TiberCAD: towards multiscale simulation of optoelectronic devices

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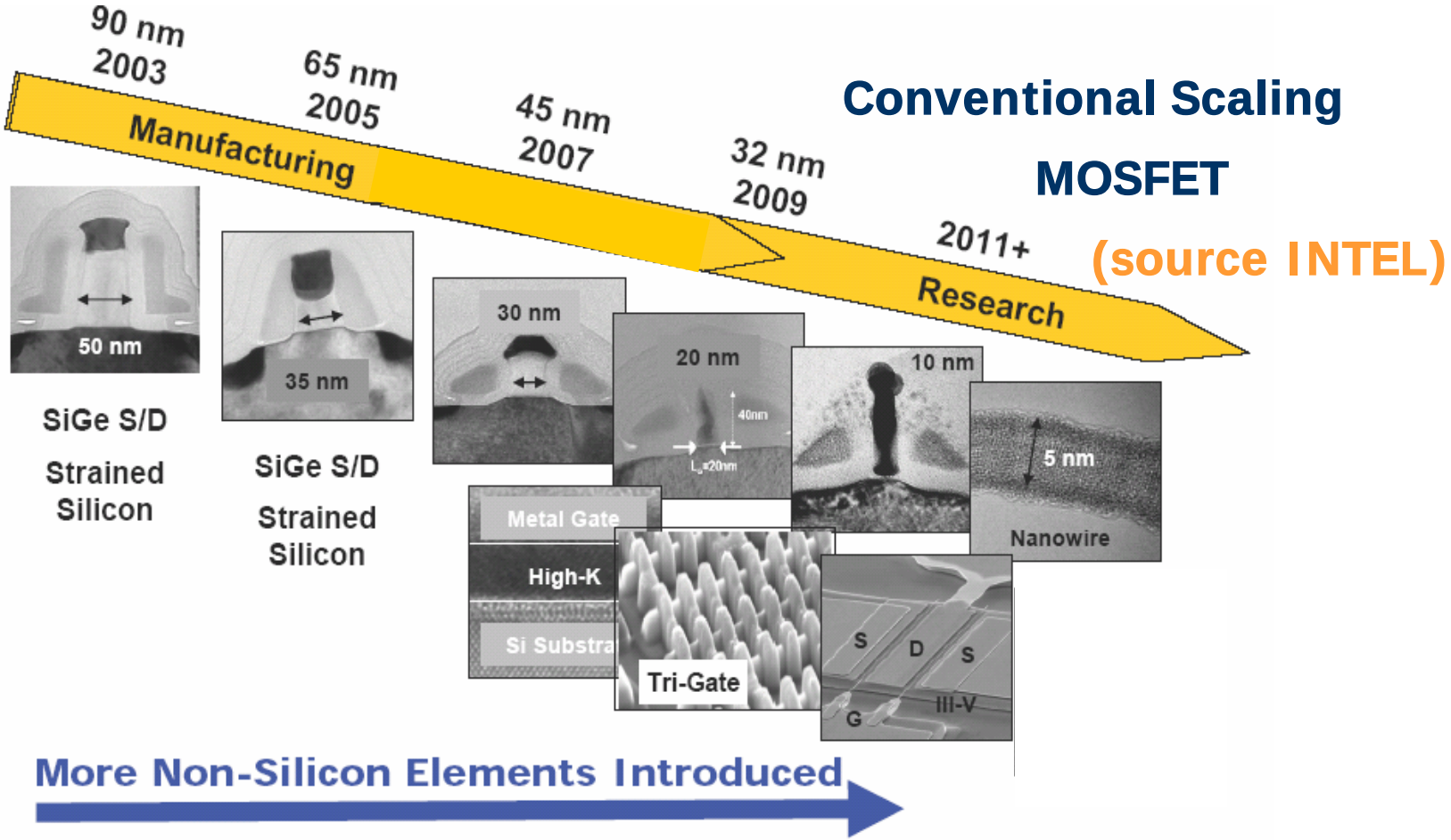
Human resources and mobility

Outline

- Introduction / the TiberCAD project
- Physical models
- Numerical implementation / Software structure
- Simulation examples
- Conclusions

Introduction: What's new in electronic devices



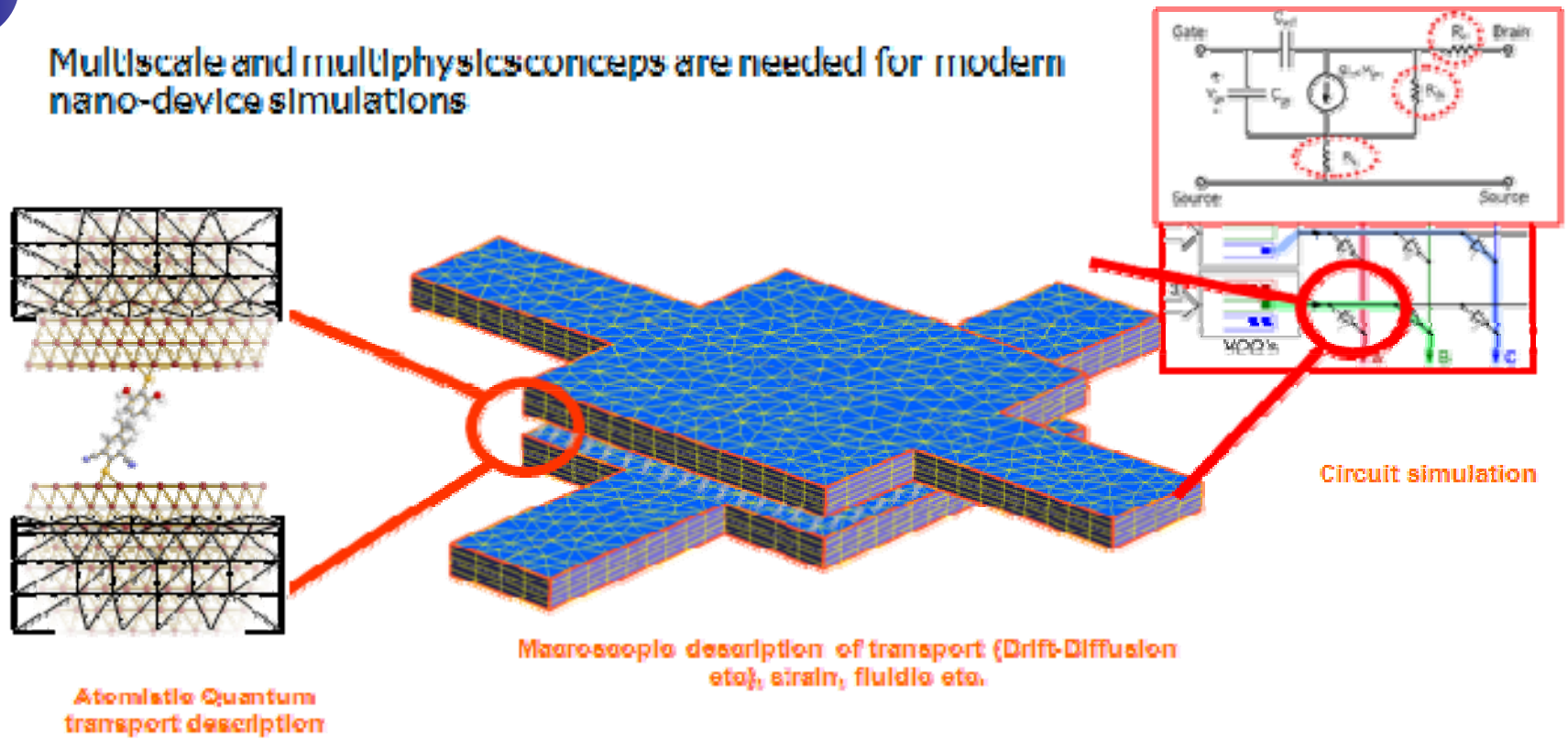
Manufacturing cost increases

TCAD request increases

TCAD complexity increases

Introduction: Multiscale scenario

Multiscale and multiphysicsconceps are needed for modern nano-device simulations



Atomistic — Quantum-classical interfaces — Continuous

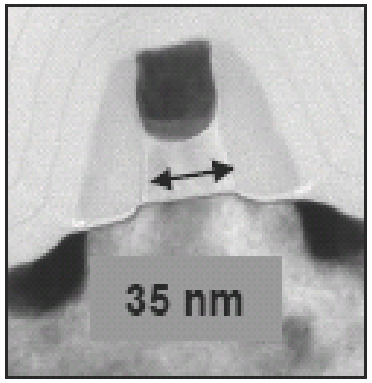
Physics — Engineering

The multiscale approach, quite common in material science, has not been used systematically for electronic transport !

