Leveraging on Nano-CMOS Competences for Diverse Applications: the Case for Modeling an Simulation

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Motivation

CMOS Technology has been relentlessly developed during the last 35 years with unprecedented records in terms of both qualitative and quantitative technological advancement and of pervasive impact on the human society.

It has also significantly stimulated the development of scientific know-how that can be exploited in close-by fields, helping their development in the frame of a beneficial synergy with micro- and nano-electronics itself.

Contents

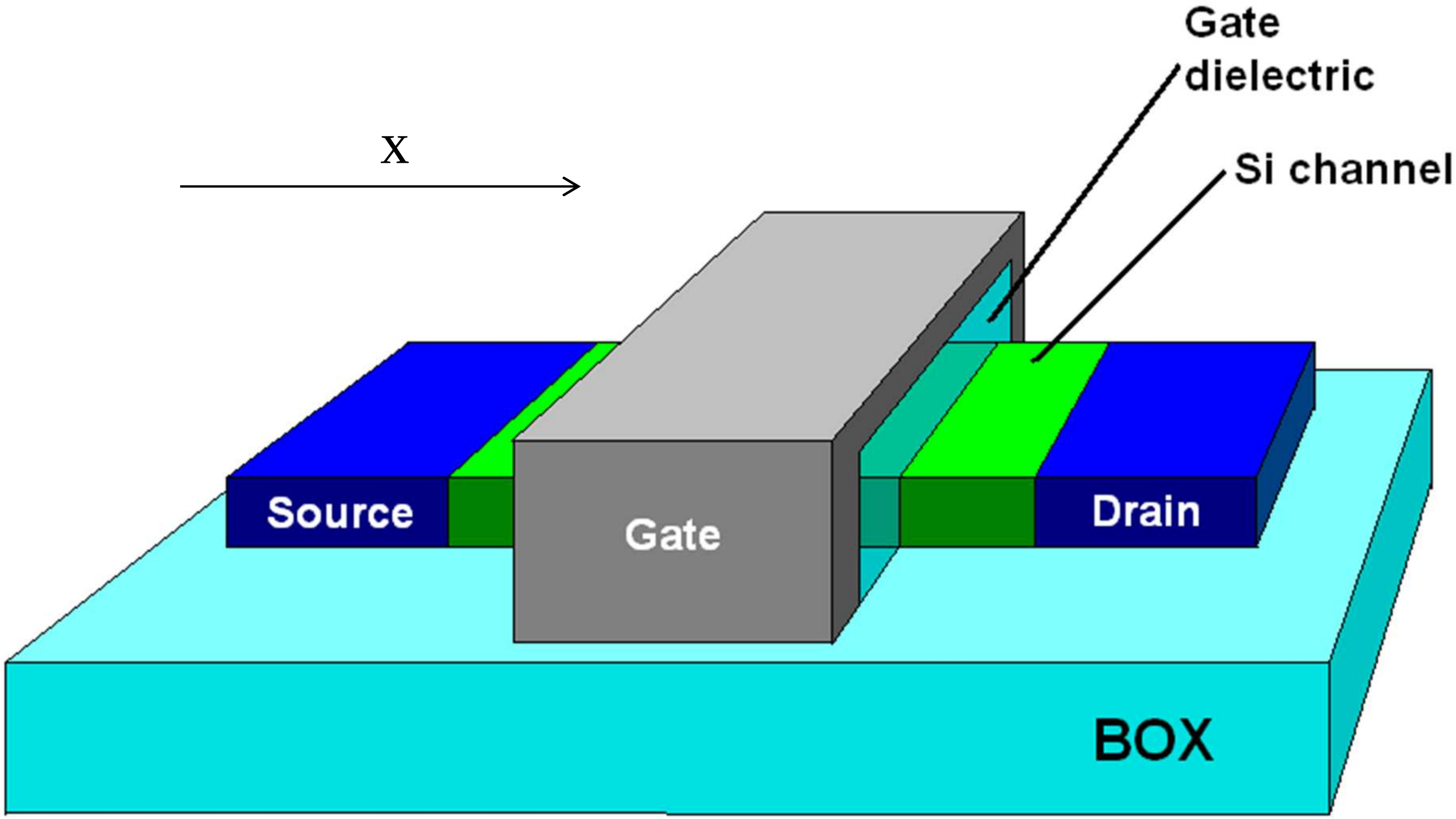
This presentation will discuss two examples in the field of modeling and numerical simulation, namely:

1. knowledge and mathematical know-how developed for the quantum-mechanical simulation of nano-scale CMOS devices can be exploited to tackle the problem of optical simulation for solar cells and optical sensors;
2. the know-how developed in the field of particle based simulation of transport in small-geometry MOSFETs significantly eases the development of numerical simulators for ionic and protein transport in nano-scale biological systems that, in turn, can be integrated within Si technology.

Outline

- 3-D Quantum Mechanical Simulation of Nano-MOSFETs vs. Electro-Magnetic simulation
  - The transverse mode representation
  - Applications to
    - ✓nMOS/pMOS I-V characteristics
    - ✓Analysis of a super-steep subthreshold slope MOSFET
  - Analogies to RCWA EM simulation
    - ✓Application to solar-cell analysis
- From Monte Carlo Device Simulation to Ionic Transport through Biological and Synthetic Nano-Scale Channels

1. Starting from advanced CMOS: the Nano-transistor.



Main strategy of simulation

- ***Self-consistent solution of***

Schrödinger equation

+ Poisson equation.

The main problem here is to solve the 3D Shrödinger equation.

Solution of 3D Schrödinger equation

$$\mathbf{H}\psi(x,y,z) = E\psi(x,y,z)$$

$$\mathbf{H} = -\frac{\partial^2}{2m_x\partial x^2} - \frac{\partial^2}{2m_y\partial y^2} - \frac{\partial^2}{2m_z\partial z^2} + U(x,y,z)$$

H is an **Hermitian** operator**.**

U(x,y,z) is the potential inside the channel.
Transport along x; confinement on the y-z plane.

The direct solution of the stationary 3D Schrödinger equation via a finite difference scheme comes across a well known instability caused by evanescent modes.

Transverse mode representation

The wave-function is expanded into the sum of x-propagating *transversal modes*

$$\psi(x,y,z)=\sum_{i=1}^{M} c_i(x)\varphi_i(y,z)$$

Where $\varphi_i(y,z)$ is the *i*-th transverse mode wave function, M is the number of involved modes. The specific set of mode wavefunction $\{\varphi(y,z)\}$ depends on the detailed mathematical formulation of the simulation method.

Toghether with arbitrary precision arithmetic it circumvents the evanescent modes problem.

