (II)

Bulk phonon model assumes an infinite silicon layer.

Are bulk phonons still appropriate for the simulation of ultrathin SOI devices?



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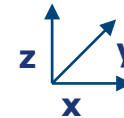
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Acoustic phonon model

- Phonons are modeled as elastic waves in an isotropic finite medium

$$\frac{\partial^2 \mathbf{u}}{\partial t^2} = s_t^2 \nabla^2 \mathbf{u} + (s_l^2 - s_t^2) \nabla(\nabla \cdot \mathbf{u})$$

- Simplified structure: single Si layer



- The solutions are:

$$u(r_{\parallel}, z) = w_n(q_{\parallel}, z) e^{iq_{\parallel} \cdot r_{\parallel} - i\omega_n t}$$

+ boundary conditions (BC) on external surfaces **Quantization of phonons**

- ✓ Free boundary conditions (vanishing stress tensor)
- ✓ Rigid boundary conditions (vanishing displacement u)

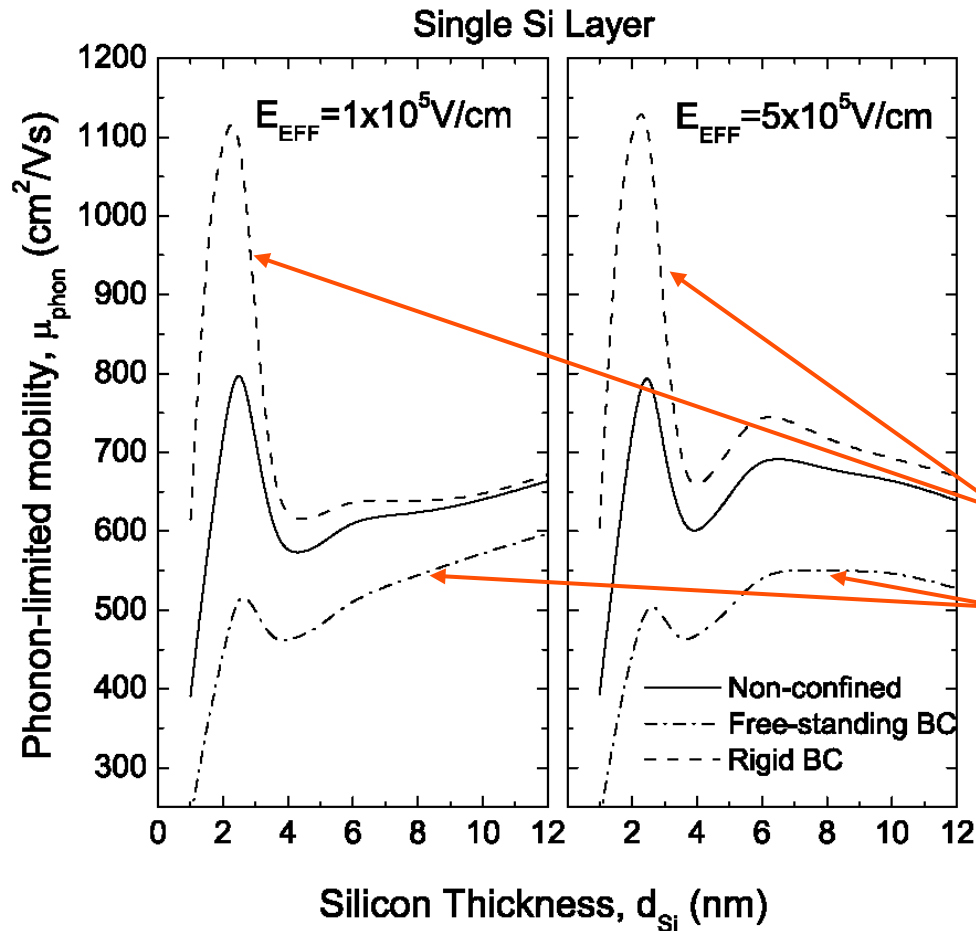


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Acoustic phonon model

Electron mobility



Important effect of phonon confinement on electron mobility

rigid BC \Rightarrow mobility increase

free BC \Rightarrow mobility decrease



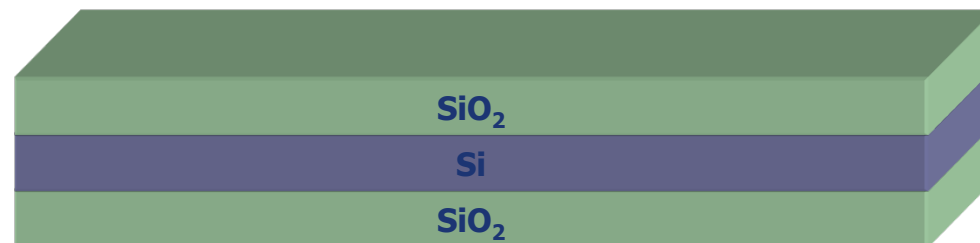
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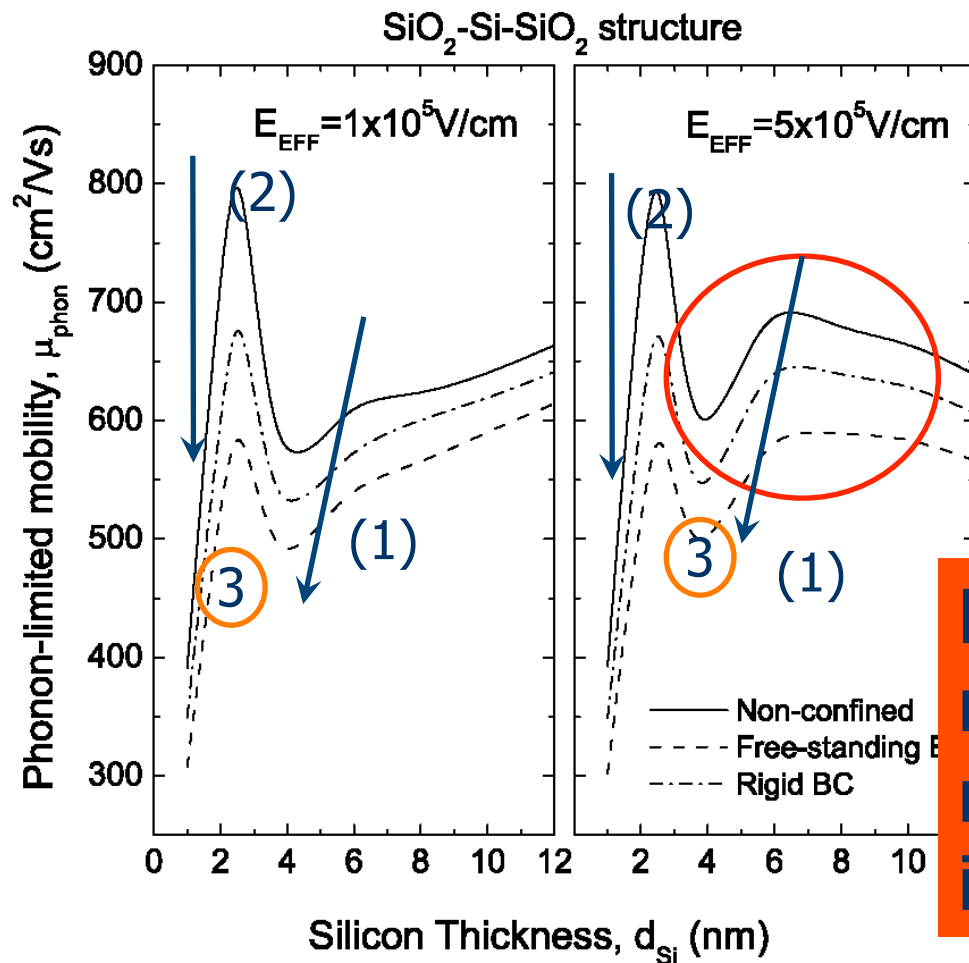
Acoustic phonon model

- Phonon confinement and quantization are reproduced
- Phonon confinement has a strong effect on the mobility
- ... but we need more realistic boundary conditions !!

We consider an improved structure



Acoustic phonon model

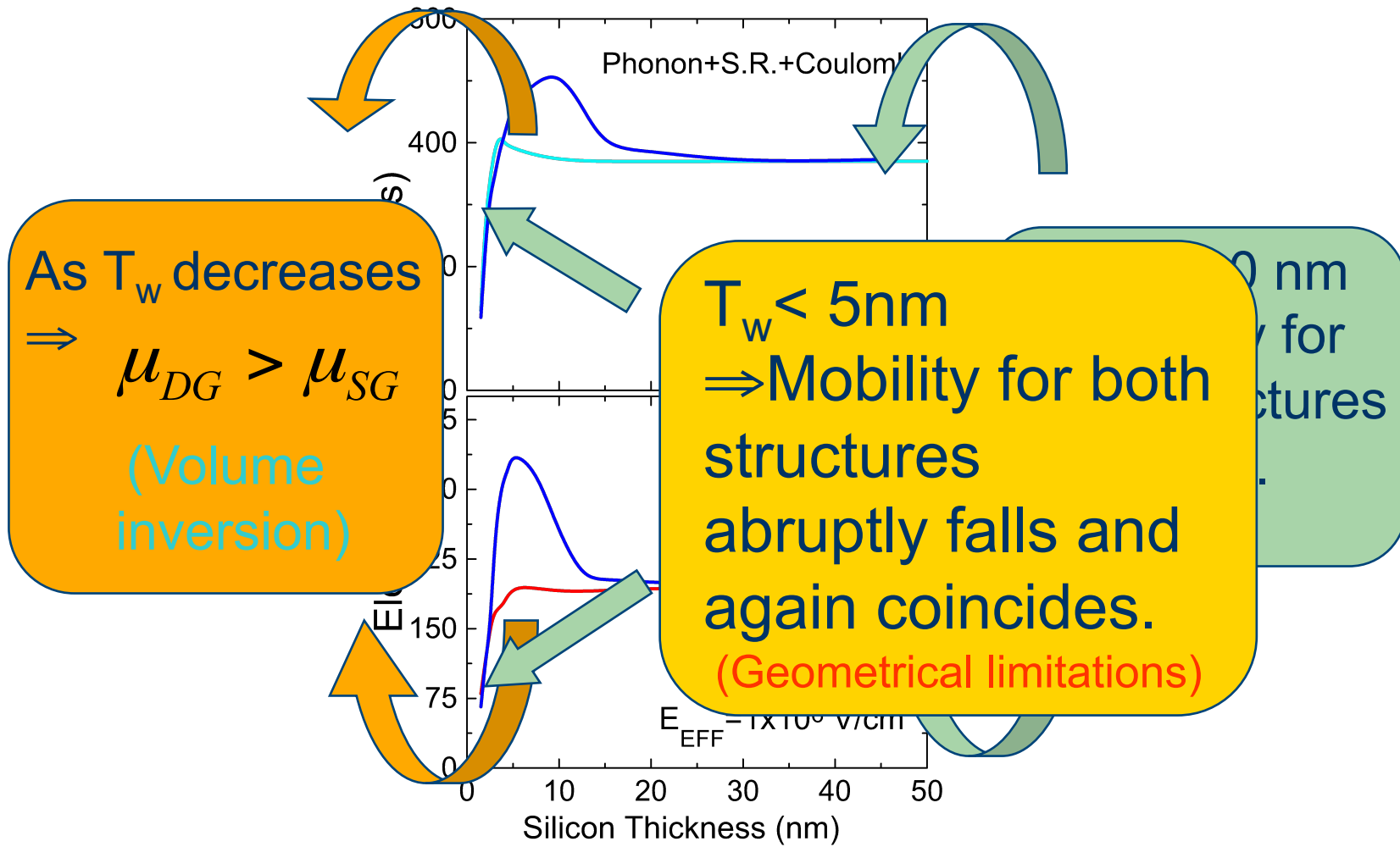


1. Both BCs imply an important electron mobility degradation.
2. The mobility peak around 2-4 nm is strongly suppressed

But, there is still a region where electron mobility is higher than in bulk inversion layers