Introduction: Multiphysics

Different physical models are needed to describe electronic devices:

MOSFET

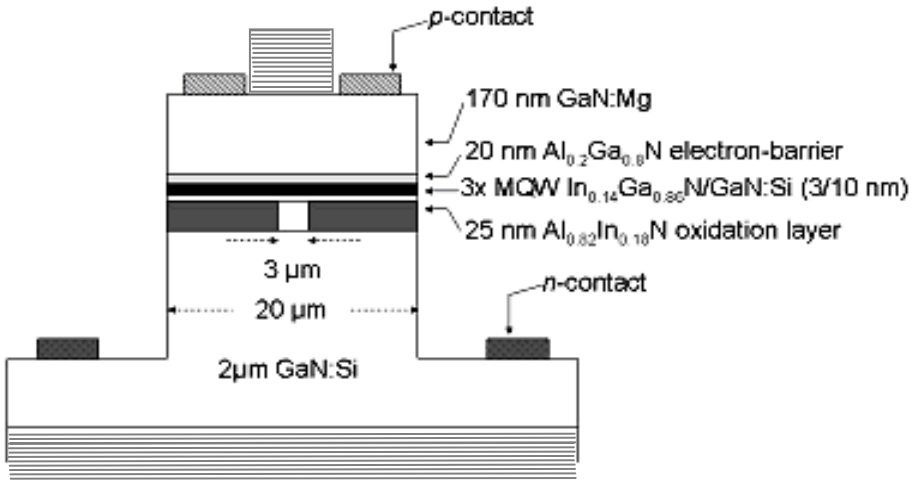


SiGe S/D

Strained Silicon

- ***Classical/Quantum transport***
- ***Strain***
- ***Temperature***
- ***Atomistic details***

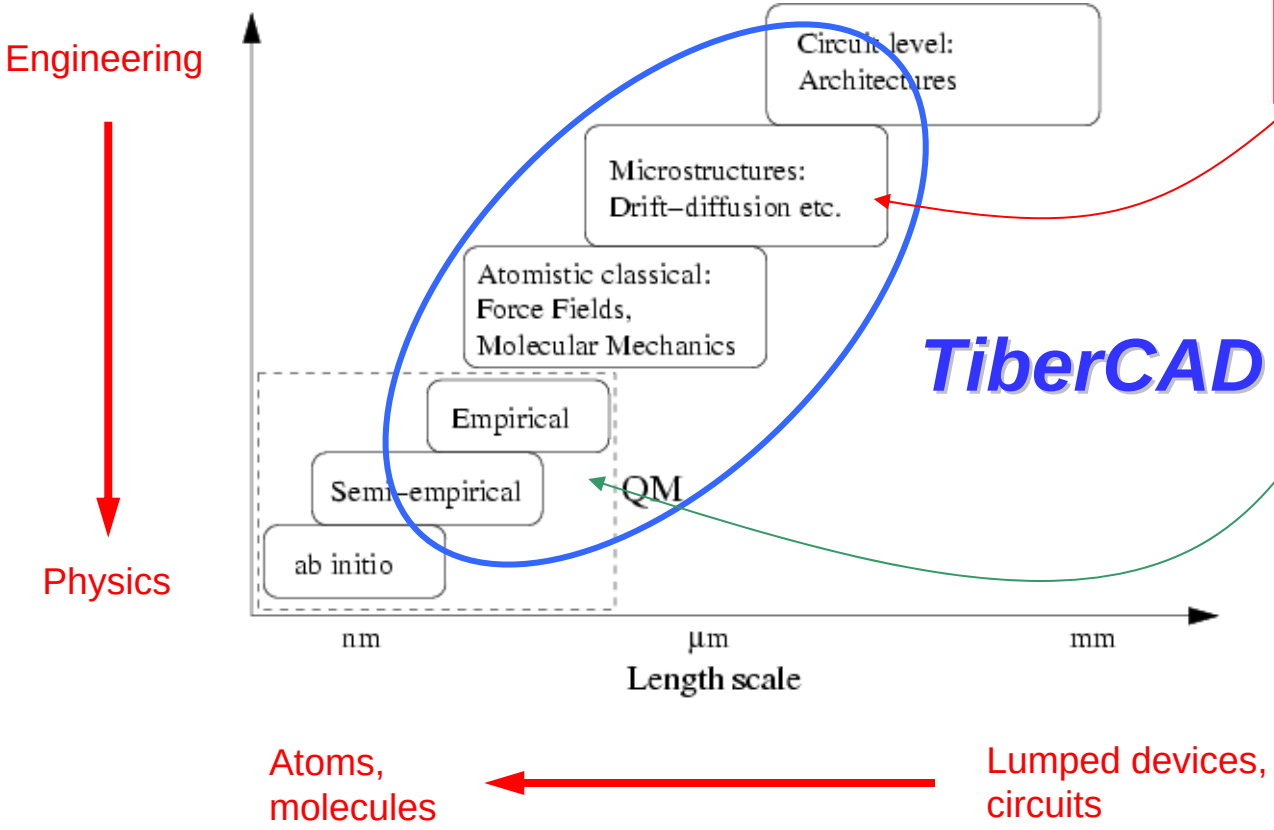
Polariton/VCSEL



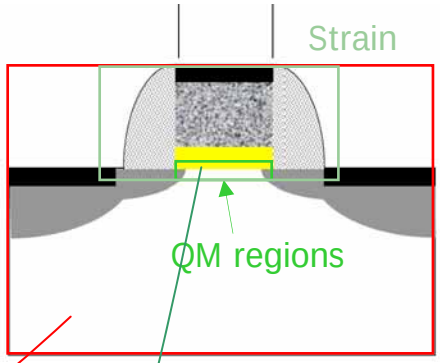
- ***Classical/Quantum transport***
- ***Electrons/holes/excitons (polaritons)***
- ***Strain***
- ***Temperature***
- ***Electromagnetic field***

Introduction: Multiscale/multiphysics

- The different simulation scales:



Example:



Physical Models: strain (linear)

define shape

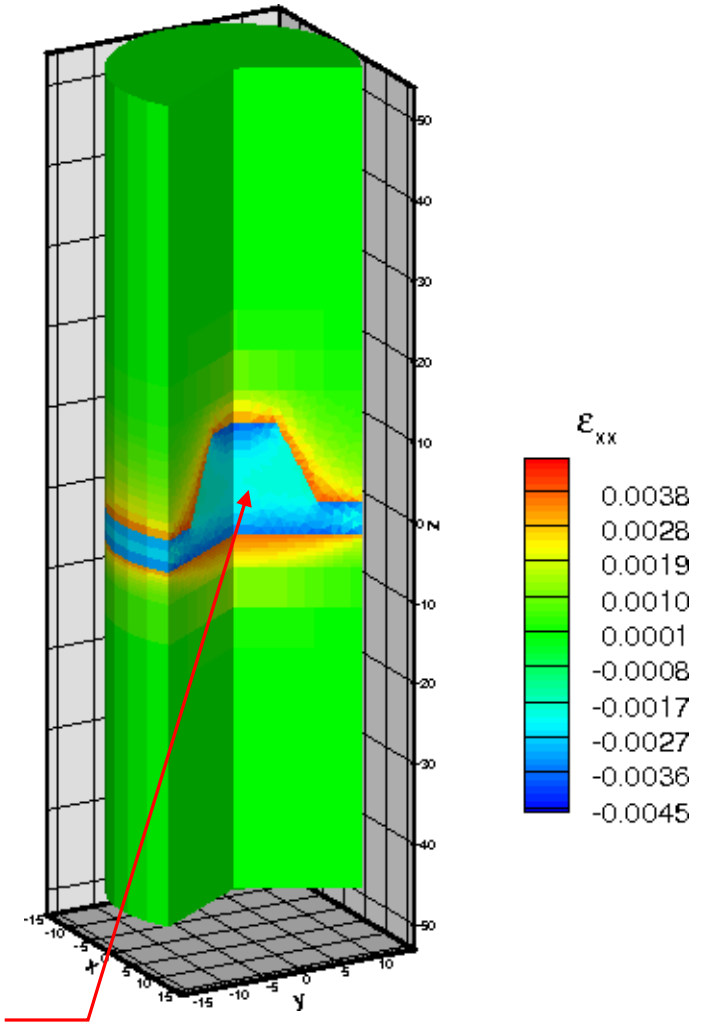
$$\varepsilon_{ij}^{0} = \delta_{ij} \frac{a_i^S - a_i}{a_i}$$