- The coefficients $c_i(x)$ can be expressed in terms of amplitudes of incoming and outgoing waves

$$c_i(x) = c_i^+(x) + c_i^-(x),\ i = 1..M$$

in vector notation: $$\mathbf{c}(x) = \mathbf{c}^+(x) + \mathbf{c}^-(x)$$

Usually we know a^+, b^-. Coefficients a^-, b^+ and function inside the channel are unknown. To solve this problem we can use either **T-*matrix*** or **S-*matrix*** formulation.

$$\begin{pmatrix} a^+ \\ a^- \end{pmatrix} = \mathbf{T} \begin{pmatrix} b^+ \\ b^- \end{pmatrix} \quad \Longleftrightarrow \quad \begin{pmatrix} b^+ \\ a^- \end{pmatrix} = \mathbf{S} \begin{pmatrix} a^+ \\ b^- \end{pmatrix}$$

Example of Transfer-matrix calculation scheme

$$\Psi(x,y,z)=\begin{cases}\sum_{n=1}^{N}(c_{1,n}^{+}e^{ik_n x}+c_{1,n}^{-}e^{-ik_n x})\varphi_n(y,z), & x\le 0\\ \sum_{n=1}^{N}d_{1,n}\chi_{1,n}(x,y,z)+d_{2,n}\chi_{2,n}(x,y,z), & 0\le x\le L_x\\ \sum_{n=1}^{N}(c_{2,n}^{+}e^{ik_n x}+c_{2,n}^{-}e^{-ik_n x})\varphi_n(y,z), & x\ge L_x\end{cases}$$

where $\chi_n(x,y,z)$ satisfies the Schrödinger equation with the following boundary conditions:

$$\chi_{1,n}\big|_{x=0}=\varphi_n,\quad \chi_{1,n}\big|_{x=L_{Canal}}=0$$

$$\chi_{2,n}\big|_{x=0}=0,\quad \chi_{2,n}\big|_{x=L_{Canal}}=\varphi_n$$

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By matching the wave function and its derivative at the left boundary and the right boundary of the channel we get:

$$\begin{pmatrix} \mathbf{c}_{left}^{+} \\ \mathbf{c}_{left}^{-} \end{pmatrix} = \mathbf{T} \begin{pmatrix} \mathbf{c}_{right}^{+} \\ \mathbf{c}_{right}^{-} \end{pmatrix}$$

This scheme has no restrictions on channel length nor potential. It can be easily generalized to N- junction devices with N leads and a coupling region of an arbitrary shape.

The scheme is described in detail in:

J. T. Londergan, J. P.Carini, D. P. Murdock, "Binding and scattering in two-dimensional systems: applications to quantum wires,waveguides, and photonic crystals" Springer, 1999.

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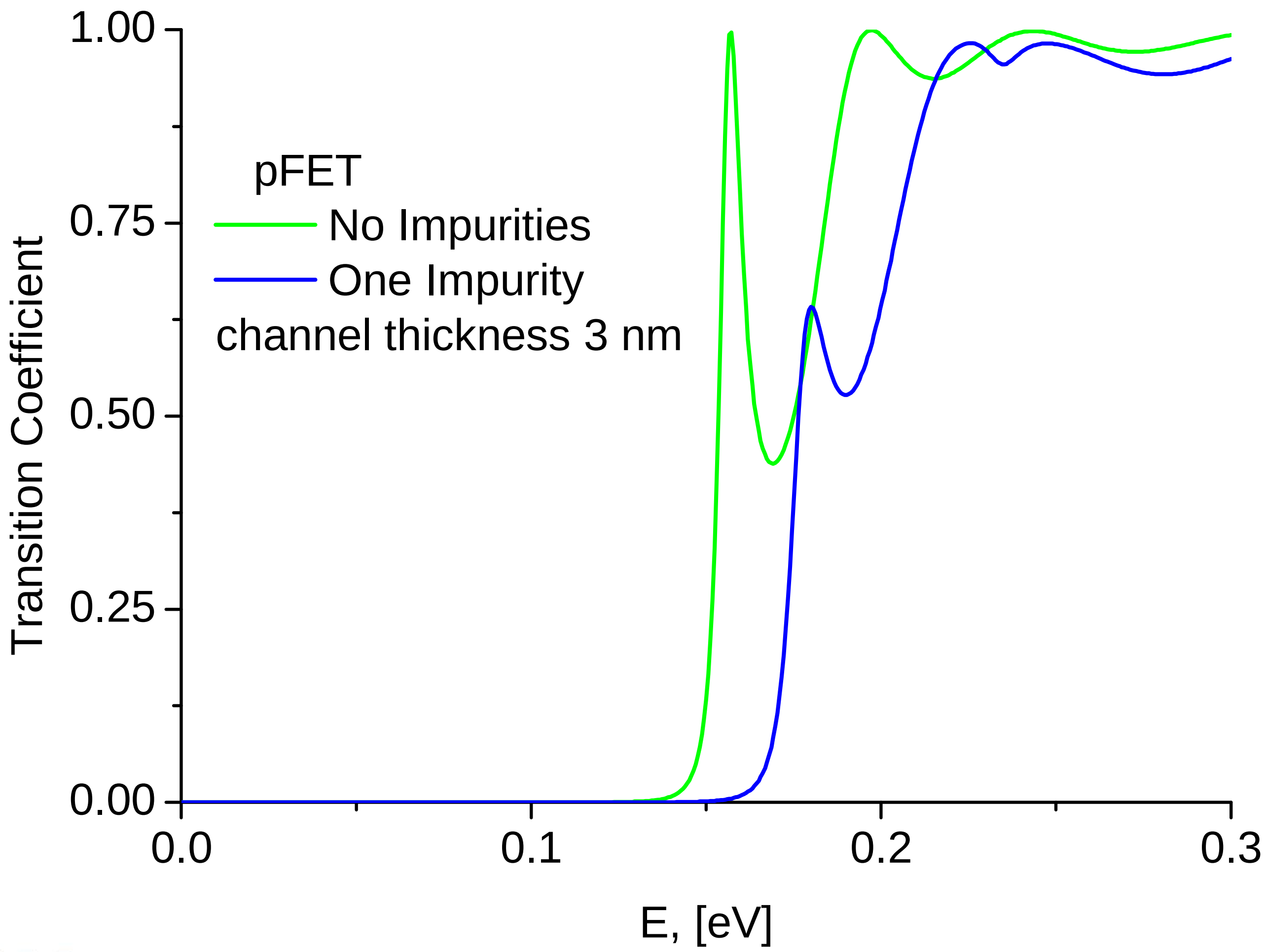
Example: hole transmission in channel

(10nm x 10nm x 5nm)