Double Gate vs Single Gate

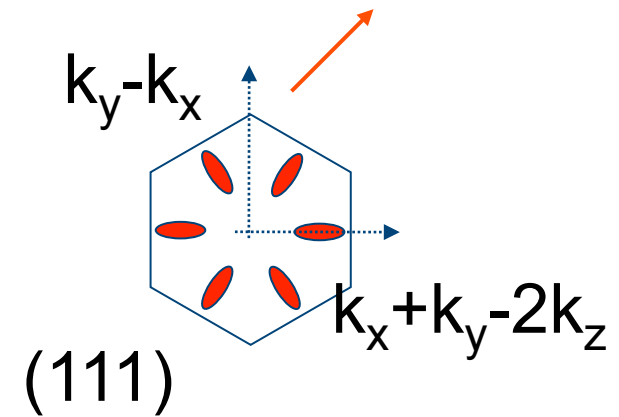
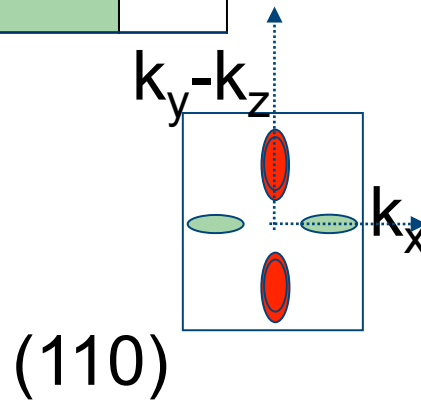
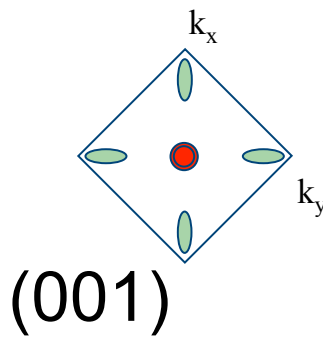
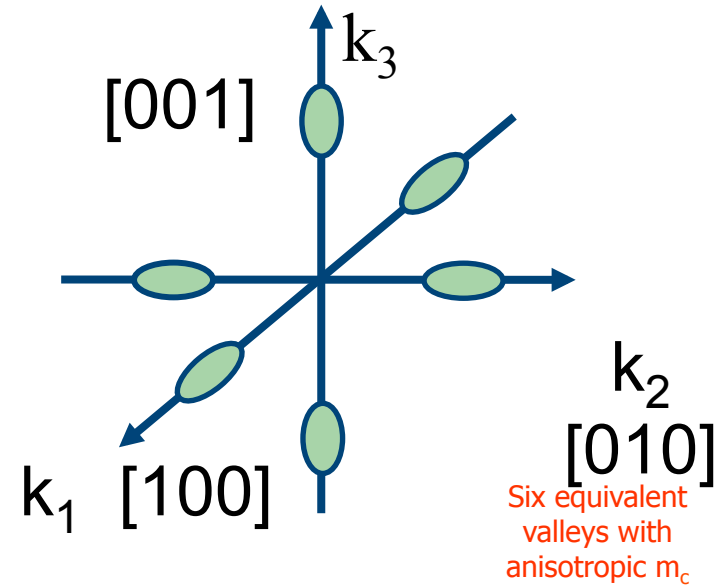


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Crystallographic orientation

Quantization direction	m_3	n_v
(100)	0.916	2
	0.19	4
(110)	0.315	4
	0.19	2
(111)	0.258	6

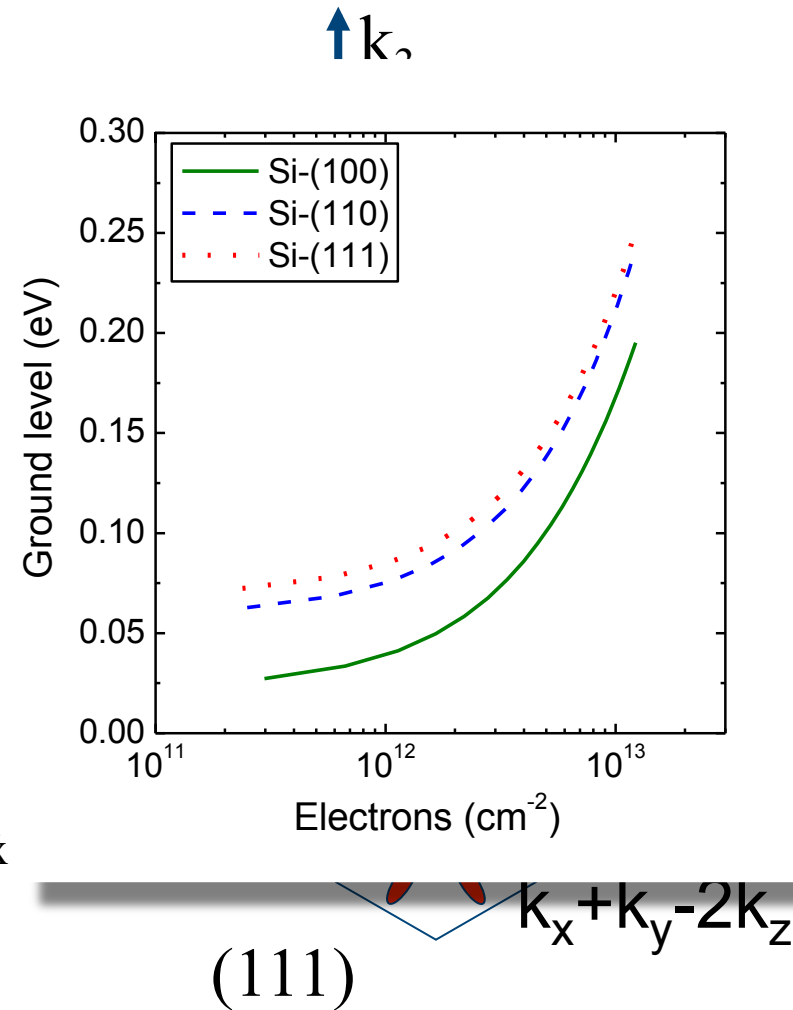
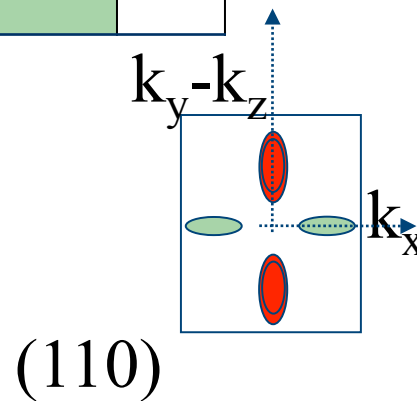
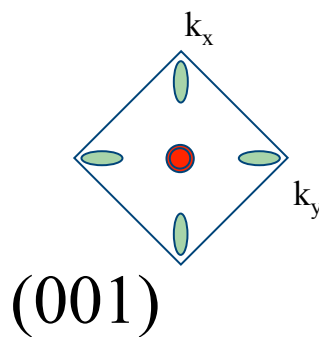


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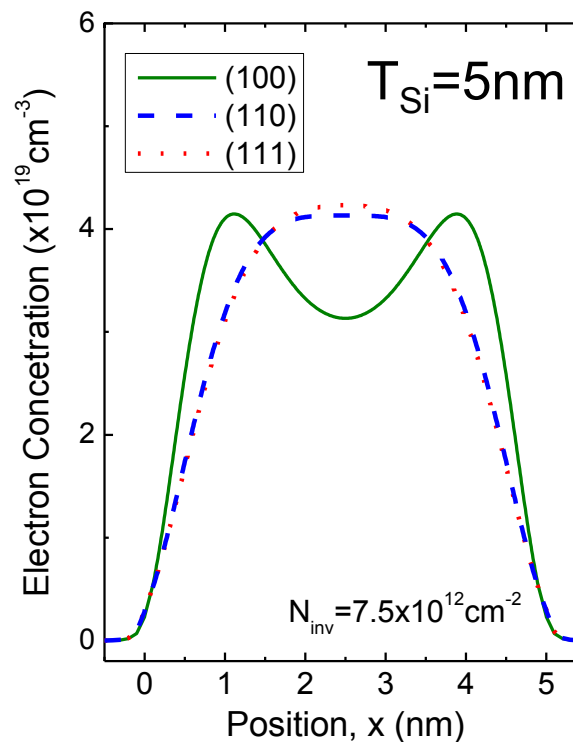
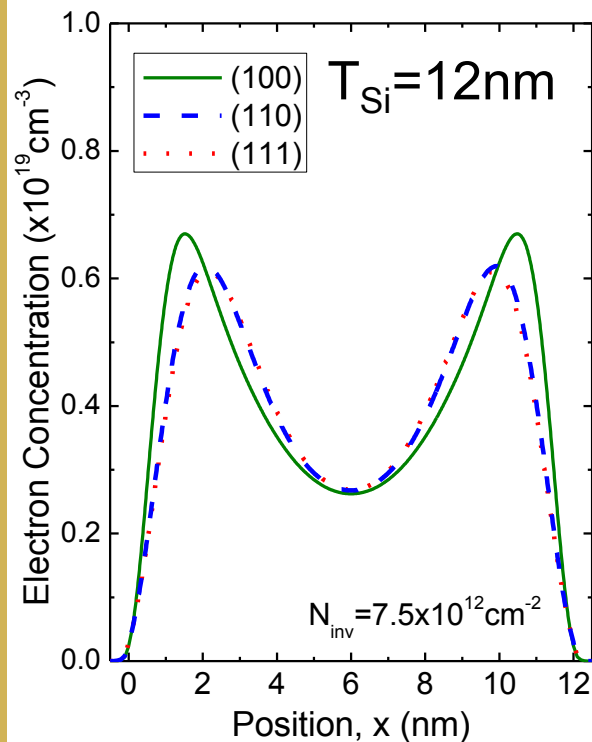


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Crystallographic orientation

The higher quantization mass in the Si-(100) quantization orientation produces lower subband-energy levels → electrons are more confined to the Si/SiO₂ interfaces



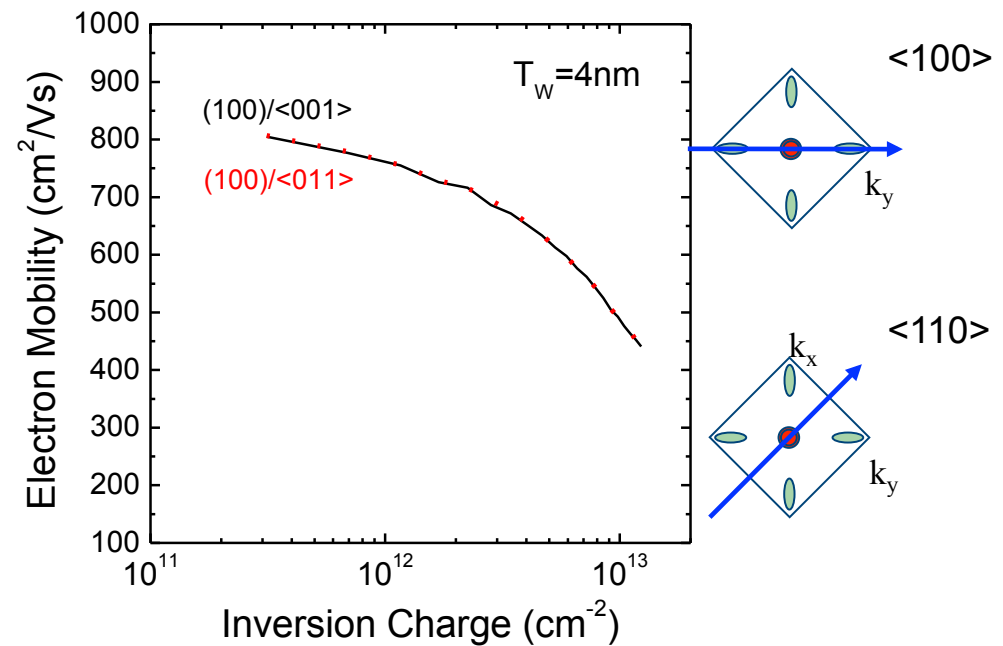
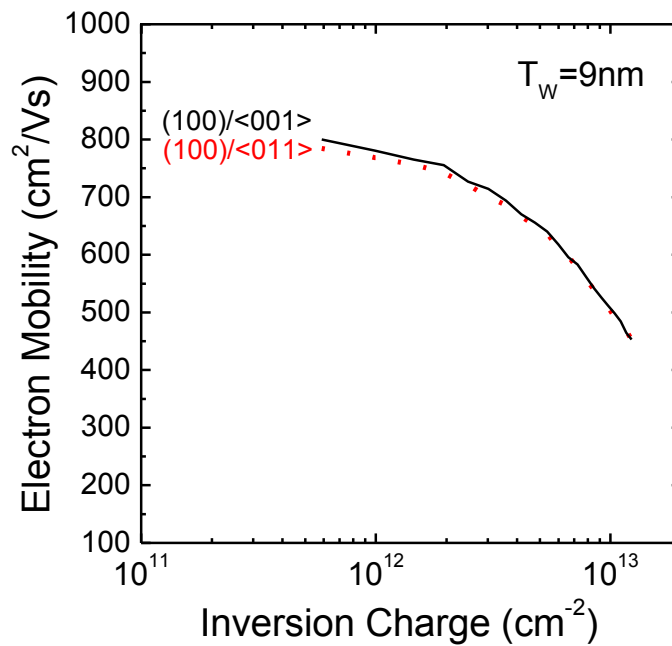
Electrons in Si-(110) and Si-(111) are more spread into the silicon layer