Minimization of the elastic energy

$$\frac{\partial}{\partial x_i}\left(C_{ijkl}(\mathbf{r})\left(\frac{\partial u_k}{\partial x_l} + \varepsilon_{kl}^{n}(\mathbf{r}) \right) \right) = 0$$

Strain tensor

$$\varepsilon_{ij}^{n} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$



GaN dot in AlGaN nanocolumn

Povolotskyi-Di Carlo, JAP **100**, 063514 (2006)

Physical Models: strain (non-linear)

self-consistency cycle

define shape

$$\varepsilon_{ij}^{0} = \delta_{ij}\frac{a_i^S - a_i}{a_i}$$

$$\frac{\partial}{\partial x_i}\left(C_{ijkl}(\mathbf{r})\left(\frac{\partial u_k}{\partial x_l} + \varepsilon_{kl}^{n}(\mathbf{r})\right)\right) = 0$$

$$\varepsilon_{ij}^{n} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \varepsilon_{ij}^{n-1}$$

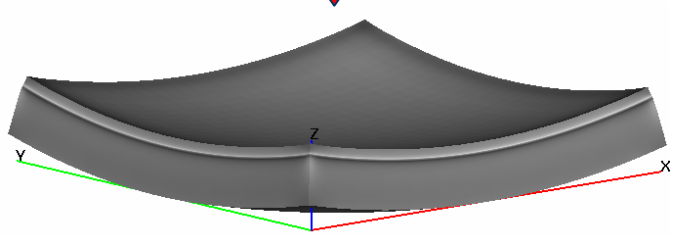
define new shape by moving nodes

$$\vec{r} \rightarrow \vec{r} + \vec{u}$$

$\|\vec{u}\| > \delta$ — yes

stop

Free-standing AlGaN/GaN



Povolotskyi-Di Carlo, JAP **100**, 063514 (2006)

Physical Models: Particle transport

- Particle transport is treated in the drift-diffusion approximation
  - Particle flux is written in terms of the electro-chemical potentials, eg.

$$j_n = \mu_n n \nabla \phi_n, \quad j_p = -\mu_p p \nabla \phi_p$$

  - Particle densities are modeled assuming local equilibrium, eg. electrons:

$$n = N_c F_{1/2}\left(\frac{\phi_n - E_c}{k_B T}\right)$$

→ – Band parameters are calculated from **k·p** parametrisations including strain

  – For electrons/holes:

$$\nabla j_n = \nabla\left(\mu_n n \nabla \phi_n\right) = -R(n,p)$$
$$\nabla j_p = \nabla\left(-\mu_p p \nabla \phi_p\right) = -R(n,p)$$

+ Poisson equation $\nabla\left(\varepsilon \nabla \varphi - P\right) = e(n - p + N_a^- - N_d^+)$

Piezo- and pyropolarization

- Exciton transport is implemented in TiberCAD and can be coupled to electron/hole transport by means of exciton generation/dissociation

Physical Models: Thermal transport

- Self-heating is a critical issue for high-power devices, but also in highly integrated circuits (could be limiting factor)

- Implementation of thermal transport is based on a thermodynamic model

  Continuity equation for the energy flux j^u:

$$\frac{\partial u}{\partial t} - \nabla j^u = \left(\frac{\partial u}{\partial t}\right)_{rad} \Rightarrow c\frac{\partial T}{\partial t} + \nabla(\kappa \nabla T) = H$$

Heat source term can be decomposed into different contributions:

- Joule
- Peltier-Thomson
- Generation-recombination effect

- Electron/hole flux has to be rewritten to include Seebeck effect:

$$j_n = \mu_n n\left(\nabla\phi_n + P_n \nabla T\right)$$
$$j_p = -\mu_p p\left(\nabla\phi_p + P_p \nabla T\right)$$

$P_{n,p}$: thermoelectric powers

Physical Models: Quantum mechanics

- Quantum mechanical models are based on envelope function approximation (single- and multiband **k·p** approach):
  - Expand the single particle states in bulk Bloch states

$$\psi(\mathbf{r}) = \sum_n f^n(\mathbf{r}) u^n_{\mathbf{k}=0}(\mathbf{r})$$

  - Solve a Schrödinger equation for the envelope functions

$$\hat{H}\vec{f} = E\vec{f}, \quad \text{eg.} \quad -\frac{\hbar^2}{2}\nabla\left(\frac{1}{m(r)}\nabla f_c(r)\right) + E_c(r) f_c(r) = E f_c(r)$$

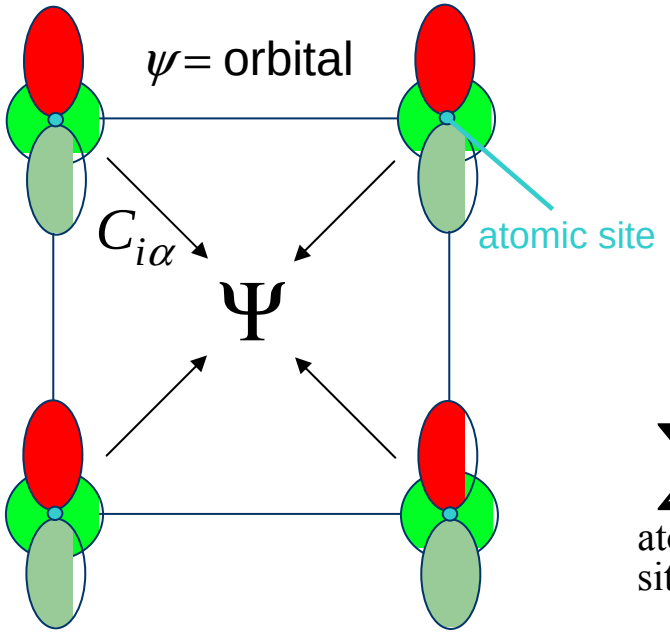
  - ✓ Calculate eigenstates of confined particles
  - ✓ Calculate optical transition probabilities
  - ✓ Calculate valence and conduction band parameters in presence of strain
  - ✓ Calculate quantum mechanical particle density:

$$n = \sum_i \sum_{\mathbf{k}\in \mathrm{BZ}} \left|\psi_{i,\mathbf{k}}(\mathbf{x})\right|^2 \frac{1}{1+\mathrm{e}^{(E-\mu_e(\mathbf{x}))/kT}}$$

Performed on an adaptative grid

Physical Models: Atomistics

- Tight-binding approach: expand wave function in atomic orbitals



$$\Psi(r) = \sum_{j,\alpha} C_{j,\alpha} \psi_{\alpha}(r - R_j)$$

Atomic site

Atomic orbital index

$$\sum_{\substack{\text{atomic} \\ \text{site, j}}} \sum_{\text{orbitals, } \beta} \left[H_{i\alpha,j\beta} - E S_{i\alpha,j\beta} \right] C_{j\beta} = 0$$

$$H_{i\alpha,j\beta} = \left\langle \phi_{i\alpha} \middle| H \middle| \phi_{j\beta} \right\rangle \qquad S_{i\alpha,j\beta} = \left\langle \phi_{i\alpha} \middle| \phi_{j\beta} \right\rangle$$

Matrix elements can be calculated by using density functional theory (DFTB in collaboration with Bremen, Frauenheim) or used as empirical fitting parameters (Empirical Tight Binding).