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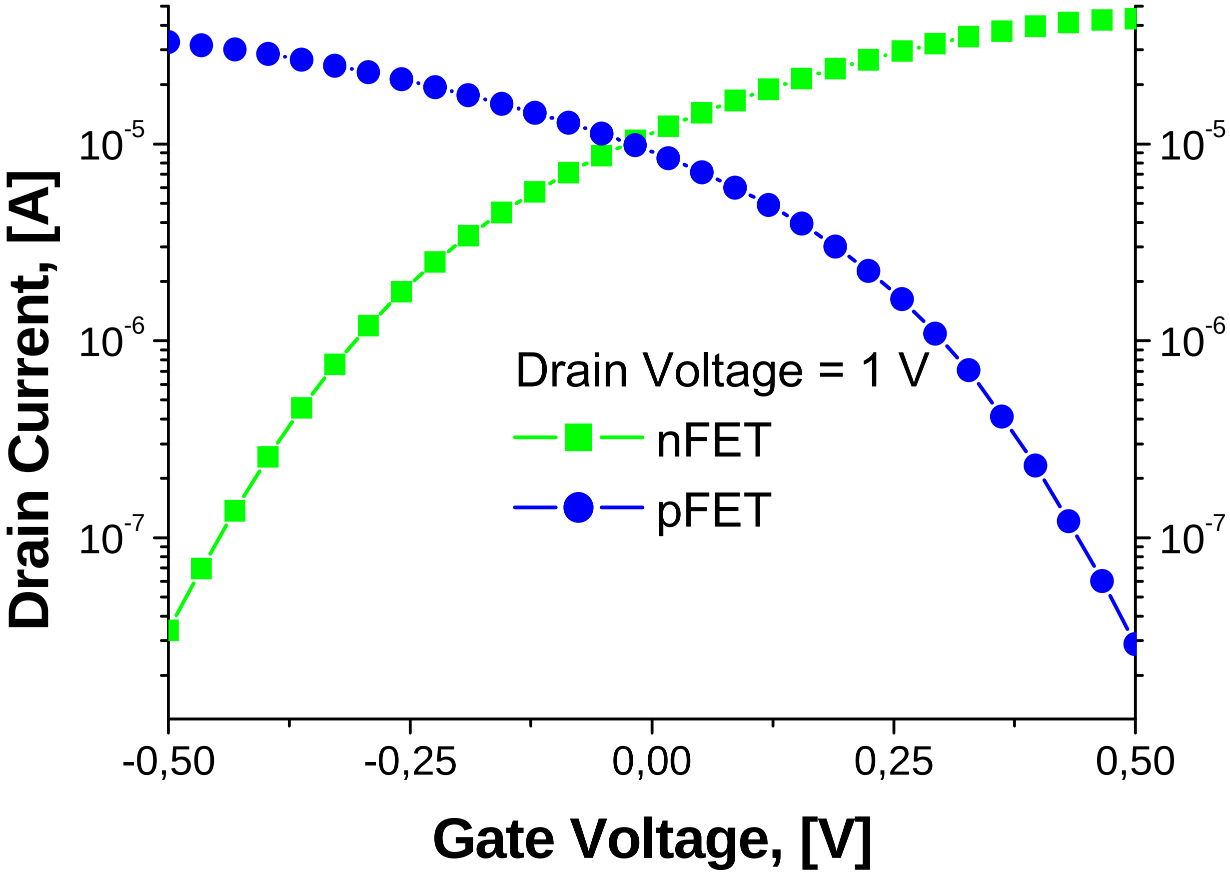
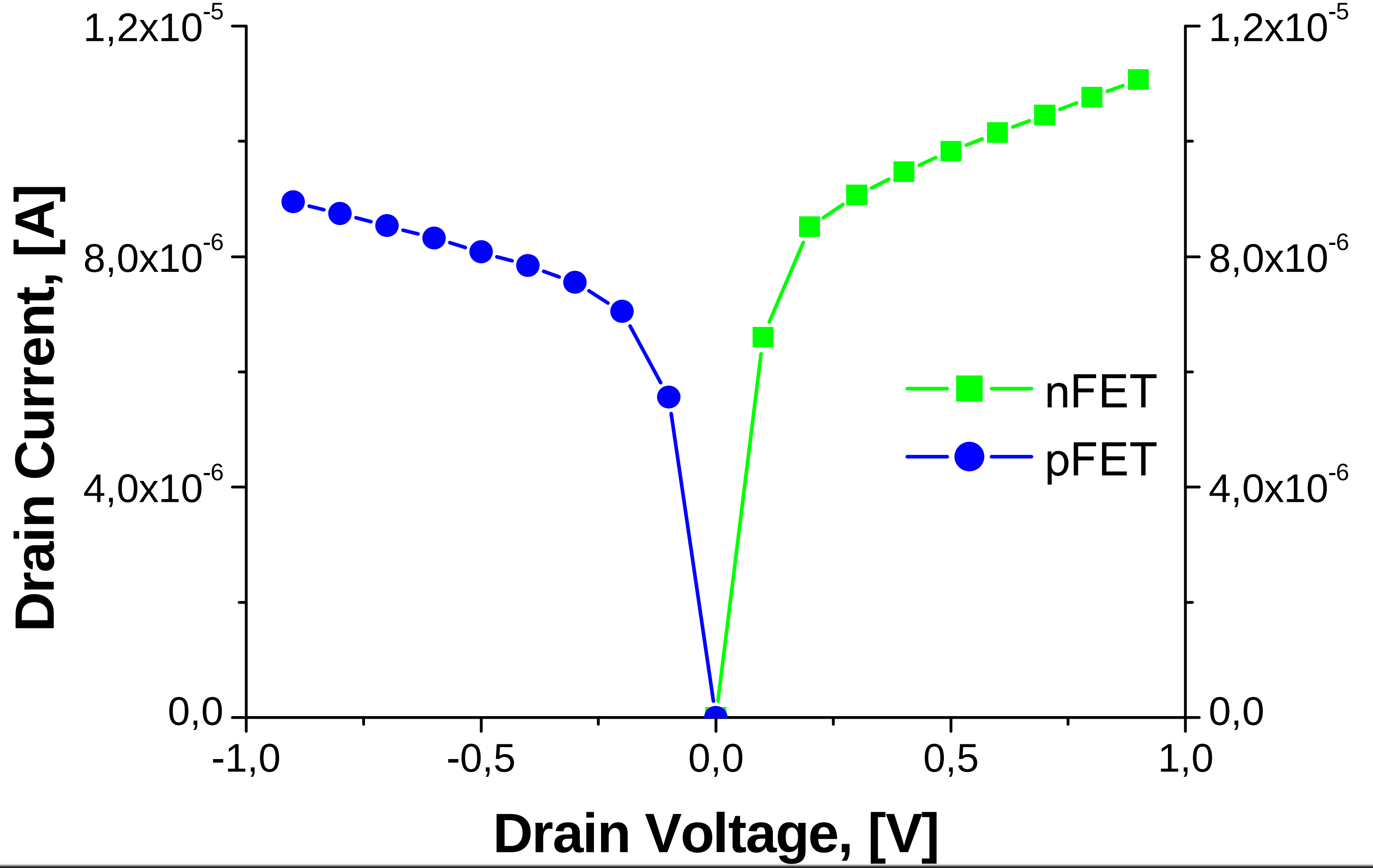
Transfer characteristics (log)

(10nm x 10nm x 5nm)



Sub-threshold swing is 71 mV per decade of current.