Less effect of surface scattering mechanisms



Crystallographic orientation

Monte Carlo calculation using phonon scattering and surface roughness scattering



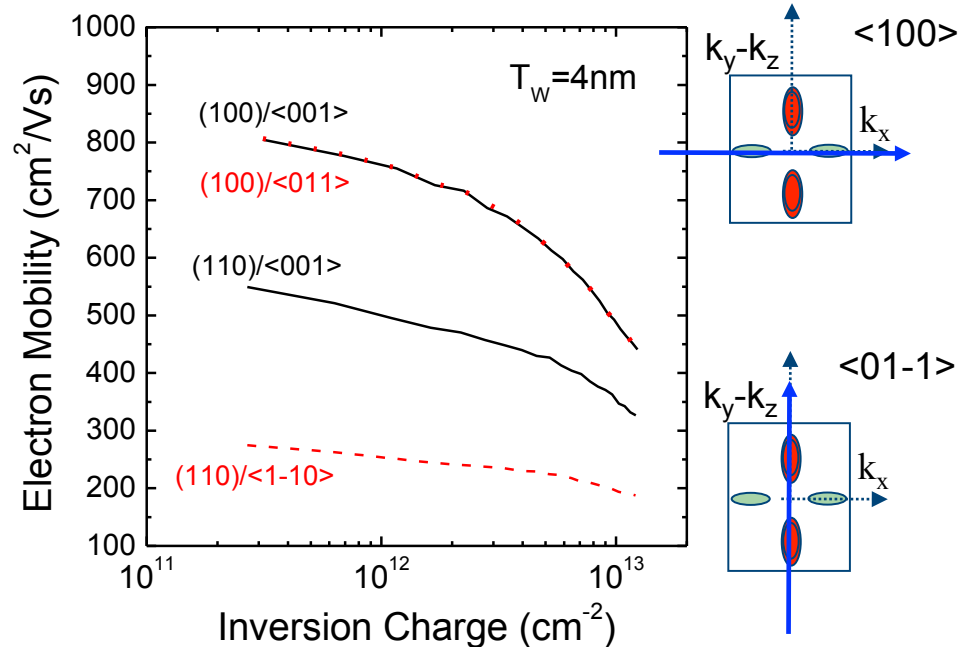
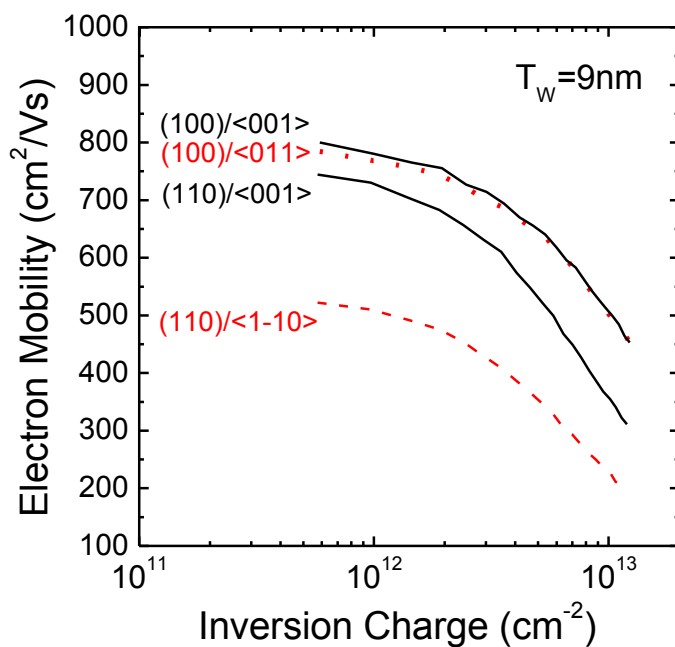
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Crystallographic orientation

Monte Carlo calculation using phonon scattering and surface roughness scattering

The effects of the surface orientation are more important as the silicon thickness decreases

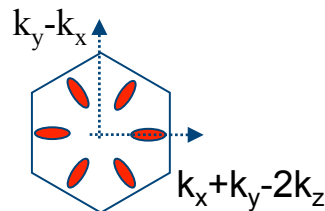


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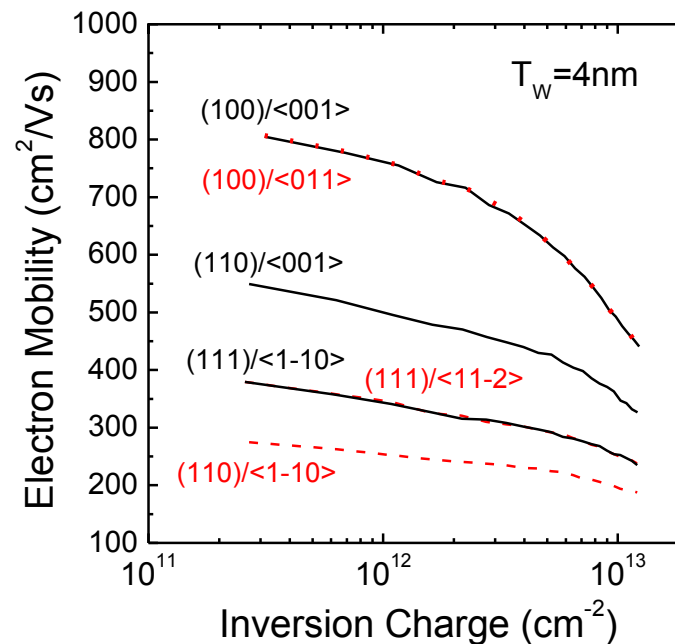
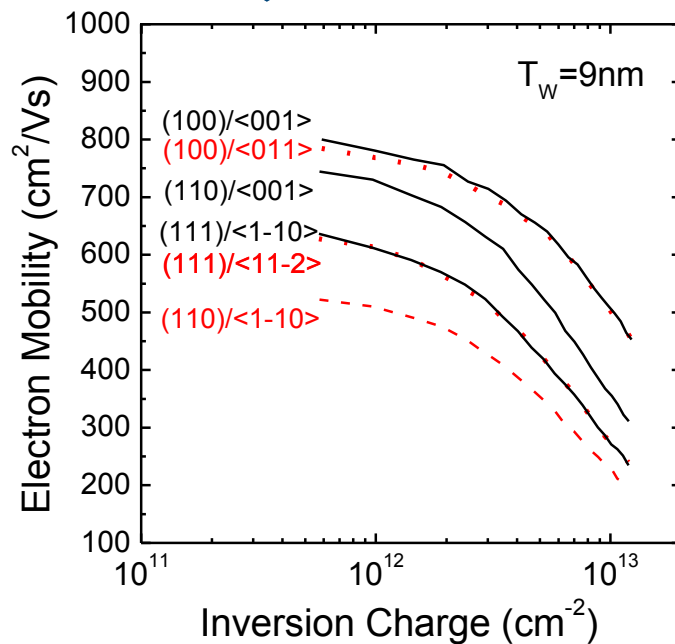
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Crystallographic orientation

Monte Carlo calculation using phonon scattering and surface roughness scattering



The effects of the surface orientation are more important as the silicon thickness decreases



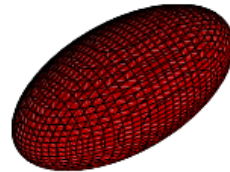
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Hole mobility

Electrons vs. holes

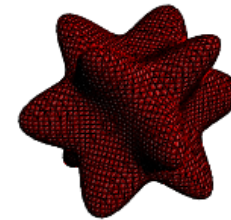
Electrons



- separable
- 1 eigenvalue equation
- $E = E_\nu + E(k_x, k_y)$

- analytic

Holes



- not separable
- N eigenvalue equations
- $E = E_\nu(k_x, k_y)$

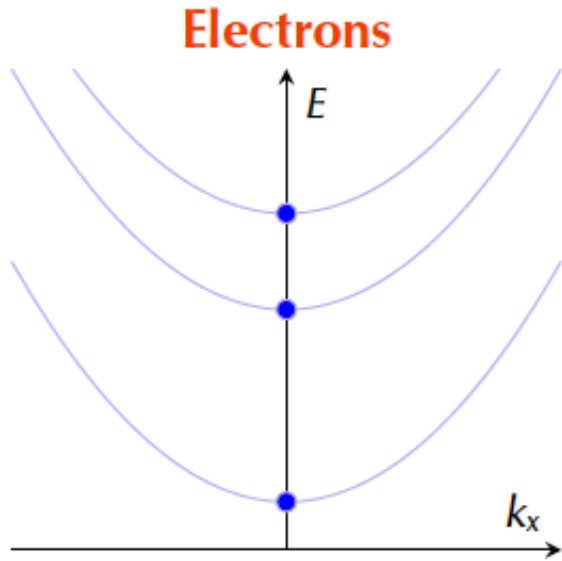
- interpolation needed

1D quantum confinement

Subband dispersion

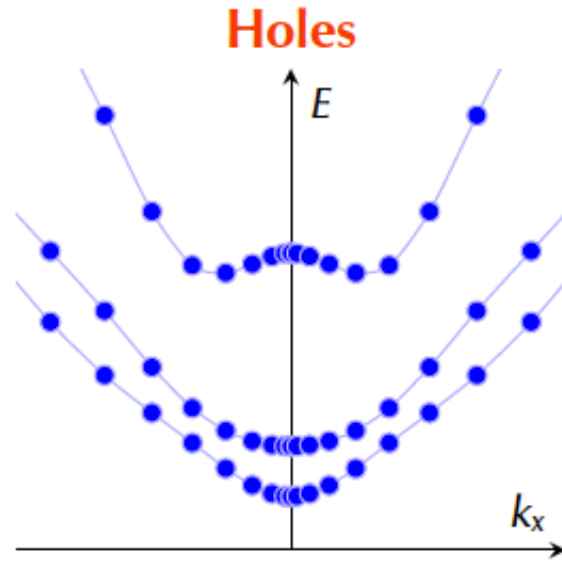


Hole mobility



$$E = E_i + \frac{\hbar^2 k_x^2}{2m_x}$$

parameter



interpolation: $E = E_i(k_x)$

Effective mass

to be computed
depends on potential well



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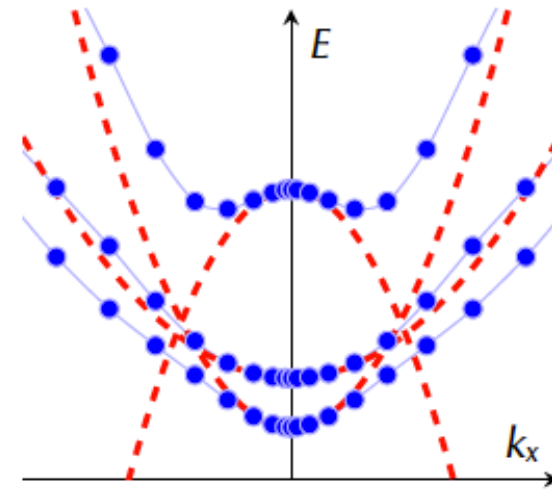
Hole mobility

Transport mass

Given subband i and direction α :

$$\frac{1}{m_i^\alpha} = \frac{1}{\hbar^2} \frac{\partial^2 E_i(k)}{\partial k_\alpha^2}$$

- ▶ non-parabolic:
 m_i^α depends on k
- ▶ if we take m_i^α at $k = 0$:
parabolic approximation
however ...



Hole mobility

k·p method

The **k·p** method

- approximate expression for the computation of band structure around $\mathbf{k} = \mathbf{k}_0$.
- an arbitrary number of bands can be considered

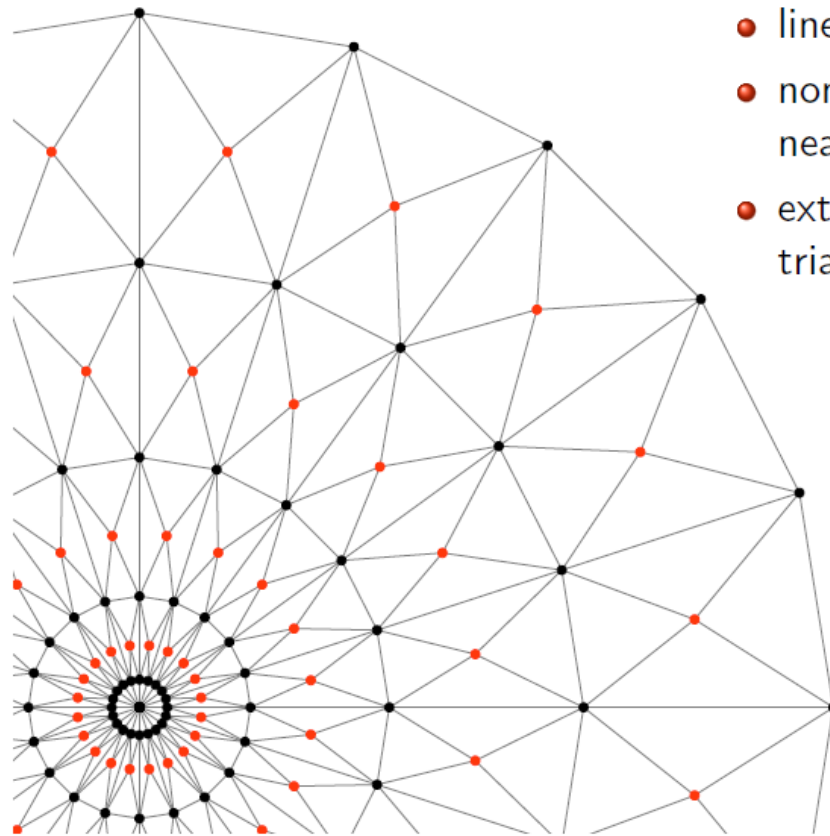
The valence band(s)

- degeneration (3 valence bands)
- spin-orbit interaction
- 6×6 **k·p** method



Hole mobility in inversion layers

The mesh (in k_{\parallel} plane)