Implementation

TiberCAD implements:

- Strain (including piezoelectric effect)
- Semi-classical transport of electrons / holes / excitons (+ Poisson)
- Heat transport
- Quantum mechanics based on **k·p** envelope function approximation
- Atomistic description via Density Functional Tight-Binding (DFTB, from Frauenheim group, Bremen) or Empirical Tight-Binding, including Quantum Molecular Dynamics
- *Quantum transport (via NEGF) has not been fully integrated*

- *1D, 2D, 3D and cylindrical symmetry*
- *Adaptive meshes*
- *Written to run in parallel (but not yet tested)*
- *Input parser with a syntax similar to commercial TCAD*
- *Interfaces with some of commercial TCAD*
- *Possibility to link user defined models*

Implementation: Numerics

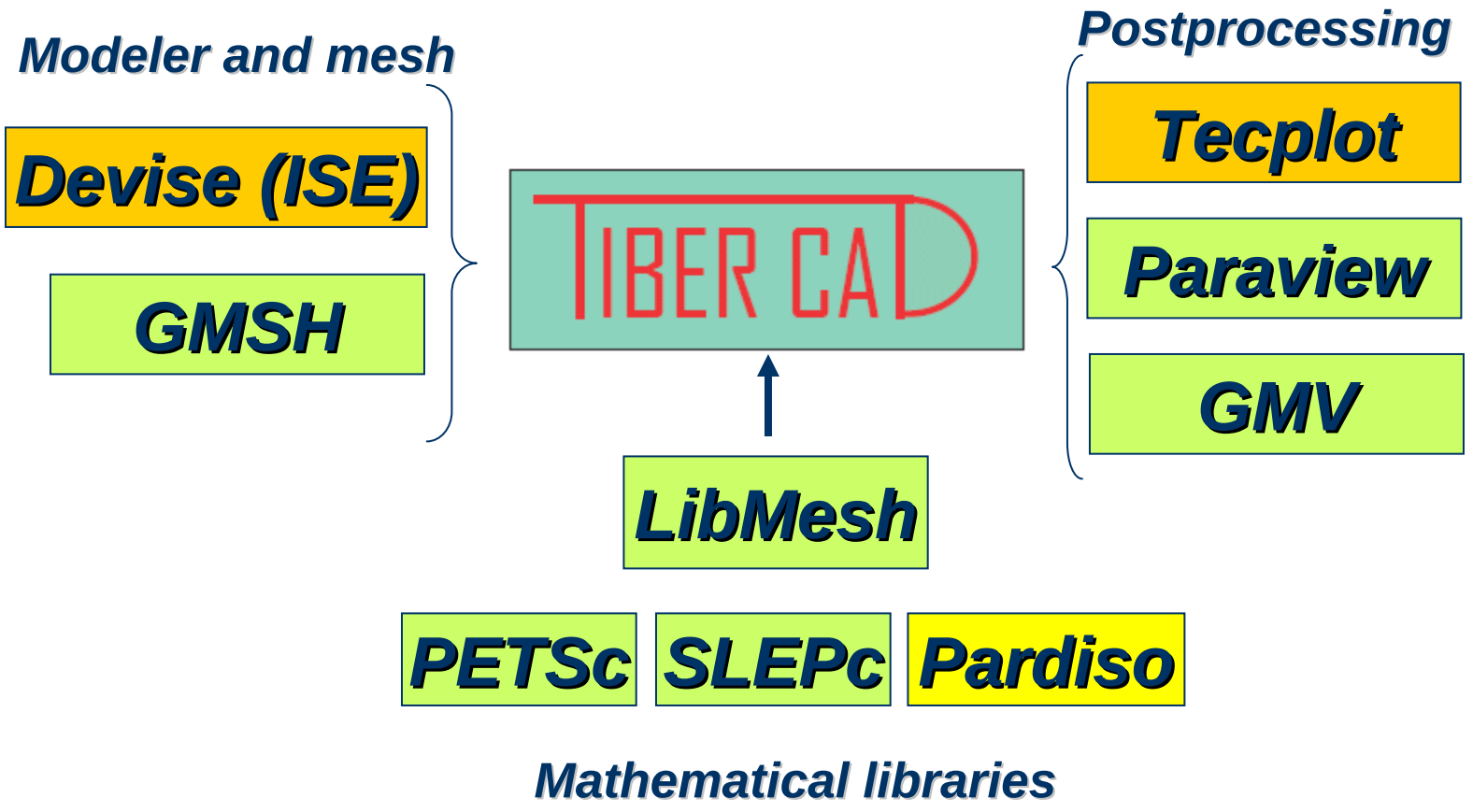
- All PDE based models are discretized by means of the **finite element method** (FEM) using the Fermi levels as variables!
  (in contrast to conventional approaches which us box integration and densities as variables)

- **ill-conditioned Jacobian** as the diffusion coefficients in the linearized continuity equations are proportional to the particle densities.
- The conditioning is improved by an appropriate **diagonal scaling**.
- The linear system is solved by means of **iterative solvers** (bi-conjugate gradient with ILU preconditioning), using the open-source library PETSc
- **Numeric Gauss integration** for integrals

Possible improvements:

- Further stabilization could be achieved using (pseudo-)residual-free bubbles
- Analytic integration where possible

Implementation: TiberCAD structure

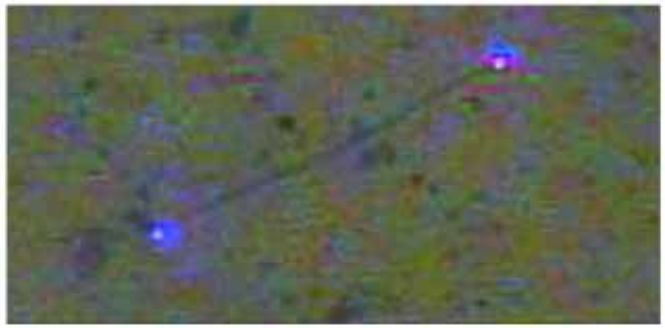


Development is done in Linux, porting to other UNIX-like environments is planned and to Windows has been achieved

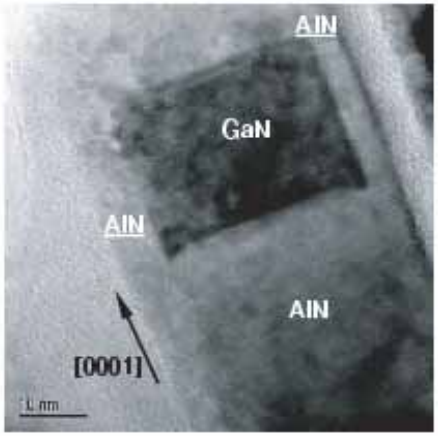
TiberCAD 1.0 is freely downloadable at www.tibercad.org

GaN/AlGaN nanocolumns

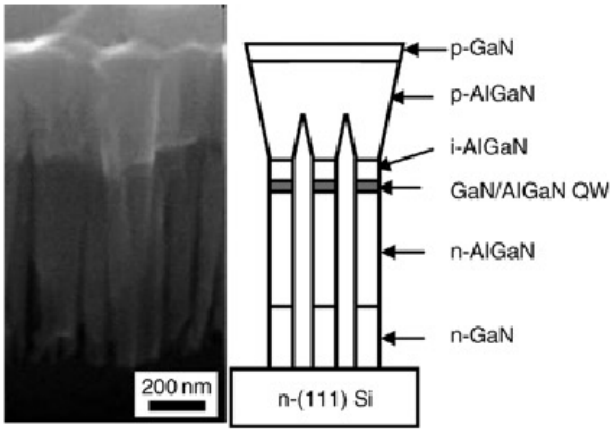
GaN/AlGaN nanowires are becoming important in LED and single photon source applications