Output characteristics
(10nm x 10nm x 5nm)



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Application: Superlattice-Based Steep-Slope Switch

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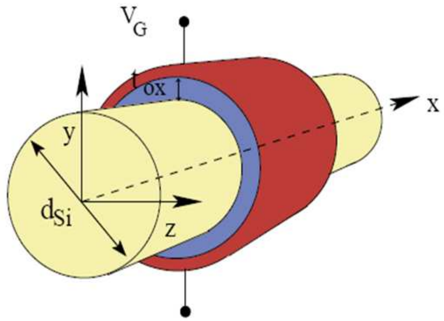
Outline

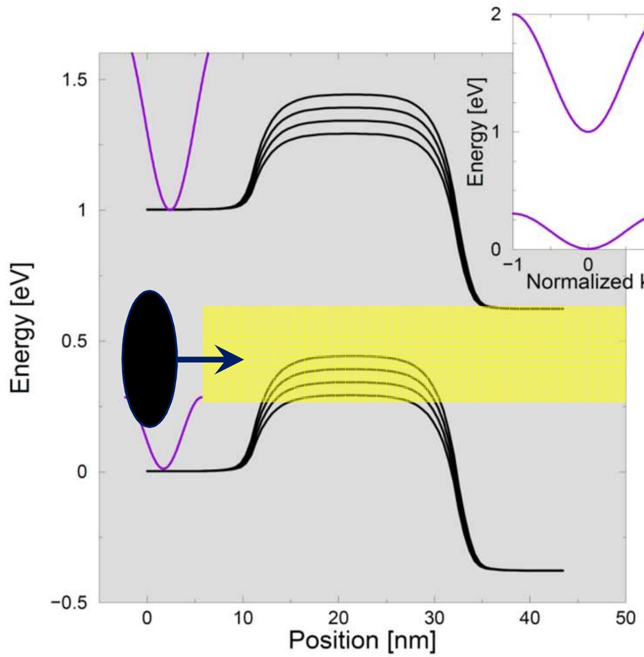
- Superlattice-Based Steep-Slope Switch
- Optimization of the subband structure
- Superlattice-based nanowire FET
- Semiconductor pairs for the superlattice
- Discussion