- linear interpolation
- non-uniform k -mesh, finer near the origin
- extra points to create a triangulation

discretization

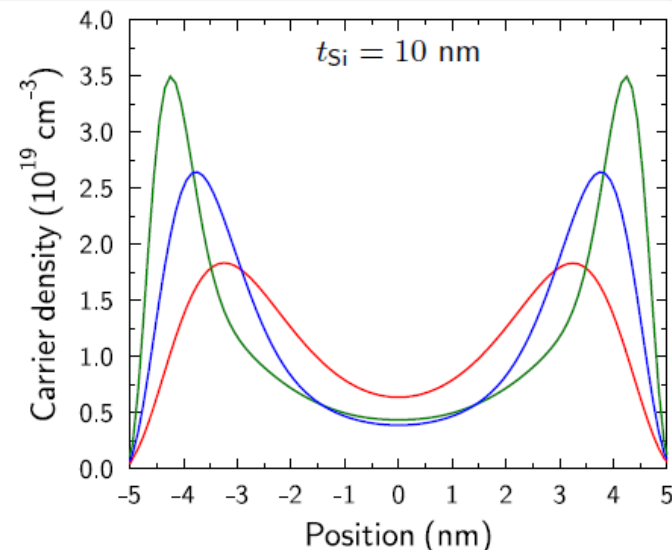
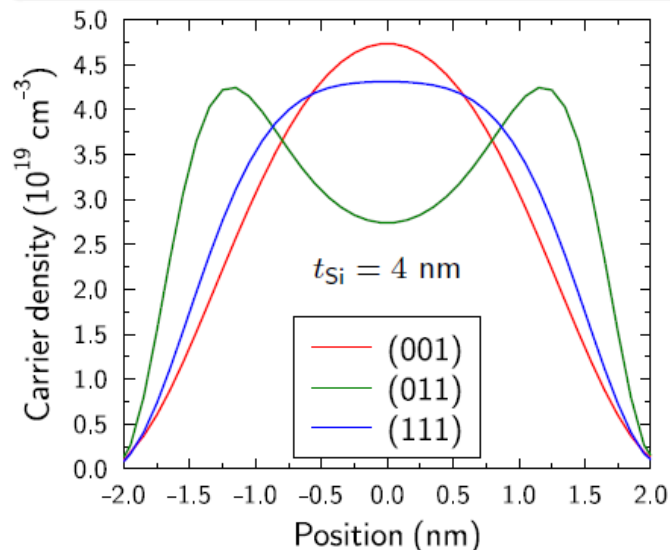


Hole mobility in DGSOI transistors

Results: inversion charge

Charge distribution

- different distance from the interface (centroid)
- one or two peaks can be present
- volume inversion can have different effects



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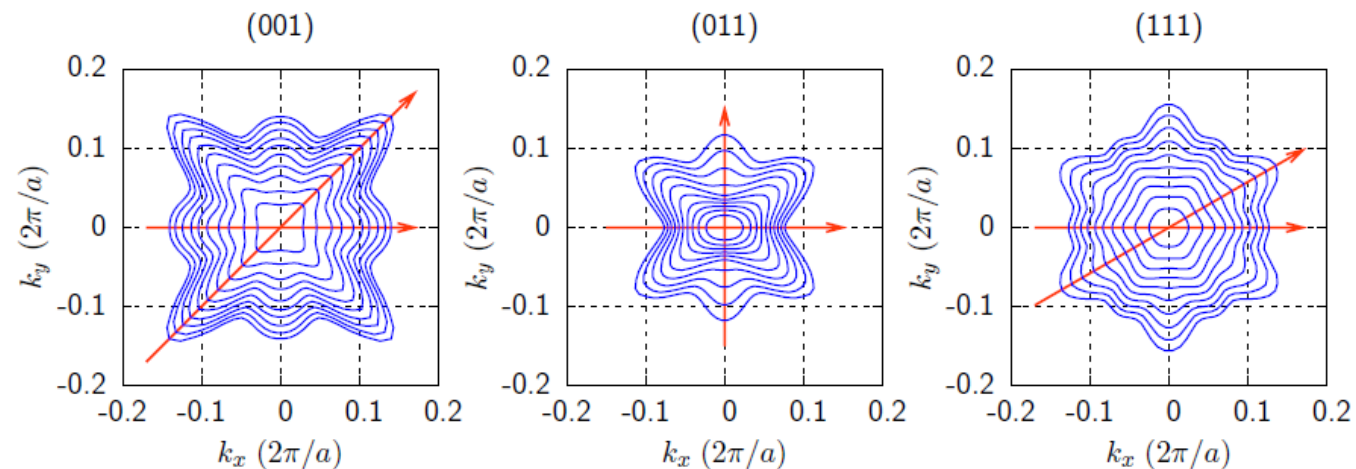
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Hole mobility in DGSOI transistors

Results: energy dispersion

Energy dispersion of first subband (10 nm)

- isotropic mobility: (001) and (111) surfaces
- non-isotropic mobility: (011) surface



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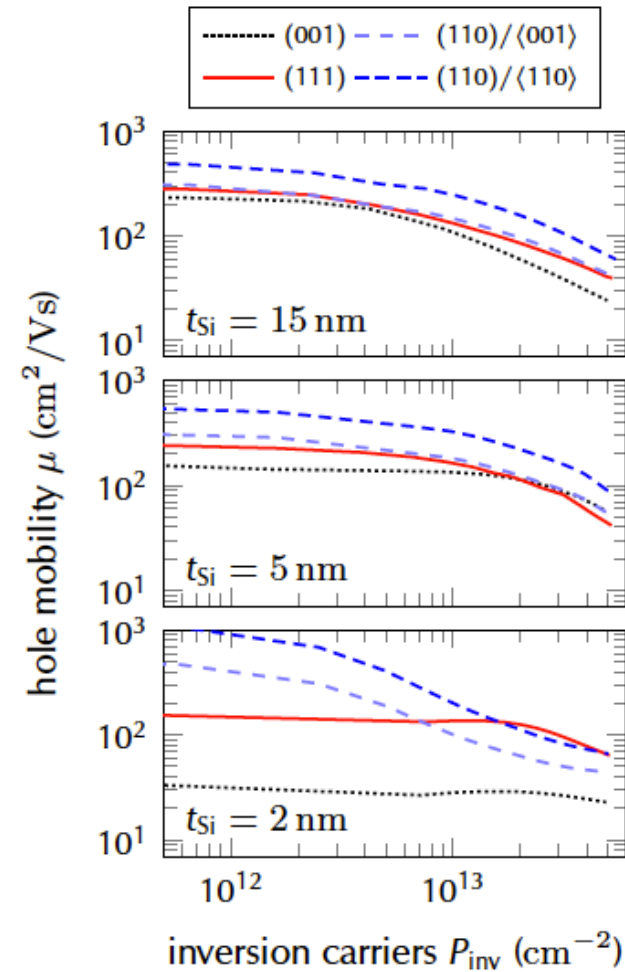
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Hole mobility in DGSOI transistors

Results: hole mobility

Mobility vs. inversion charge

- ▶ **negligible** dependence on channel direction for (100) and (111)
- ▶ **strong** dependence on channel direction for (110)
- ▶ weak dependence on P_{inv} at small t_{si} (but not for (110))
- ▶ enhancement factor of (110) and (111) increases at small t_{si}



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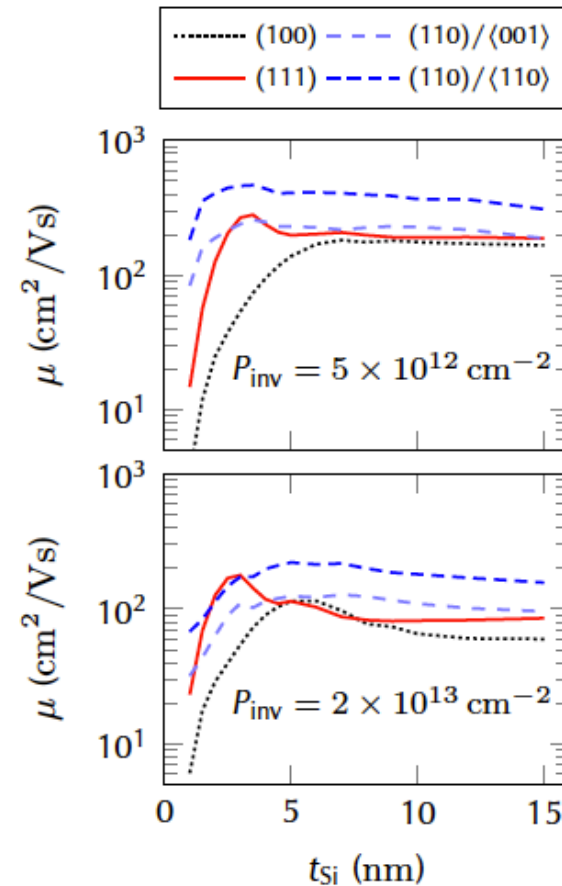
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Hole mobility in DGSOI transistors

Results: hole mobility

Mobility vs. t_{Si}

- ▶ strong mobility reduction as small t_{Si} in every case
- ▶ for (110) and (111) surface the reduction happens at smaller t_{Si}
- ▶ performance improvement of (110) and (111) increases at small t_{Si}



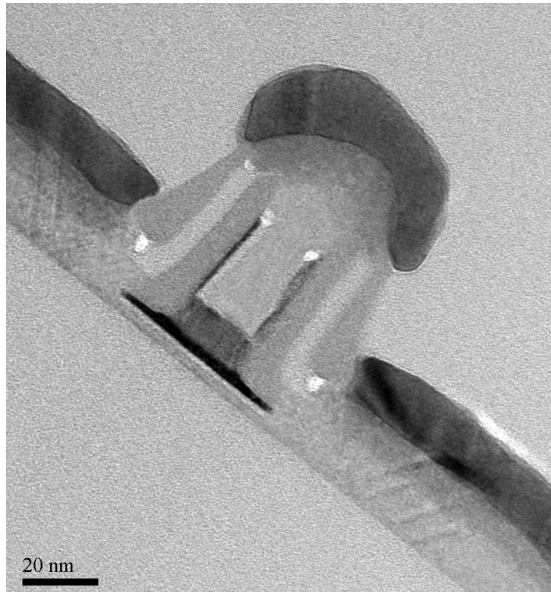
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CMOS Scaling

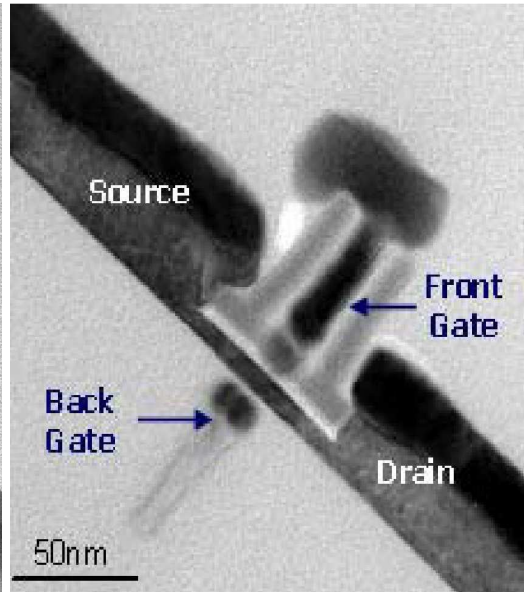
- **SOI: Thickness based & number of gates**

(Courtesy of LETI)



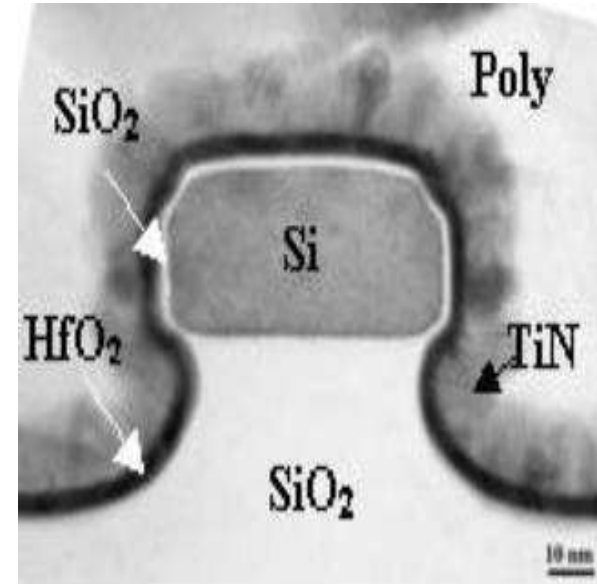
Planar FDSOI

$$T_{Si} \approx L_G / 4$$



Double gate SOI

$$T_{Si} \approx L_G / 2$$



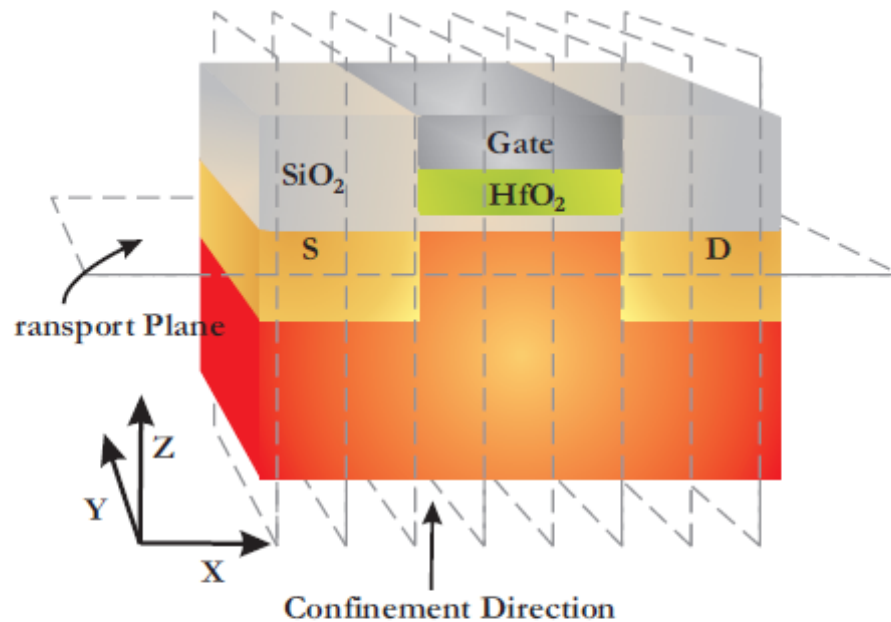
Tri-Gate/FinFET

$$T_{Si} \approx W \approx L_G$$



Multi-subband Monte Carlo simulation

Based on the space-mode approximation [Venugopal et al 2002]