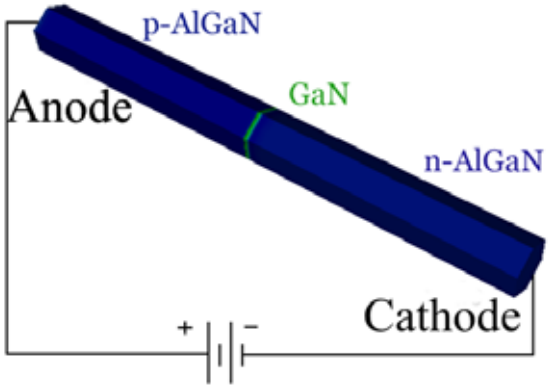
Johnson et al. Nature materials 1, 106 (2002)



Ristic et al. phys. stat. sol. 202, 367 (2005)

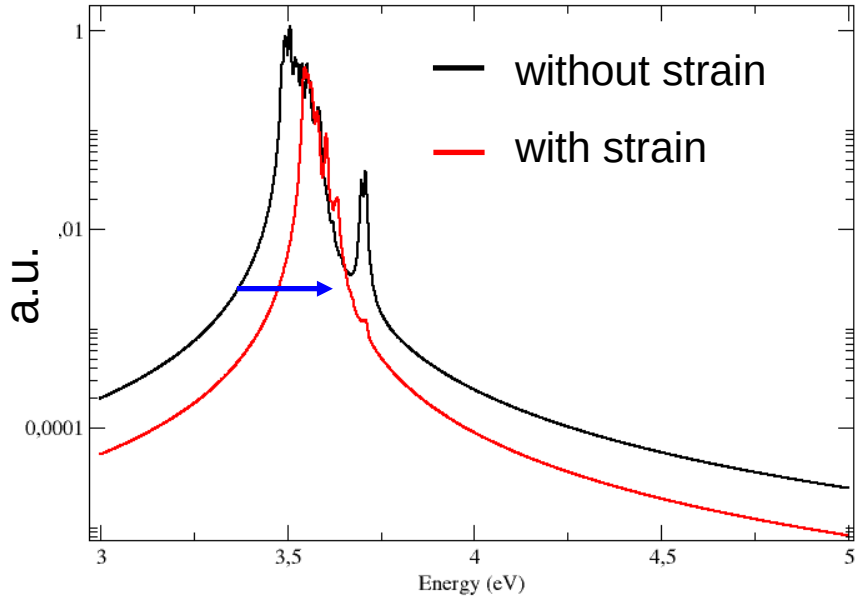


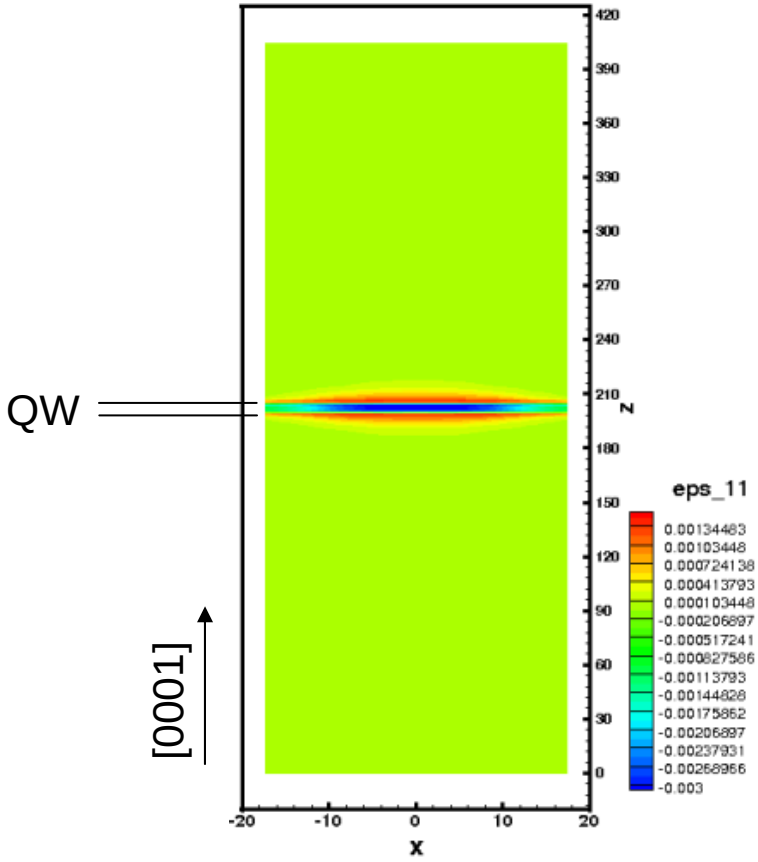
simulation



Sekiguchi et al. Electronics Letters (2008)

Nanocolumn: k•p emission spectra

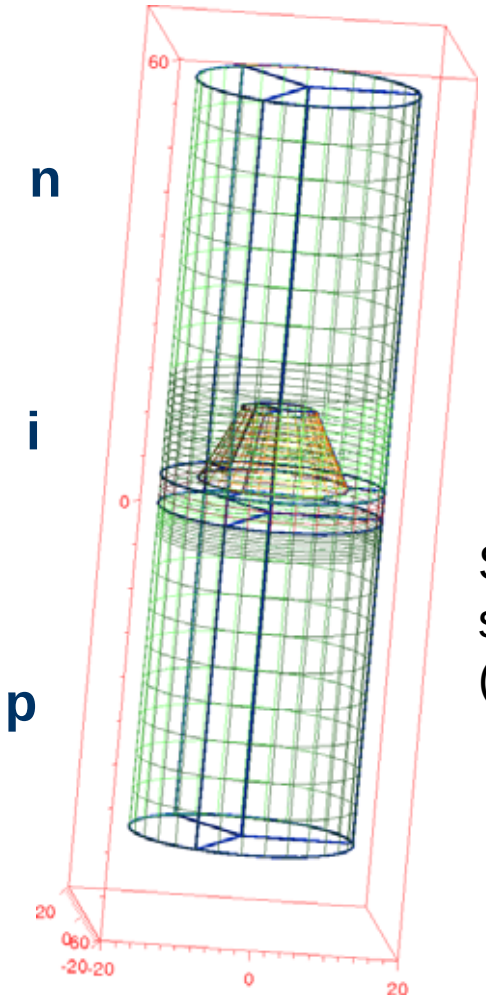


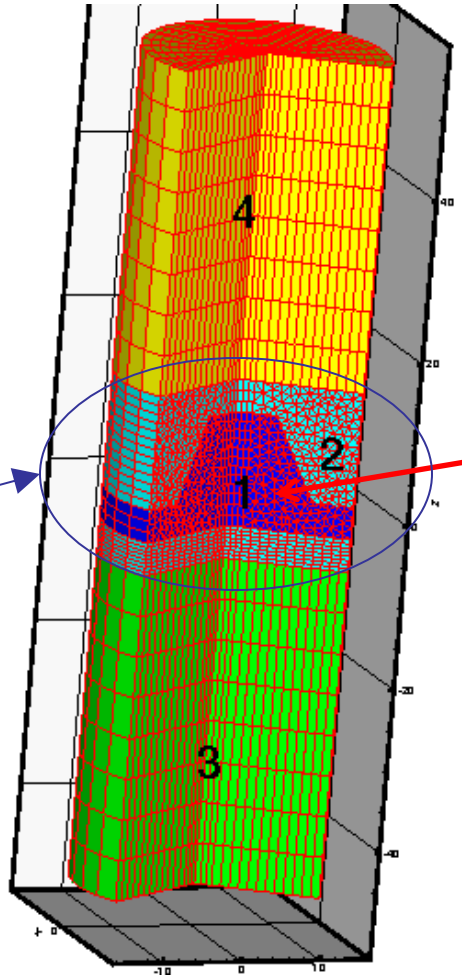


- 6x6 k.p model for valence band and single band for conduction band.
- modified Hamiltonian to include strain effects (Bir-Pikus)
- A blue shift is observed due to compressive strain

Conical GaN dot in nanowire

- 3D simulation of AlGaN nanocolumn with conic quantum dot
- solve strain, Drift-Diffusion/Poisson, self-heating and Schrödinger equation