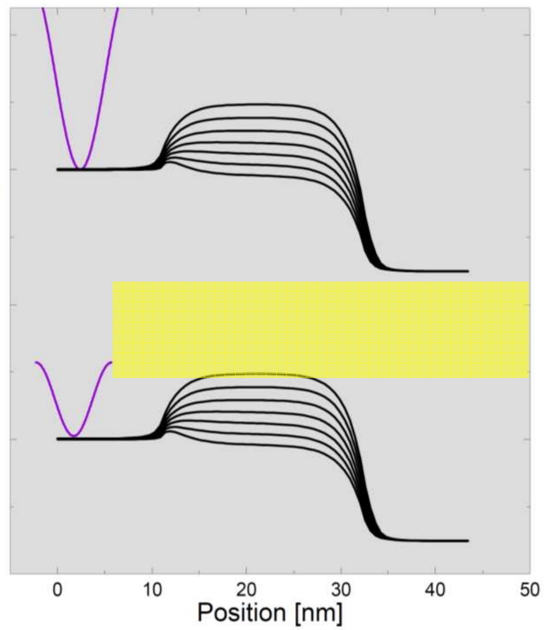
Device concept

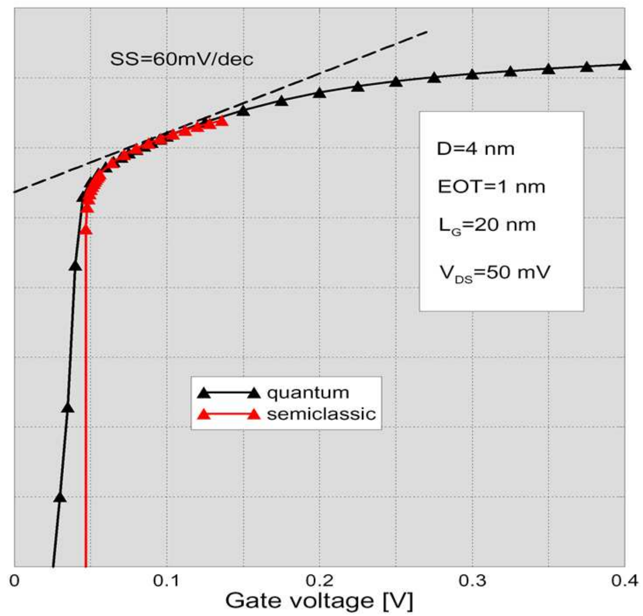


transverse quantization

1D transport problem







Semiclassical and Q.M. turn-on characteristics

OFF STATE

ON STATE

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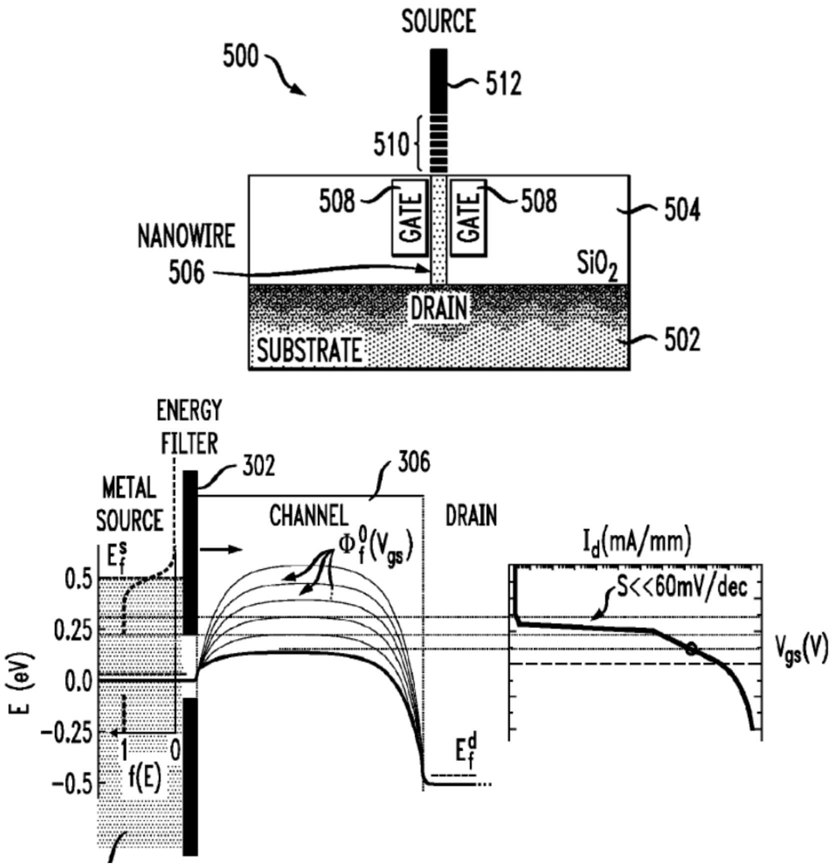
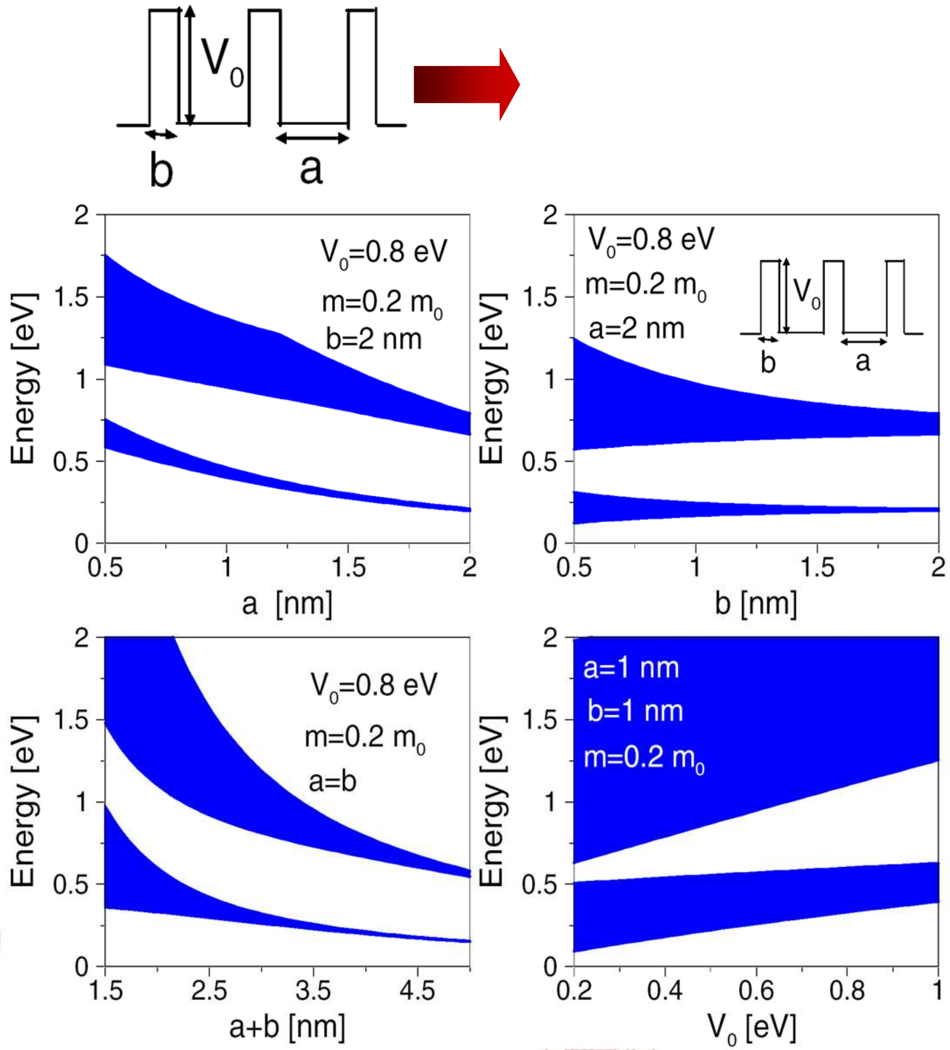
How to filter out high-energy electrons?

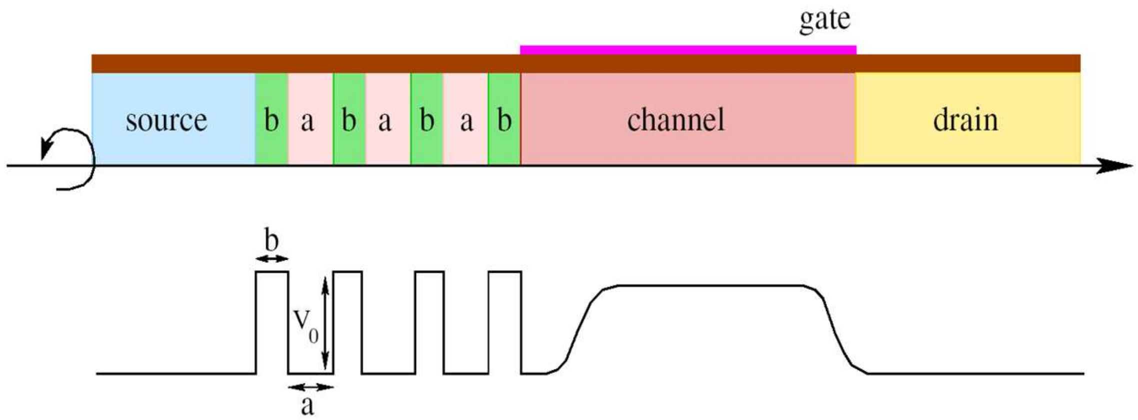
superlattice structure between the source and the channel