Boltzmann Transport Equation

$$\frac{\partial f}{\partial t} + \frac{\vec{p}}{m} \cdot \nabla_{\vec{r}} f + \vec{F} \cdot \nabla_{\vec{p}} f = \left. \frac{\partial f}{\partial t} \right|_{coll}$$

Poisson's Equation

$$\nabla (\epsilon \nabla V(x, z)) = -\rho(x, z)$$

Schrödinger Equation

$$-\frac{\hbar^2}{2m_z^*} \frac{\partial^2}{\partial z^2} \Psi_j(z) - qV(z) \Psi_j(z) = E_j \Psi_j(z)$$



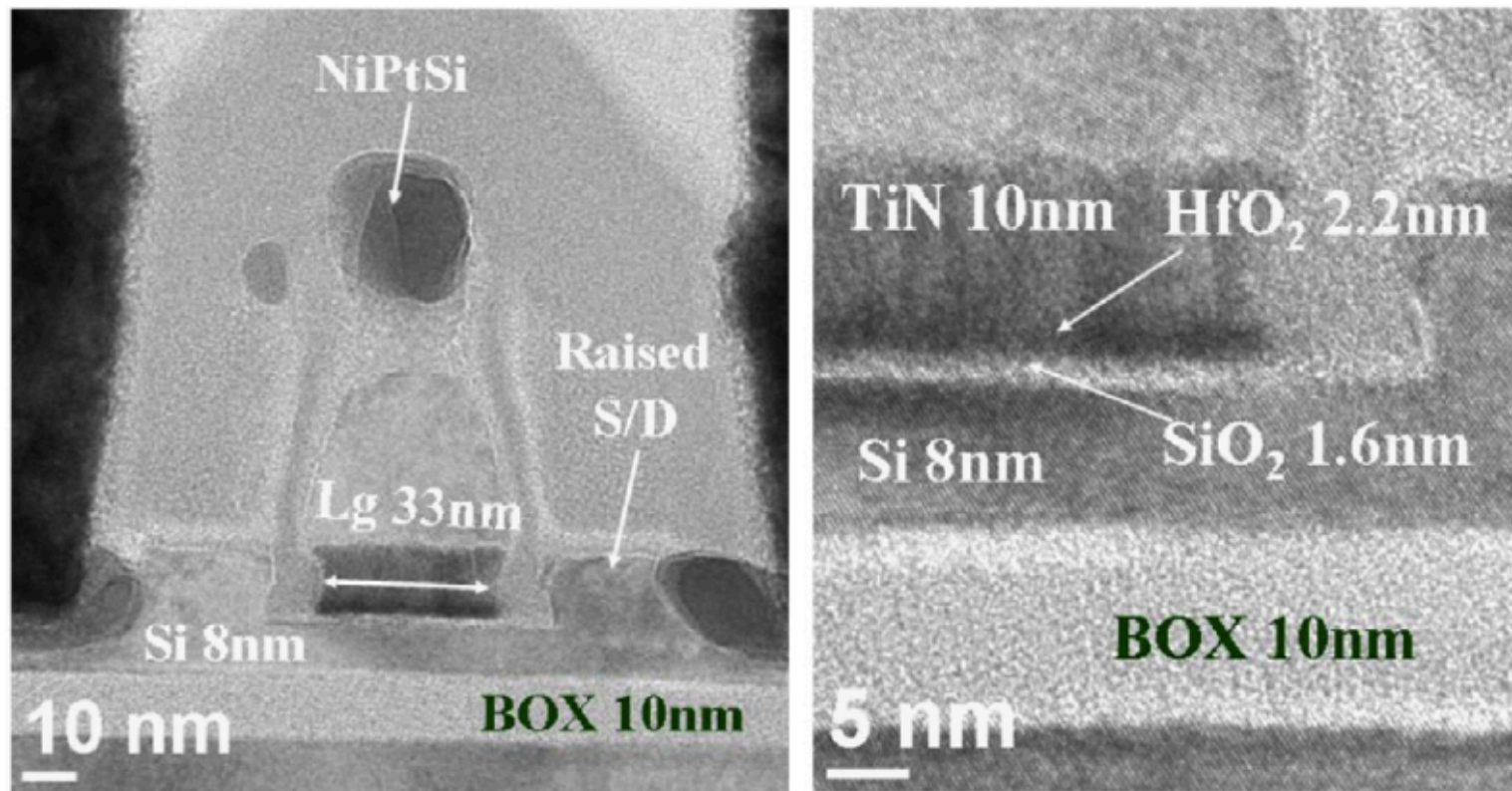
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Multi-subband Monte Carlo simulation

Model Validation

From C. Fenouillet-Beranger et al, SSE 54 (2010) 849–854



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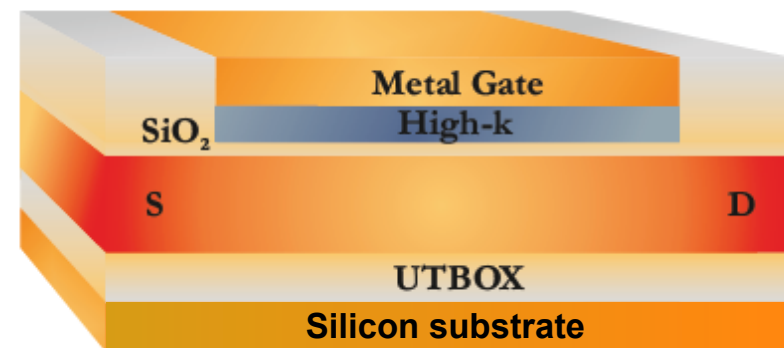
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Multi-subband Monte Carlo simulation

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From C. Fenouillet-Beranger et al, SSE 54 (2010) 849–854

- ✧ $L_G = 33\text{nm}$
- ✧ Midgap metal gate
- ✧ $T_{\text{high-k}} = 2.2\text{nm}$
- ✧ $T_{\text{SiO}_2} = 1.6\text{nm}$
- ✧ $T_{\text{Si}} = 8\text{nm}$
- ✧ Lightly doped channel
- ✧ Gaussian doping profiles in S/D
- ✧ $T_{\text{BOX}} = 10\text{nm}$



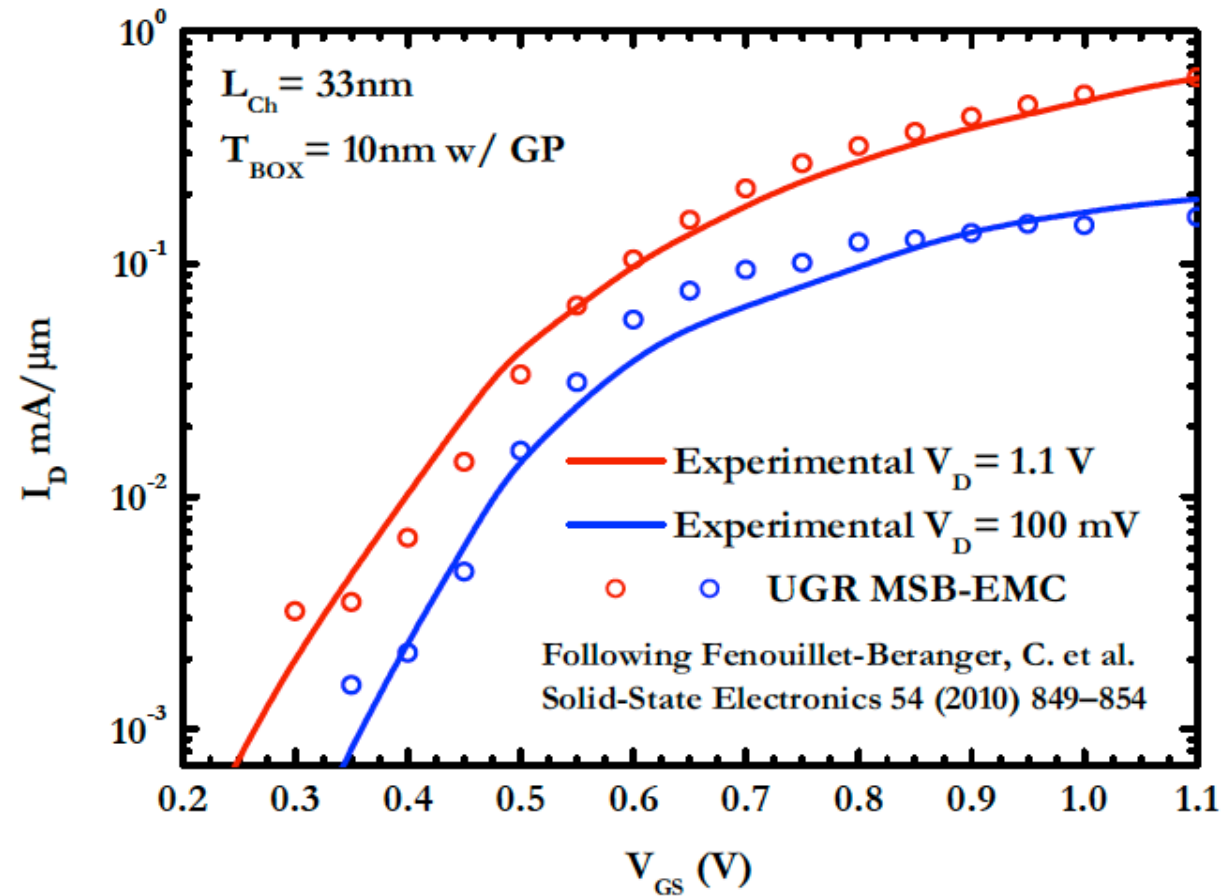
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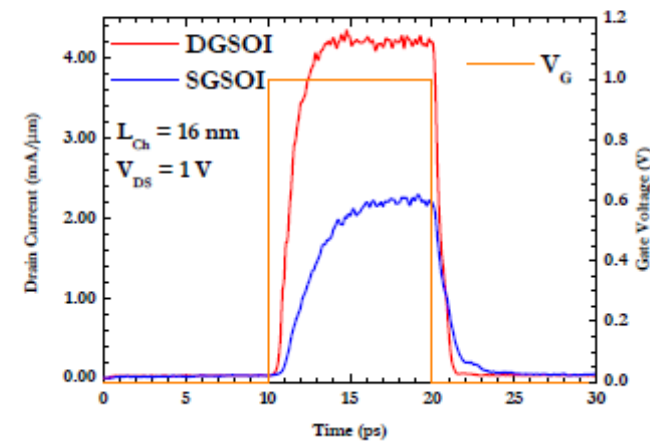
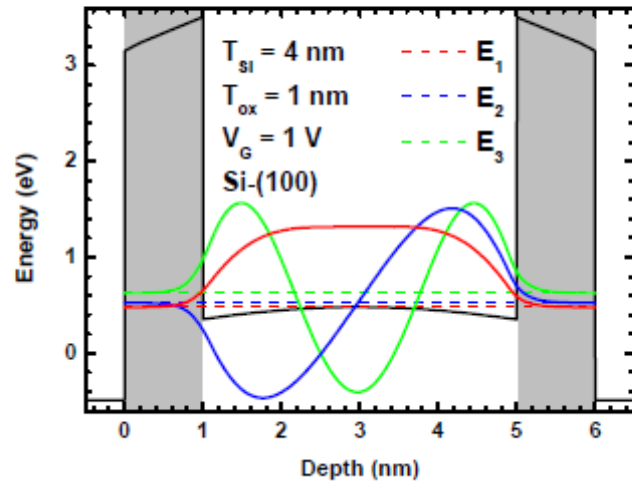
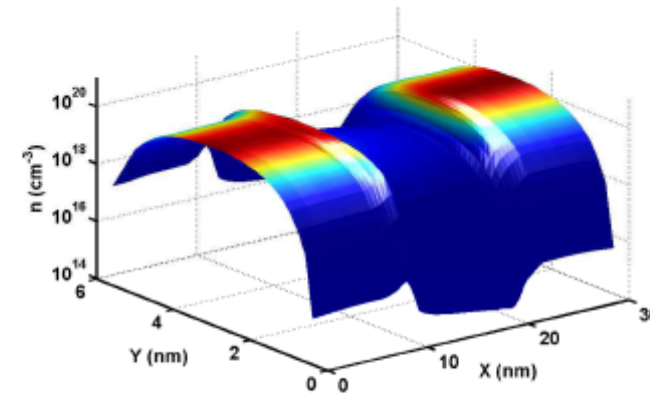
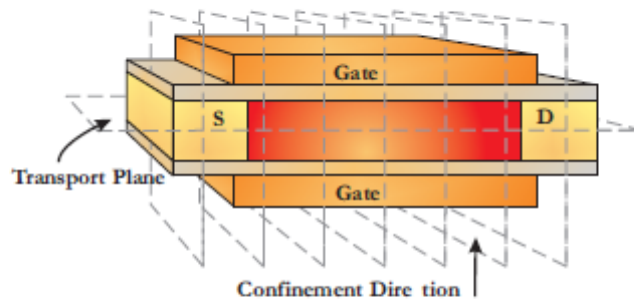