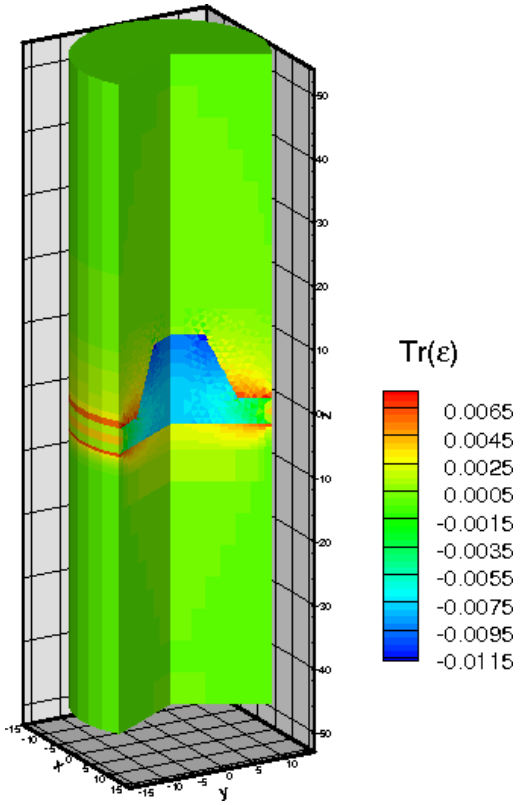
GaN quantum dot

Schrödinger is solved only here (region 1 + 2)

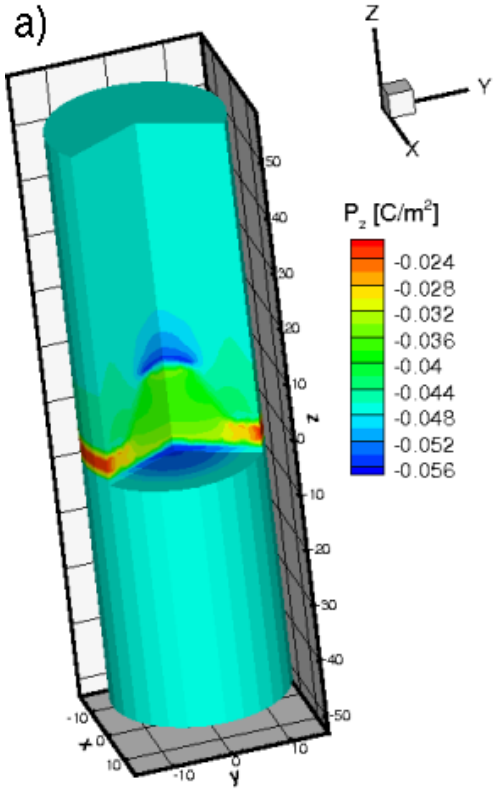
Conical $Al_{0.3}Ga_{0.7}N/GaN$ Quantum dot 5 nm-wide

Strain and Polarization

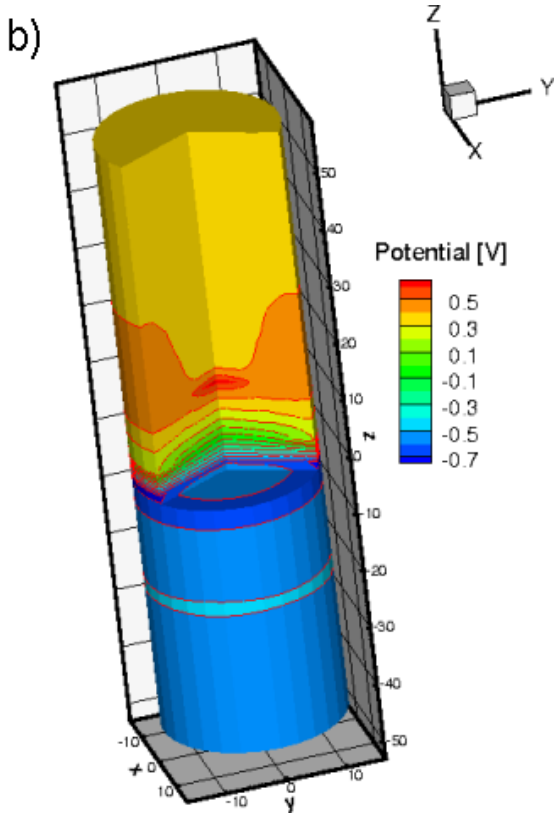
Strain - Rel. volumic change (dV/V):



Piezo- and Pyro-polarization P_z:

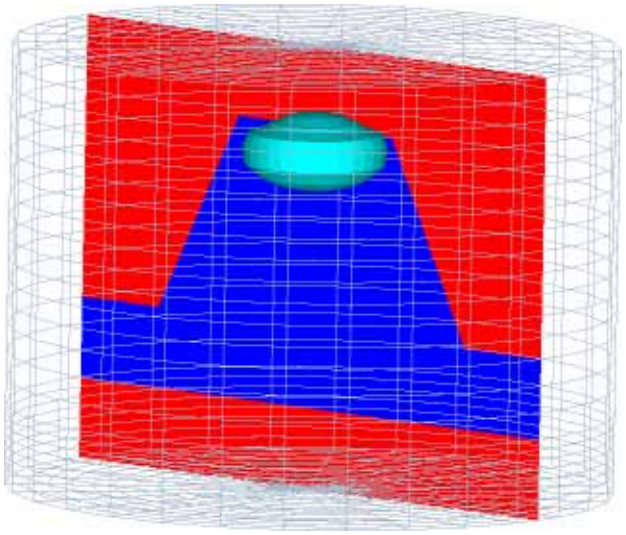


Electrostatic potential:

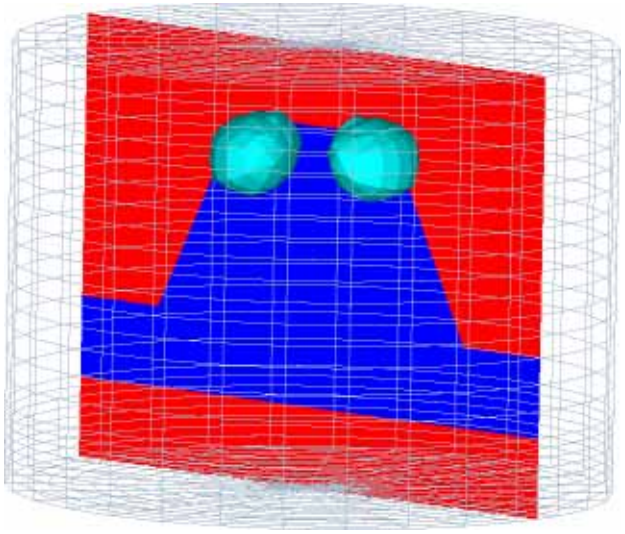


Quantum states

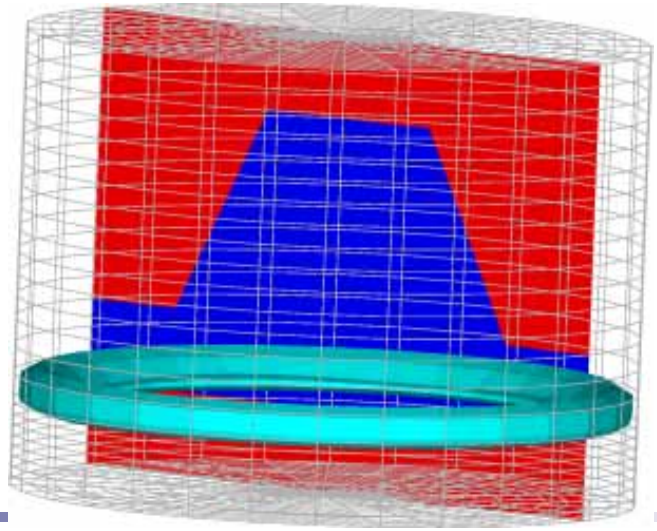
1st electron state:



2nd electron state:



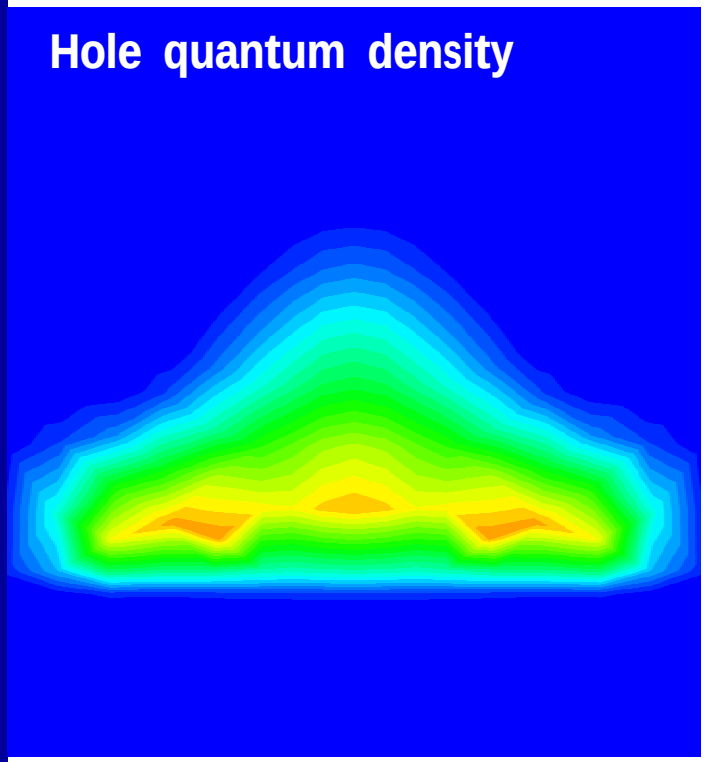
1st hole state:

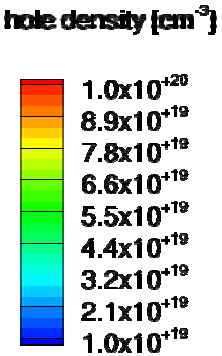


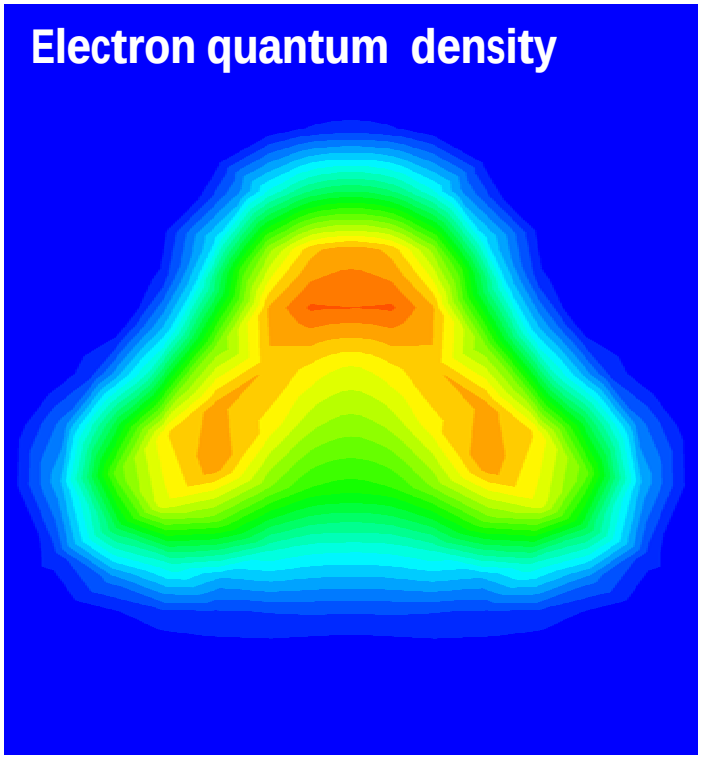
Spatial separation of electrons and holes mainly due to electric polarization