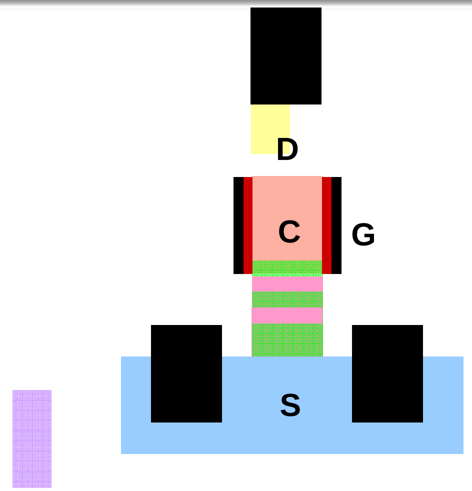


M. Bjoerk et al., United States Patent Application Publication, no. US 2009/0200540 A1, 13 August 2009.



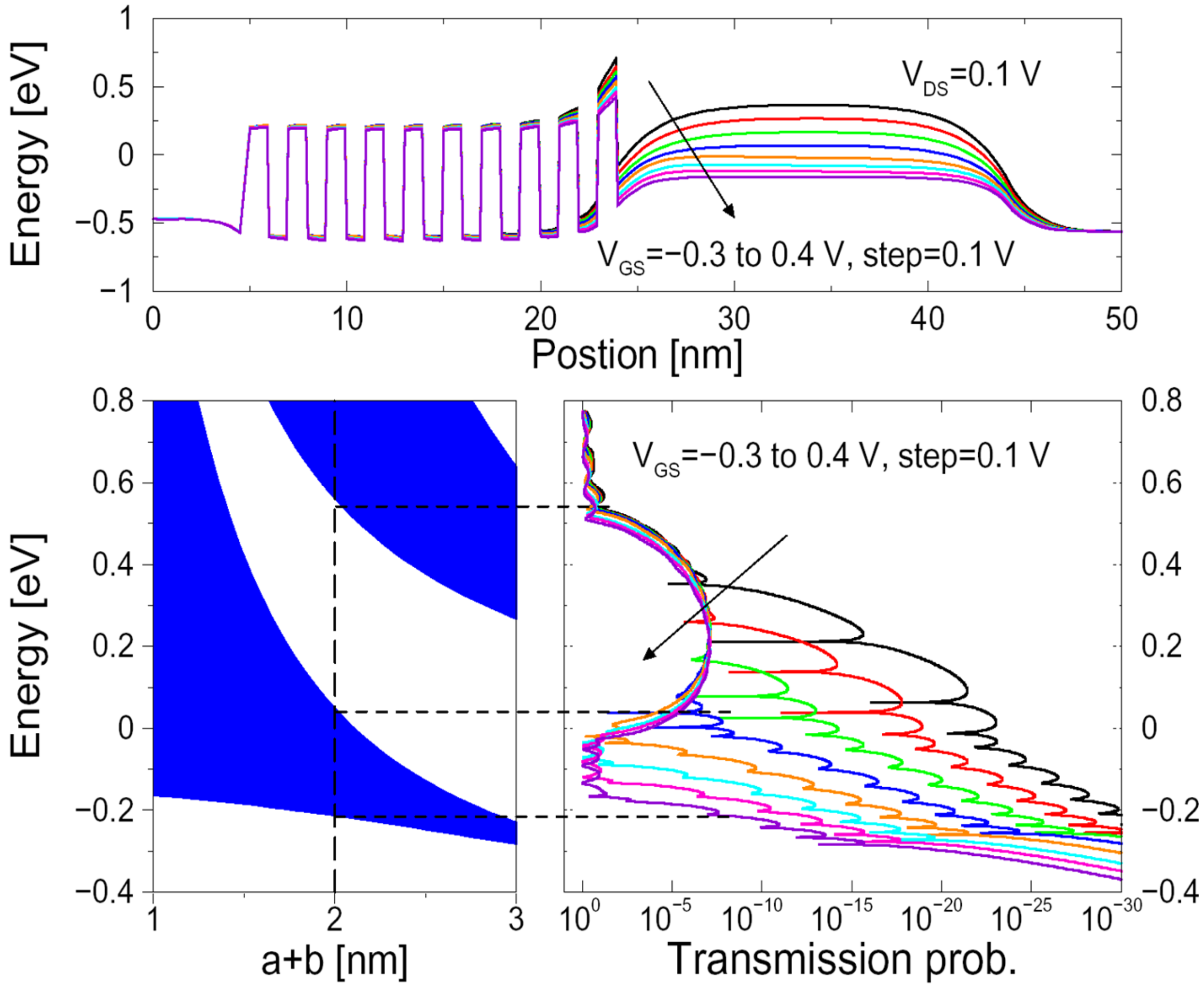
Self consistent simulation





- Self-consistent solution of the open-boundary Schrödinger-Poisson problem.
- Effective mass approximation with cylindrical coordinates.
- Every region characterized by its specific transport mass, dielectric constant and electron affinity.
- Energy-adaptive mesh in order to achieve an accurate description of the resonant states generated within the superlattice.

Superlattice minibands



Two regions where the transmission probability is close to one

They correspond to the minibands given by the Krönig-Penney model.

This very simple model provides surprisingly good results, despite the inherent assumption of an infinite number of spatial periods.

Superlattice Steep-Slope FET: Discussion

- We have presented an investigation on a novel device concept meant to achieve a steep subthreshold slope by filtering out the high-energy electrons entering the device.
- The filtering function is entrusted to a superlattice in the source extension region.
- The structure could possibly be fabricated by deposition of a number of appropriate semiconductor layers within a manufacturing process of vertical nanowires.
- Simulation results indicate that an SS = 26 mV/dec can be achieved using GaAs/AlGaAs as the constituent materials of the superlattice.
- Major improvements are possible with the appropriate selection of the semiconductor pair, e.g. the GaN/AlGaN system

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From Quantum Mechanics for CMOS to Advanced Optical Simulation

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2.Light in Nano-Scale Optoelectronics: the Macroscopic Maxwell Equations

$$\nabla \cdot \mathbf{B} = 0 \quad \nabla \cdot \mathbf{D} = \rho$$

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \quad \nabla \times \mathbf{H} - \frac{\partial \mathbf{D}}{\partial t} = \mathbf{J}$$

Assume: $\mathbf{D}(\mathbf{r}) = \varepsilon_0 \varepsilon(\mathbf{r})\mathbf{E}(\mathbf{r})$, $\mathbf{B}(\mathbf{r}) = \mu_0 \mu(\mathbf{r})\mathbf{H}(\mathbf{r})$, $\mu(\mathbf{r}) \approx 1$

$\mathbf{H}(\mathbf{r}, t) = \mathbf{H}(\mathbf{r})e^{-i\omega t}$, $\mathbf{E}(\mathbf{r}, t) = \mathbf{E}(\mathbf{r})e^{-i\omega t}$. $\rho=0$, $\mathbf{J}=0$

So

$$\nabla \cdot \mathbf{H}(\mathbf{r}) = 0 \quad \nabla \cdot \left[\varepsilon(\mathbf{r})\mathbf{E}\right] = 0$$

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$$\nabla \times \mathbf{E}(\mathbf{r}) - i\omega\mu_0 \mathbf{H}(\mathbf{r}) = 0 \qquad \nabla \times \mathbf{H}(\mathbf{r}) + i\omega\varepsilon_0 \varepsilon(\mathbf{r}) \mathbf{E}(\mathbf{r}) = 0$$

$$\boxed{\nabla \times \left(\frac{1}{\varepsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) \right) = \left(\frac{\omega}{c} \right)^2 \mathbf{H}(\mathbf{r})}$$

If $\varepsilon(\mathbf{r})$ have no imaginary part, the operator Ξ:

$$\hat{\Xi}\mathbf{H}(\mathbf{r}) = \nabla \times \left(\frac{1}{\varepsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) \right)$$ is **Hermitian** operator.

This equation is fully analog to Schrodinger equation. So, to solve ***Maxwell*** equations with this conditions we can apply the same formalism and methods as for the ***Schrodinger*** equation and vice versa. This fact is widely used for theory and modeling **photonic crystals**.