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Multi-subband Monte Carlo simulation

FDSOI, DGSOI, VMT including steady state and transient simulations

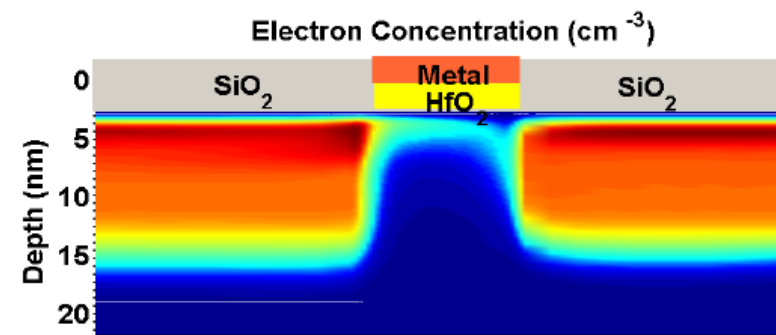
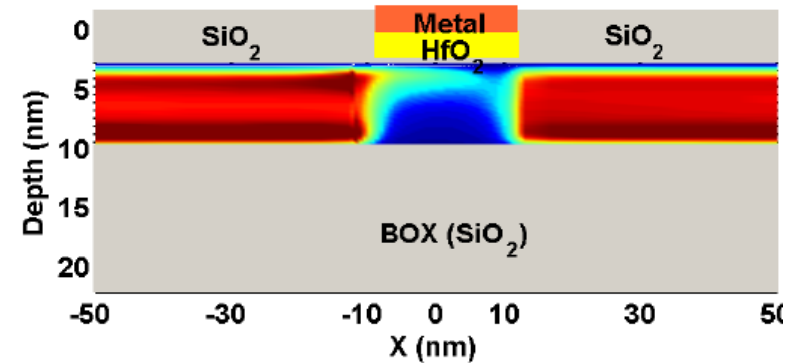
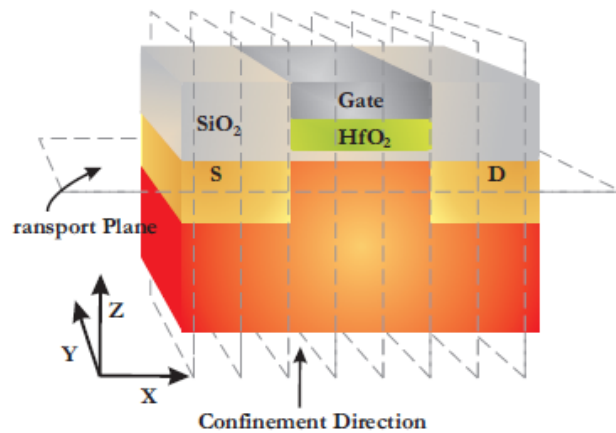
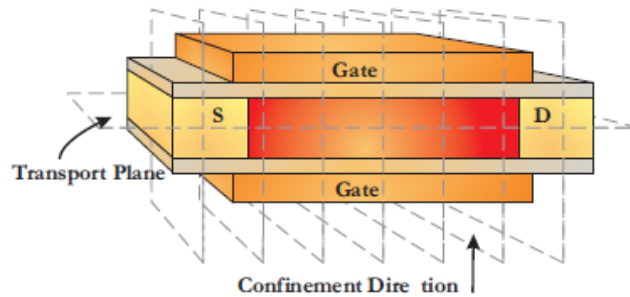


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Multi-subband Monte Carlo simulation

Charge distribution along the channel:
SOI versus Bulk



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Outline

- A. Carrier transport properties in DGSOI
 - 1. Volume inversion.
 - 2. Electron mobility.
 - 3. Crystallographic orientation.
 - 4. Strained channels.
 - 5. Hole mobility.

- B. Ensemble Monte Carlo simulation
 - 1. Quantum corrections.
 - 2. Multisubband Monte Carlo simulations

- C. Multigate nanowires



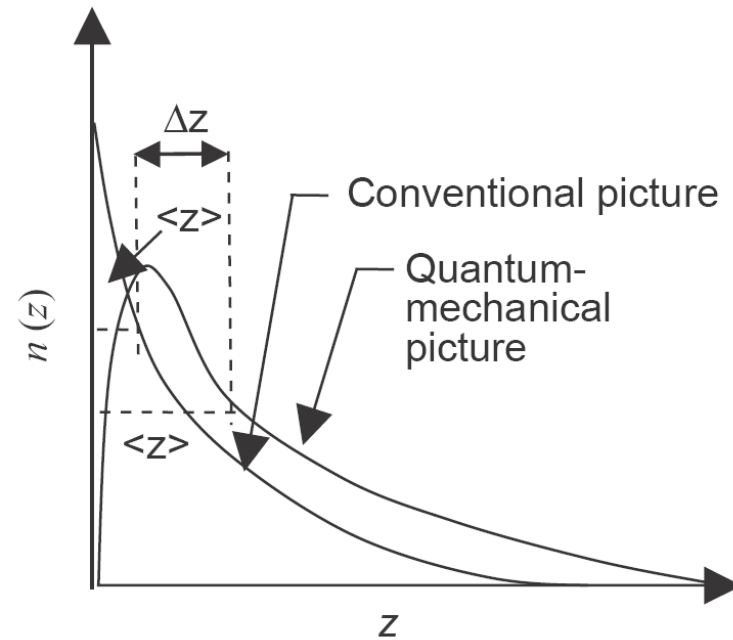
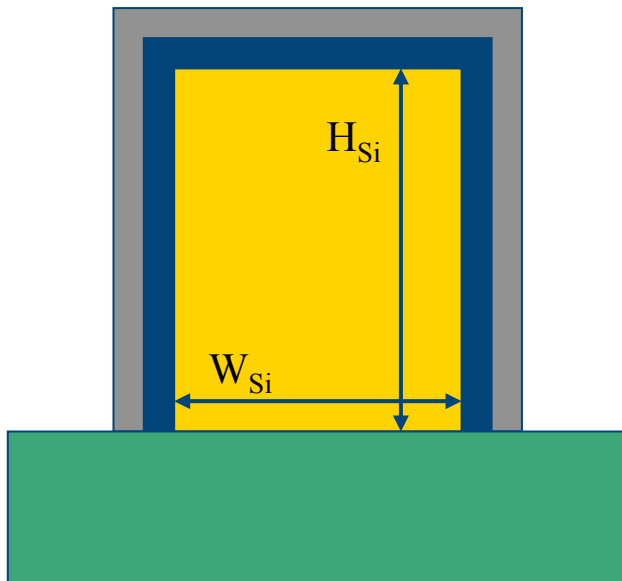
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Multigate transistors

Silicon substrate in the nanometer range

$$H_{Si} = W_{Si} < 20\text{nm}$$



Multi-Gate transistors: 2D confinement



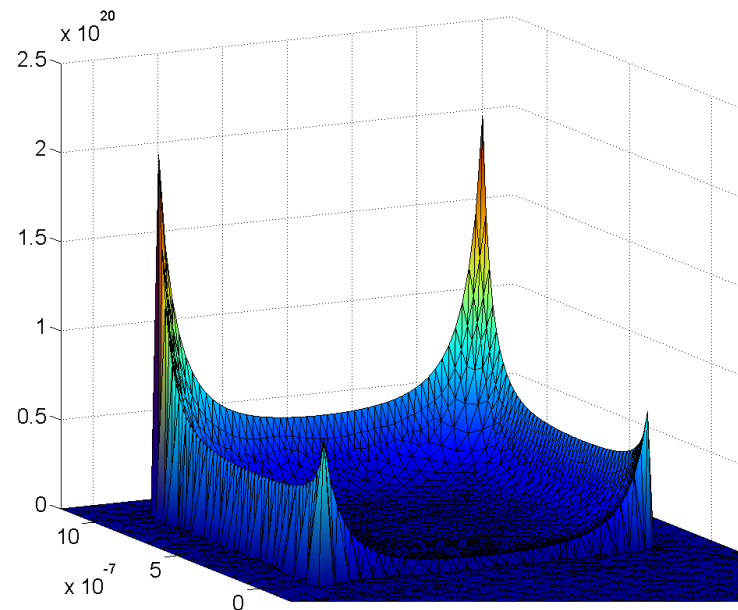
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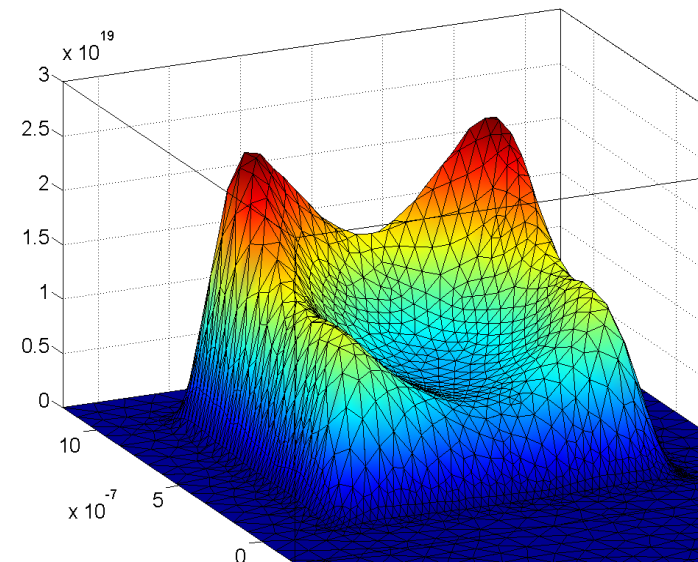
MUGate: Quantum effects