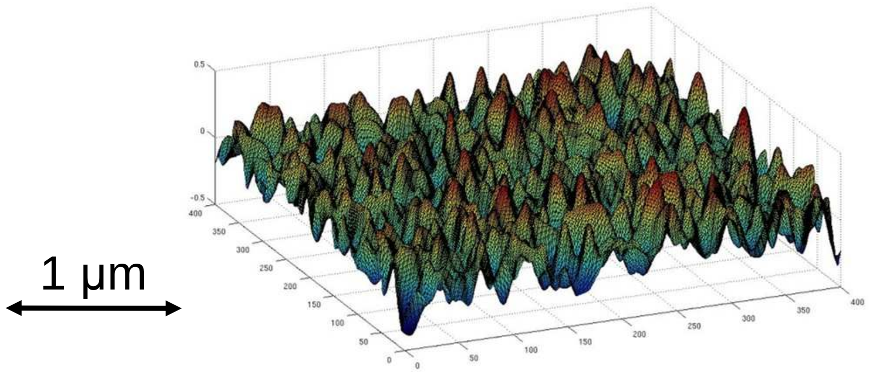
See for example:

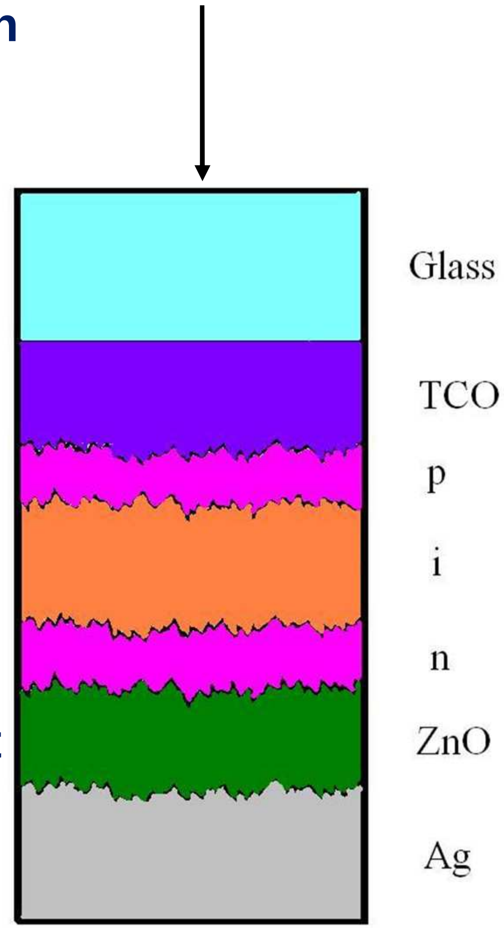
Joannopoulos J., Johnson S.G., Winn J.N., Meade R.D., Photonic Crystals. (Second edition), Princeton Univ. Press, Princeton (2008).

If $\varepsilon(\mathbf{r})$ have nonzero imaginary part, the operator Ξ is not **Hermitian** but most of the techniques from quantum theory still work with minor changes. For example **T-*matrix*** or **S-*matrix*** formalism.

Advanced Optical Simulation: Introduction

- **Photon management required to enhance the absorption**
- **Advanced optical modeling to deal with:**
  - **Multi-layer thin structures (10nm÷1000nm)**
  - **Nano-metrics rough interfaces**





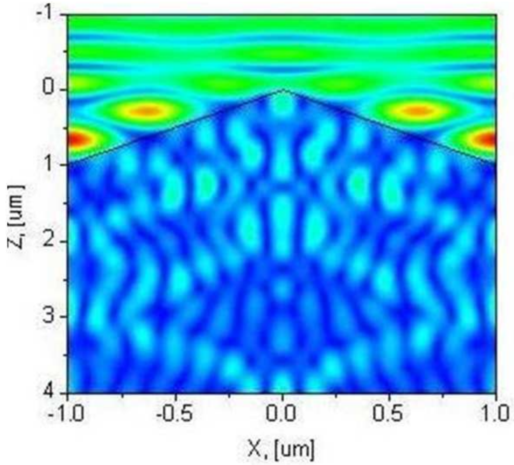
- **Near field optics requires rigorous approaches that implies the solution of the Maxwell equations.**
- **Trade-off between accuracy and computational resources.**
- **RCWA (Rigorous Coupled Wave Analysis) leads to efficient and numerically stable solvers of Maxwell equations.**

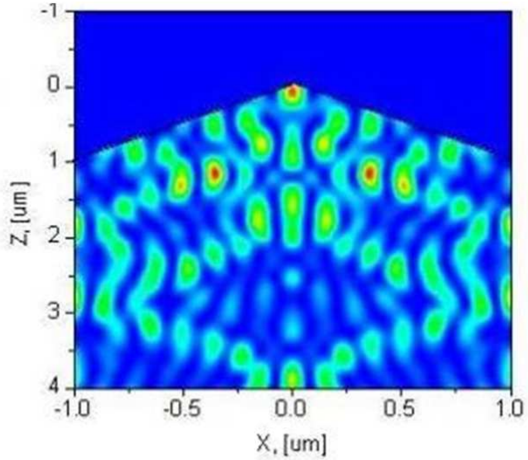
I. [illegible] M. Zanuccoli, V. Vyurkov, E. Sangiorgi, C. Fiegna, "*Efficient [illegible] of the Fourier Modal Method (RCWA) for the Optical [illegible] Optoelectronics Devices***", IWCEI 2010**

Applications: Triangular Groove (2-D)