Electron Distribution in a Trigate MOSFET

$H_{Si} = W_{Si} = 10\text{nm}$; $T_{ox} = 2\text{nm}$; $V_G = 1\text{V}$



Classical
 $n_{\max} = 2 \times 10^{20} \text{cm}^{-3}$



Quantum
 $n_{\max} = 2.5 \times 10^{19} \text{cm}^{-3}$

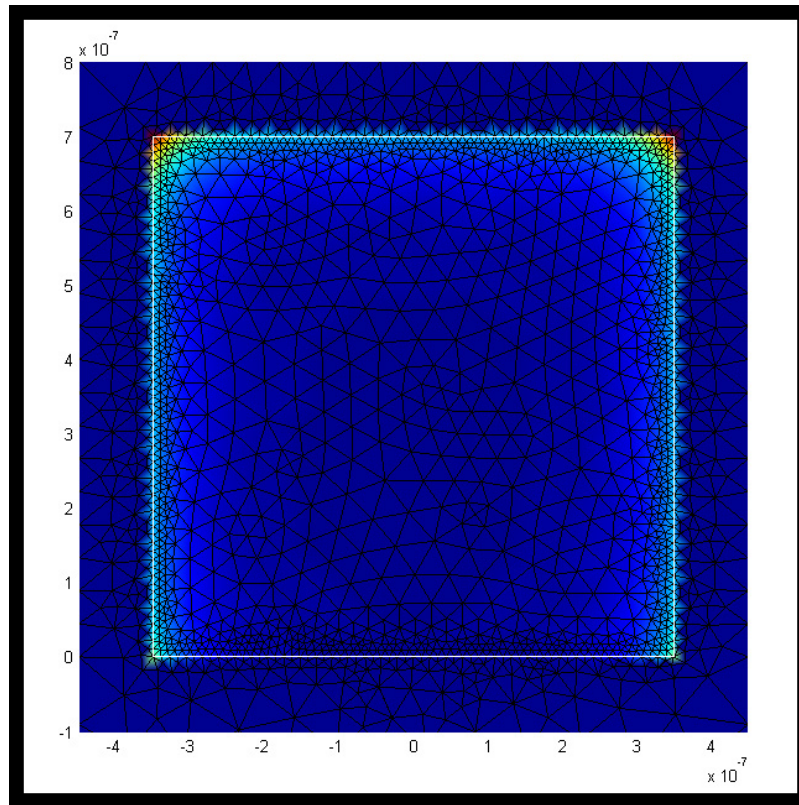


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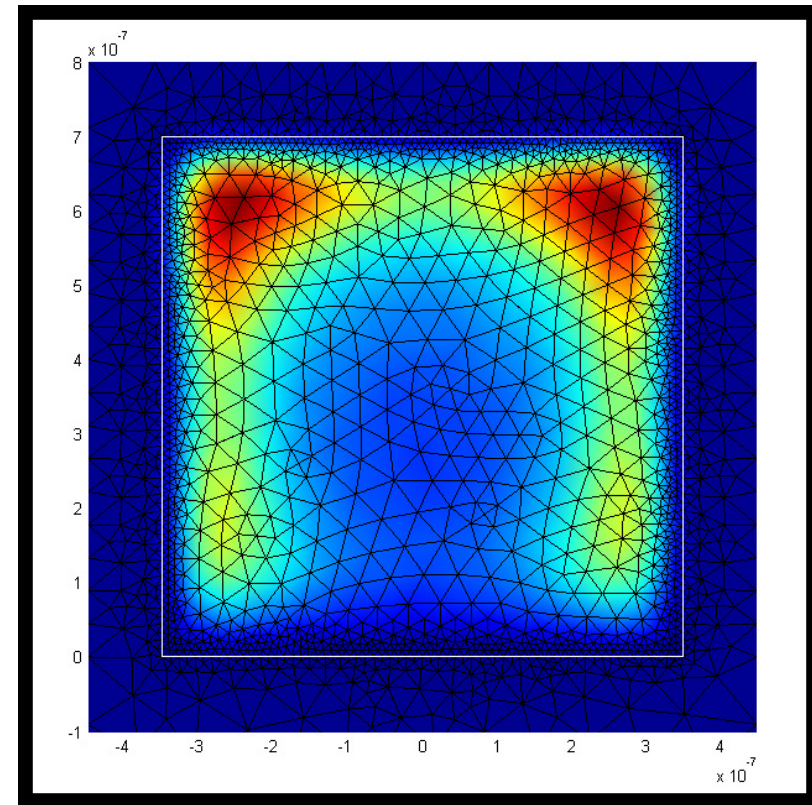
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MUGate: Quantum effects

Top view of the electron distribution in a Trigate MOS



Classical



Quantum

MUGate:1D Electron transport

2D Poisson-Schrödinger

Electrostatic of Multi-Gate FETs: E_n , $\psi_v(y,z)$, n

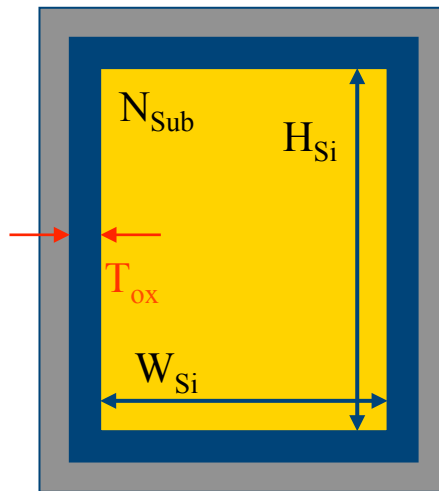
Monte Carlo simulator
acoustic & intervalley phonons
& surface roughness

Phonon limited mobility
(dominant at low fields)



MUGate:1D Electron transport

Device under study: Quantum Wire with square cross section $H_{Si} = W_{Si}$ and different crystallographic orientations



$$H_{Si} = W_{Si} = 15\text{nm}; 10\text{nm}; 5\text{nm}$$

$$\text{Gate voltage} = [0.2, 1.5]\text{V}$$

$$\text{Undoped substrate, } \phi_m = 4.61\text{eV}$$

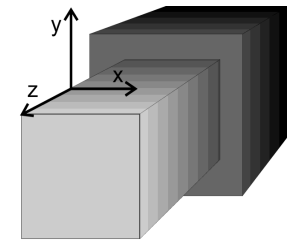
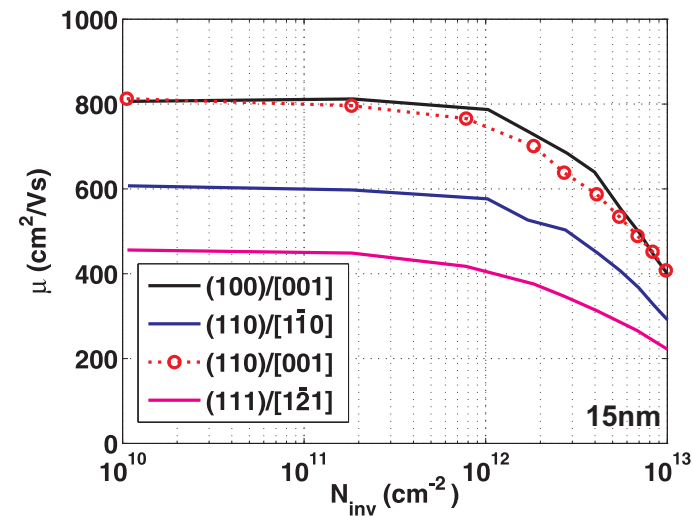
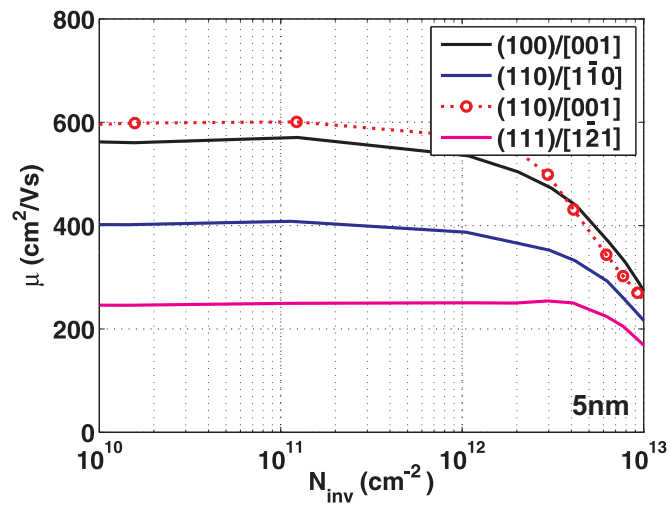
Energy values & Wave functions necessary to get 95% of the total charge $\rightarrow H_{Si} = W_{Si} > 15\text{nm} \rightarrow$ High number of E_n & $\psi_v(y,z)$.



MUGate:1D Electron transport

- Phonon-limited mobility in a square wire with different orientations (YZ-plane)/[z-direction]:

There is a strong dependence on the size and on the orientation



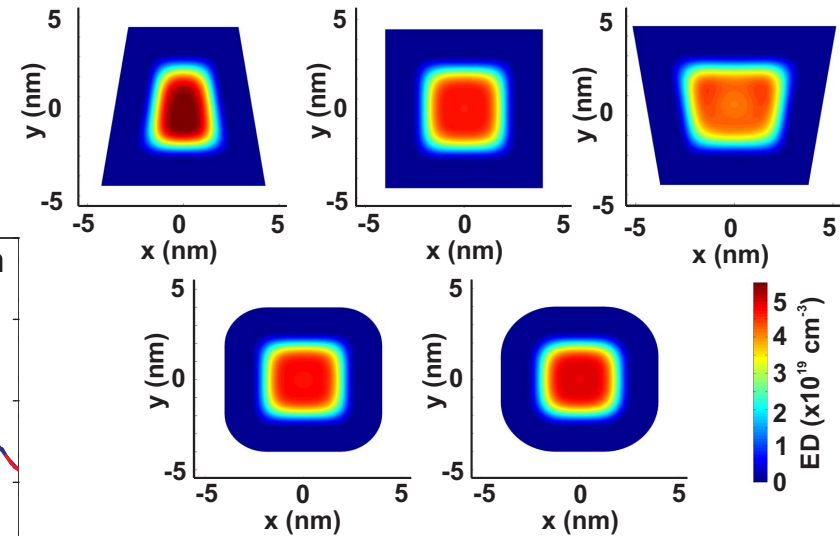
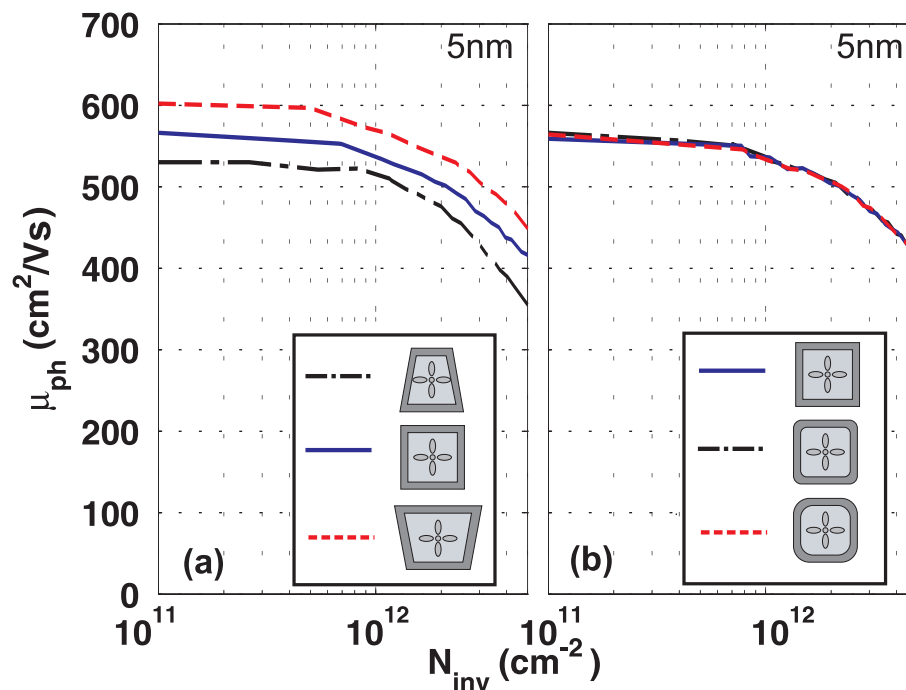
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MUGate:1D Electron transport

- Phonon-limited mobility in (100)/[001] devices with different geometries:

The effects of the geometry variability are more noticeable in small devices.



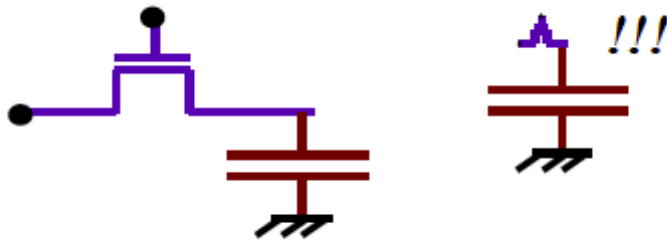
The mobility is not affected by the presence of rounding corners.



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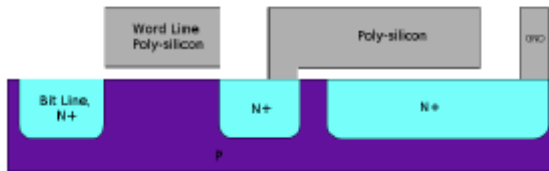
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Design of 1T-DRAM cell



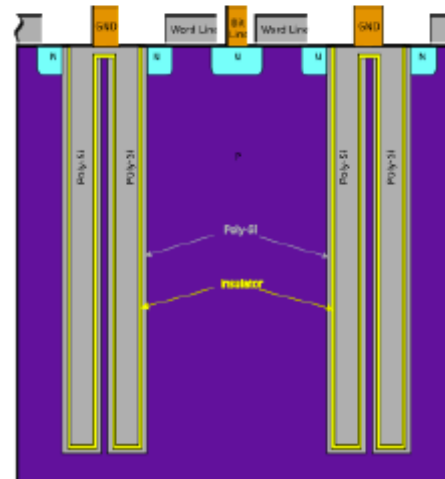
DRAM in 1968

(Dennard)



**Minimum capacitance requirement
25 fF/cell**

DRAM today



Standard

Simple concept

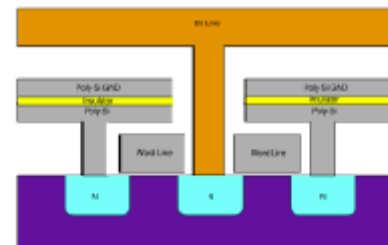


Complexity

Capacitance

Leakage

Resistance



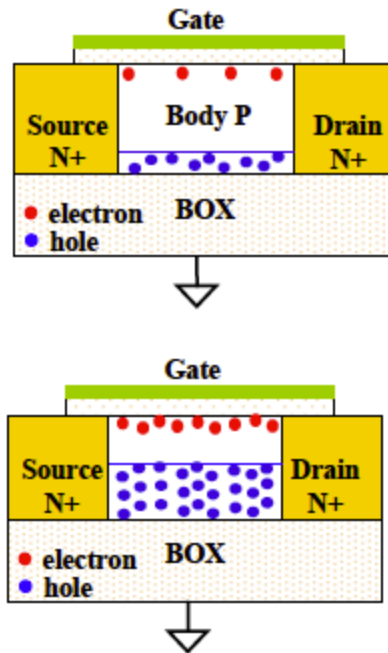
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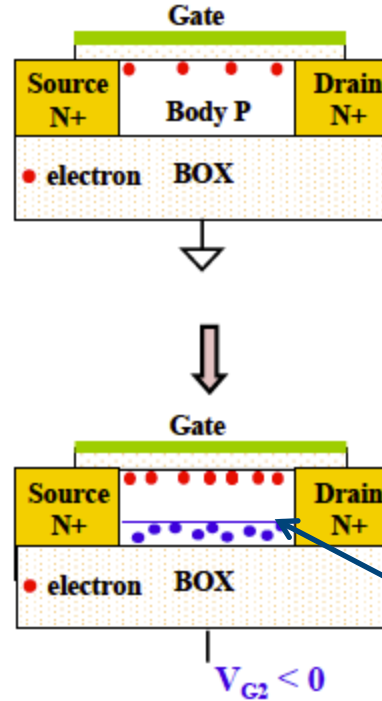
Design of 1T-DRAM cell