1

TE, E





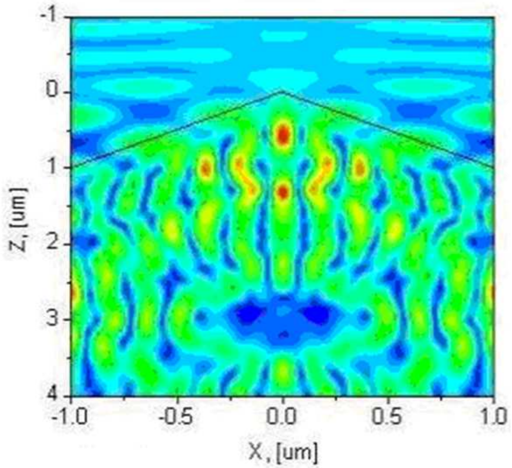
2

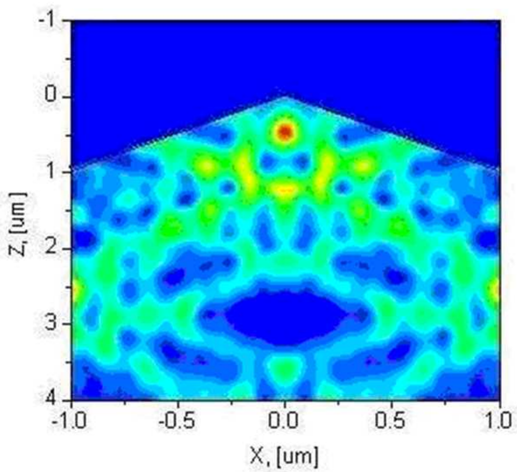
TE, Abs

λ=738nm, $M_x = 30$

3

TM, H





4

TM, Abs

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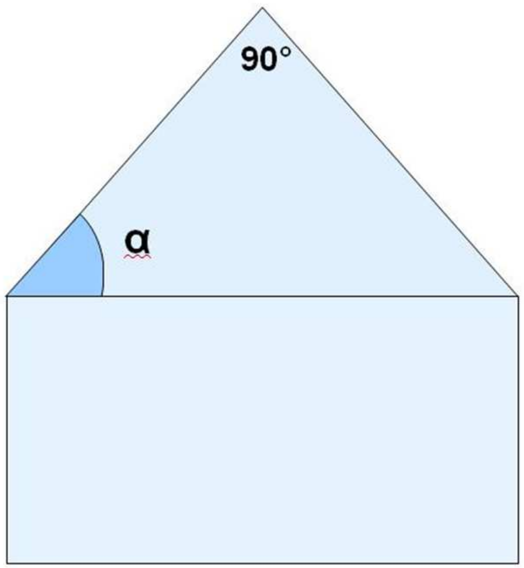
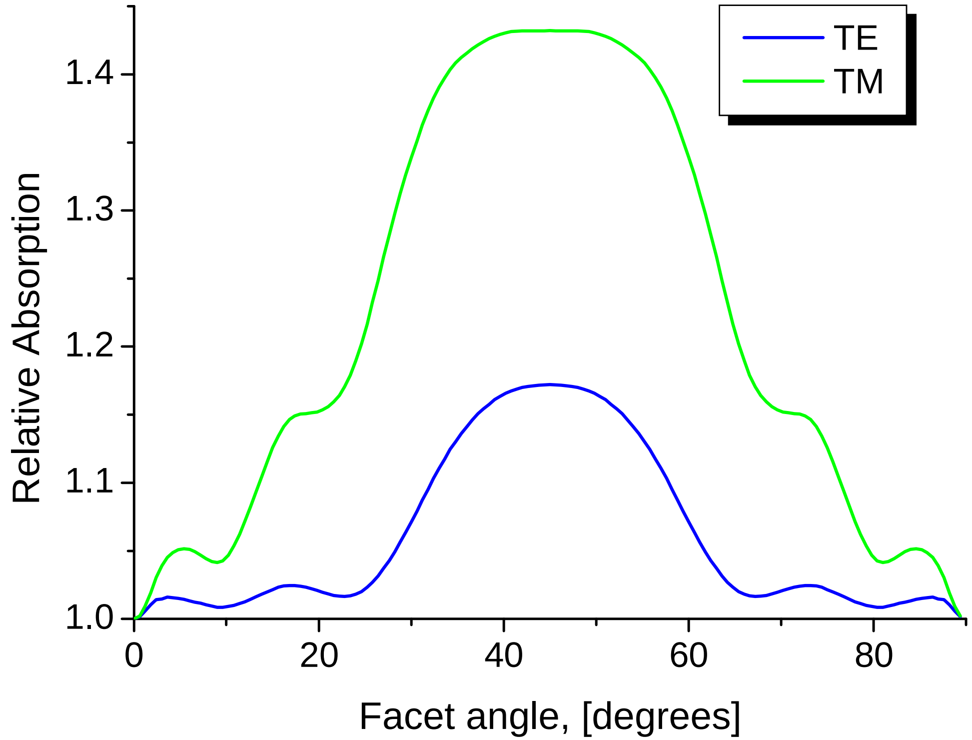
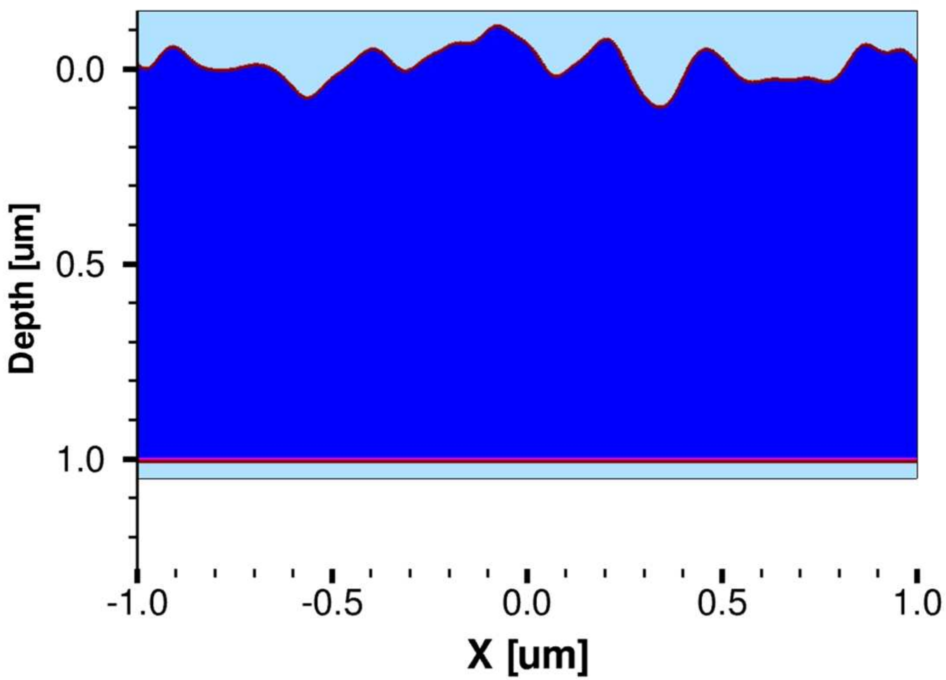
Applications: triangular groove
(2D periodic texturing for solar cells)

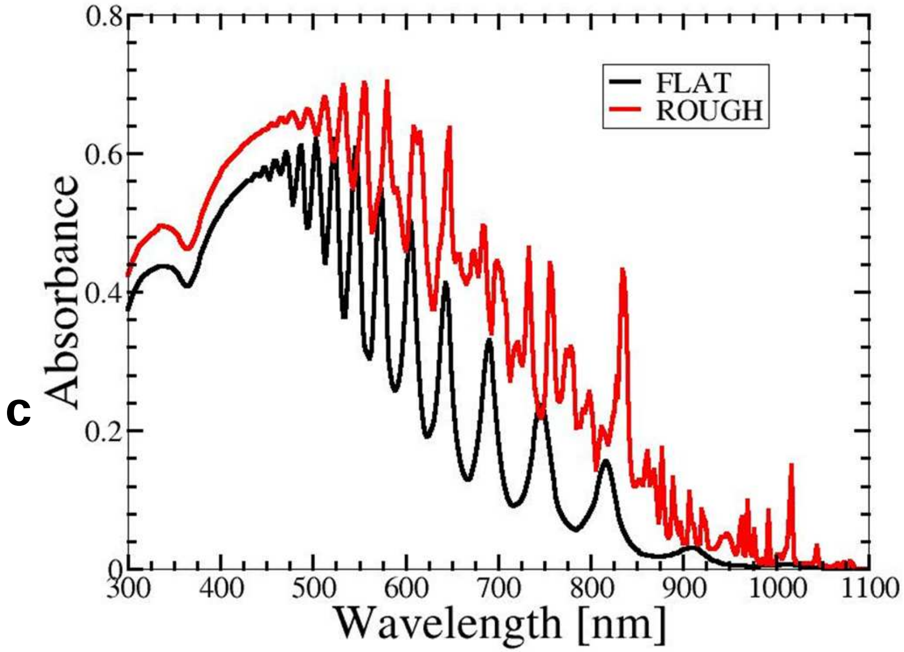
- Dependence of relative absorption on facet angle α at λ=738nm.





Rough Interface Simulation





- **2-D geometry**
- **Gaussian distribution of heights**
- **Heigh (R.M.S.) = 50nm, Correlation Length = 75nm**