The alternative: FB-1T-DRAM

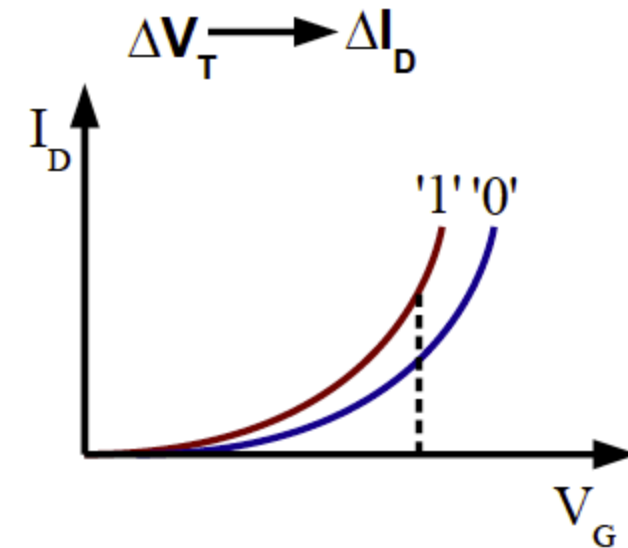
PD-SOI



FD-SOI



[Wann'93], [Okhonin'01], [Ranica'04]



Supercoupling effect

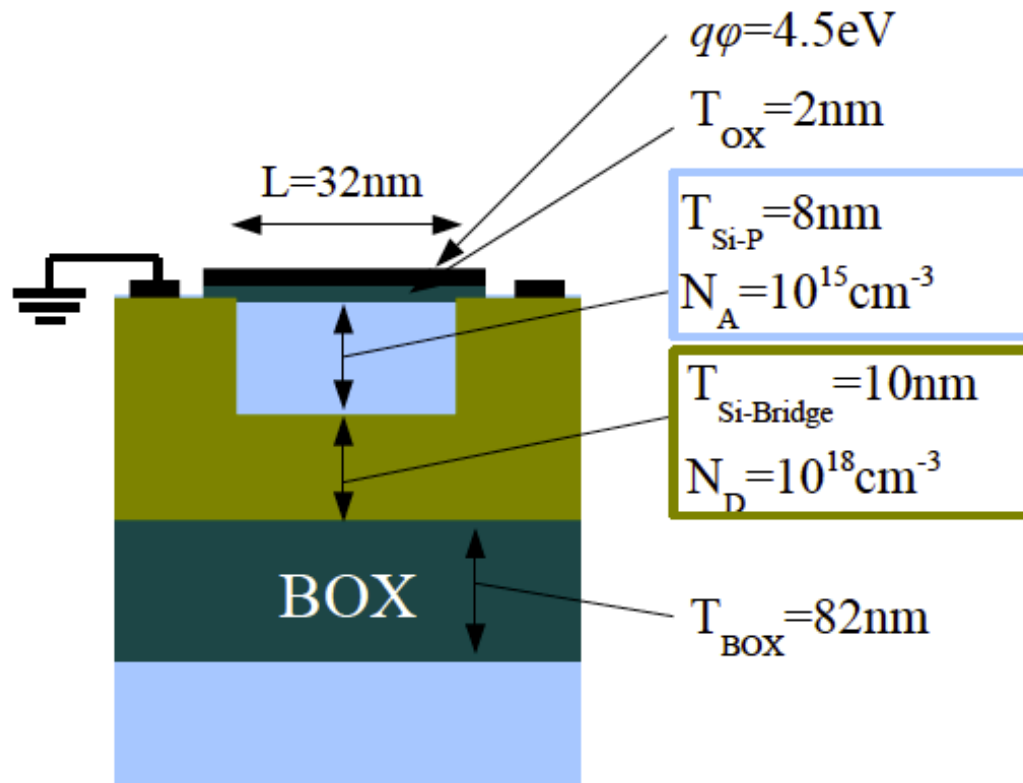


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Design of 1T-DRAM cell

Reference Device



2D

SRH

Band to Band tunneling

Impact Ionization

$T=25^\circ\text{C}$



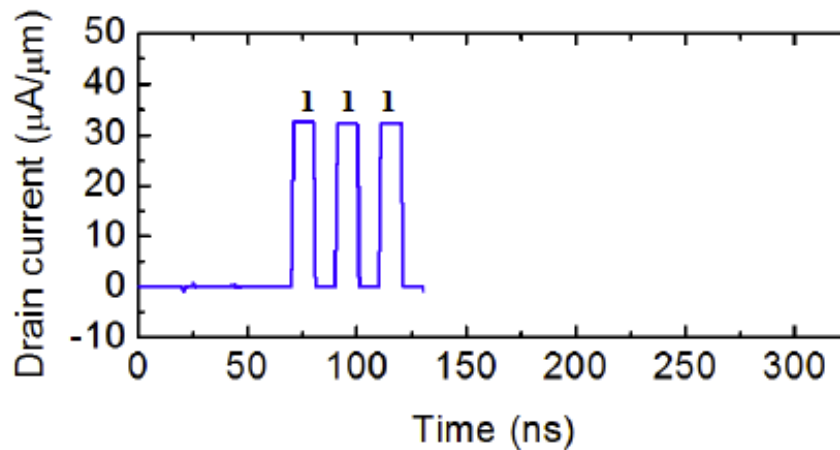
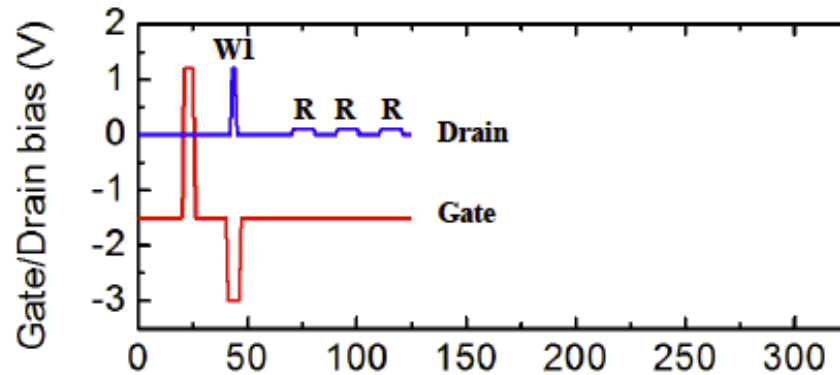
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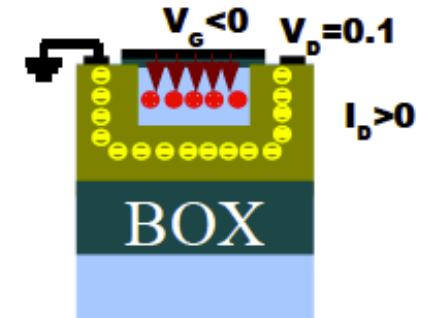
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Design of 1T-DRAM cell

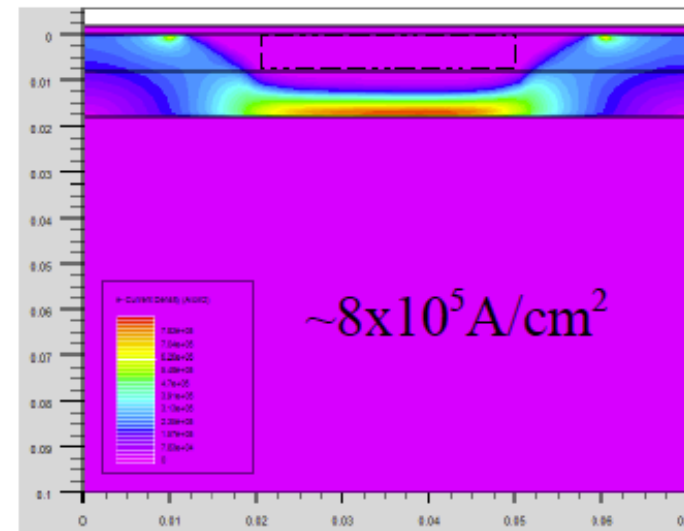
Transient simulation



Reading '1'

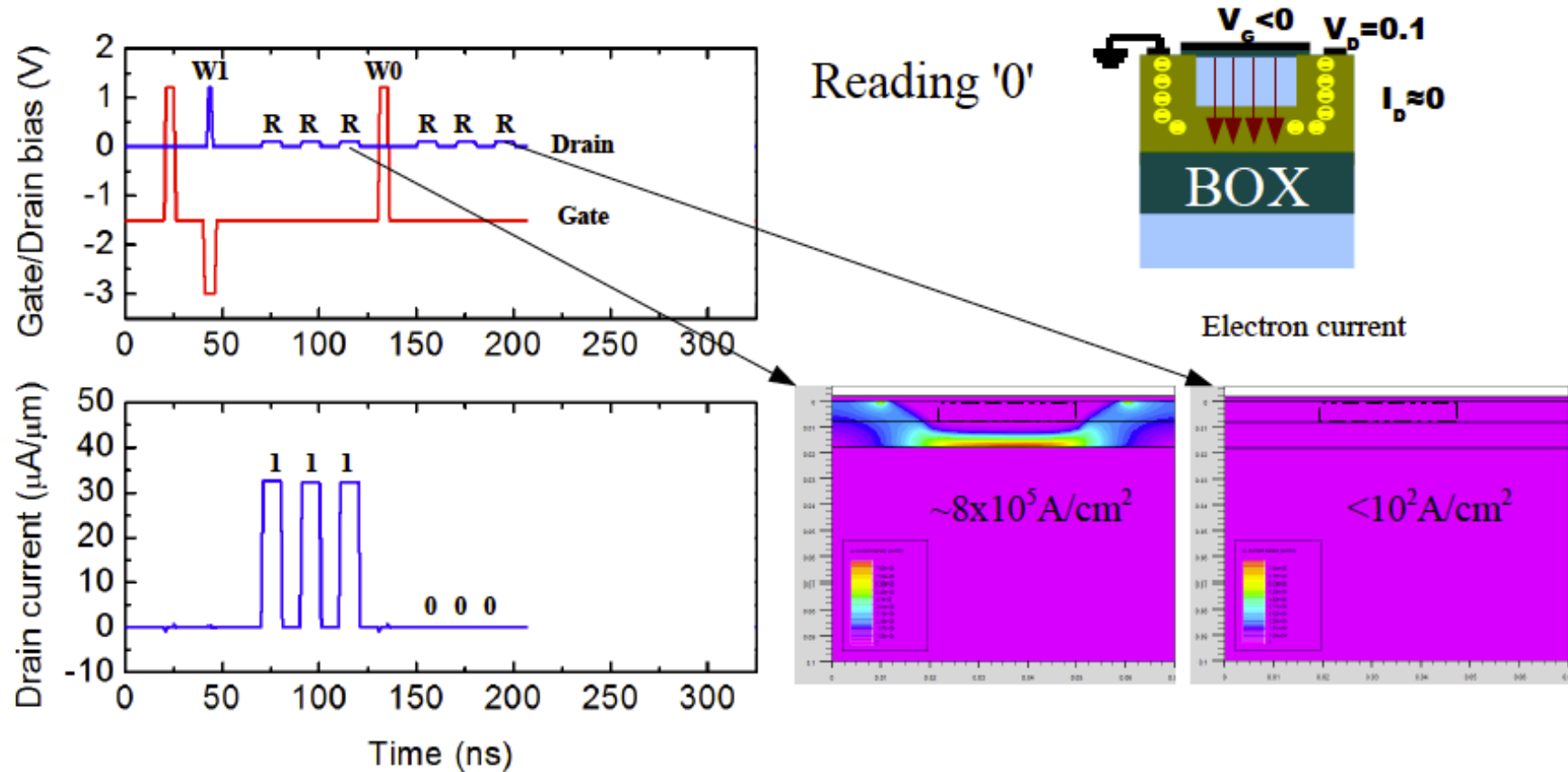


Electron current



Design of 1T-DRAM cell

Transient simulation



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Conclusions

- Simulation is an important and necessary tool for today's devices.
- It's a very complex task when you deal with real devices, but it can be faced at different complexity levels.
- It provide us with information with help us to better understand and improve our devices.



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Thank you for your attention

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