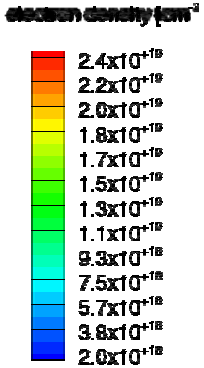
Charge density at 4.5 V

Quantum density in the dot

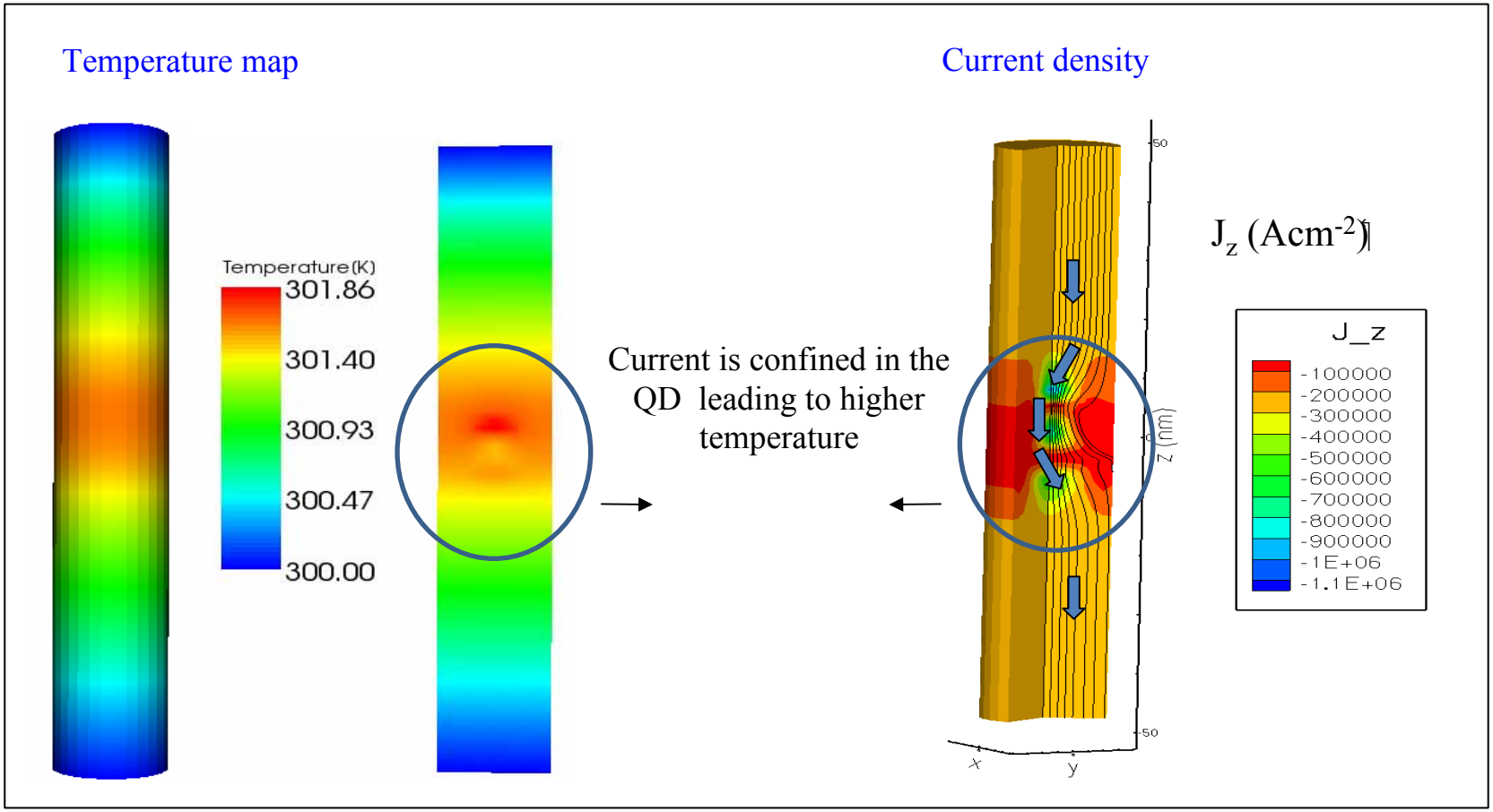




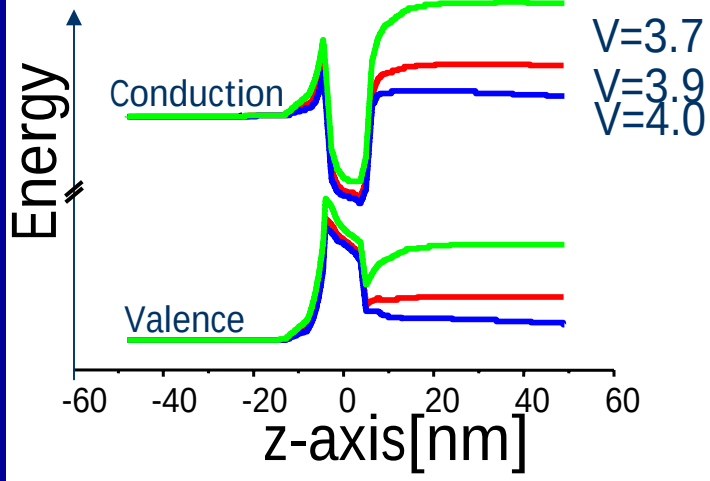


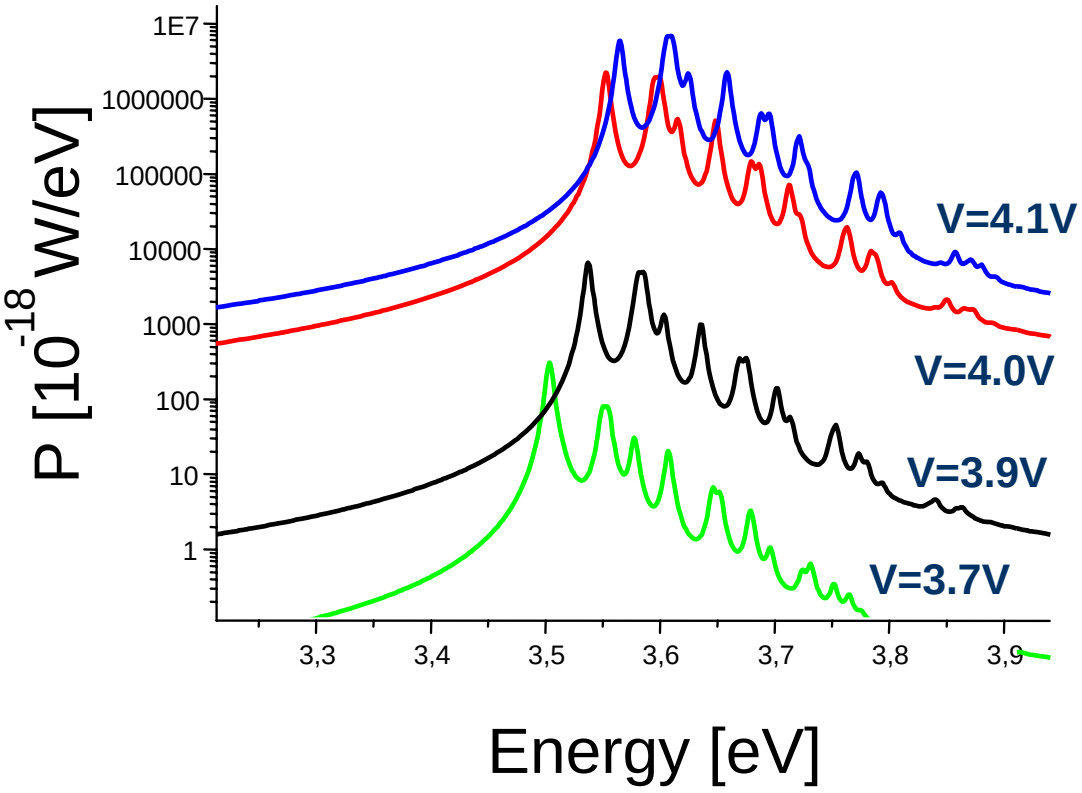


Temperature distribution



Electroluminescence of conic quantum dot



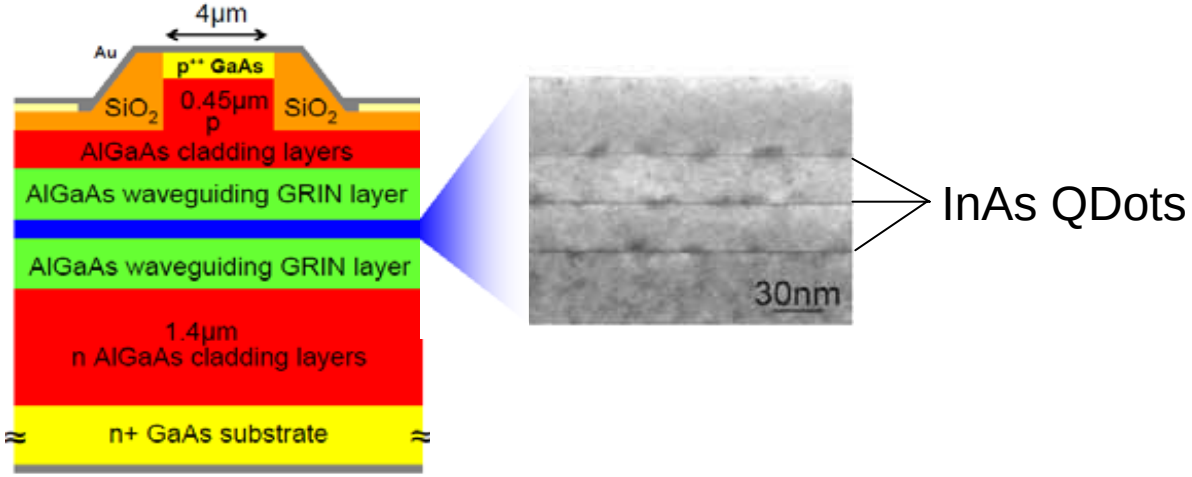


A 0.5 eV blue shift of the fundamental emission peak is obtained going from 3.7V (below threshold) to 4.1 (above threshold) due to the combined effect of polarization and screening .

Due to the screening of the polarization field we have also an increase of the optical power

InAs quantum dot LASER

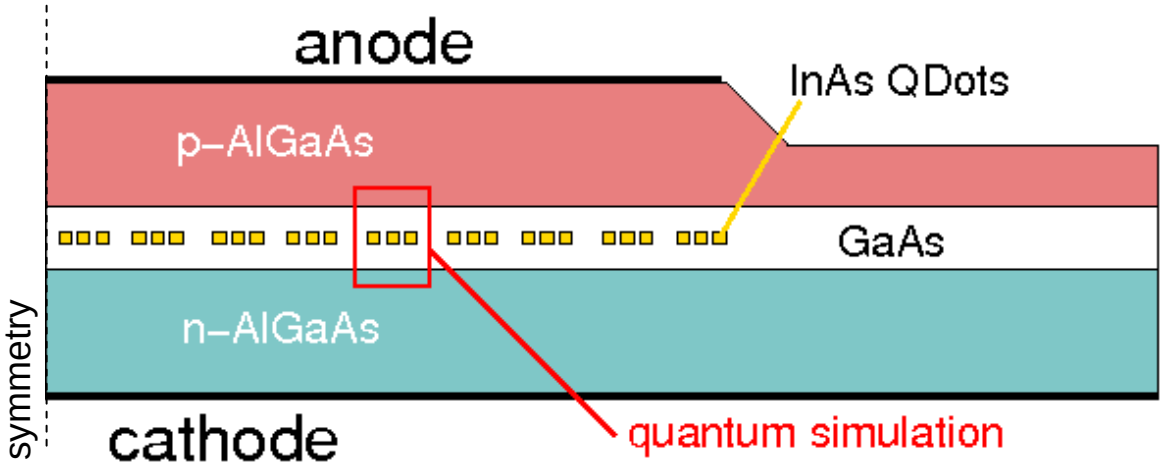
- 2D simulation of simplified InAs QDot LASER structure
- solve strain, Drift-Diffusion/Poisson and Schrödinger equation



M. Buda et. al., IEEE Journal of Quantum Electronics, 2003

Simplified structure for simulation:

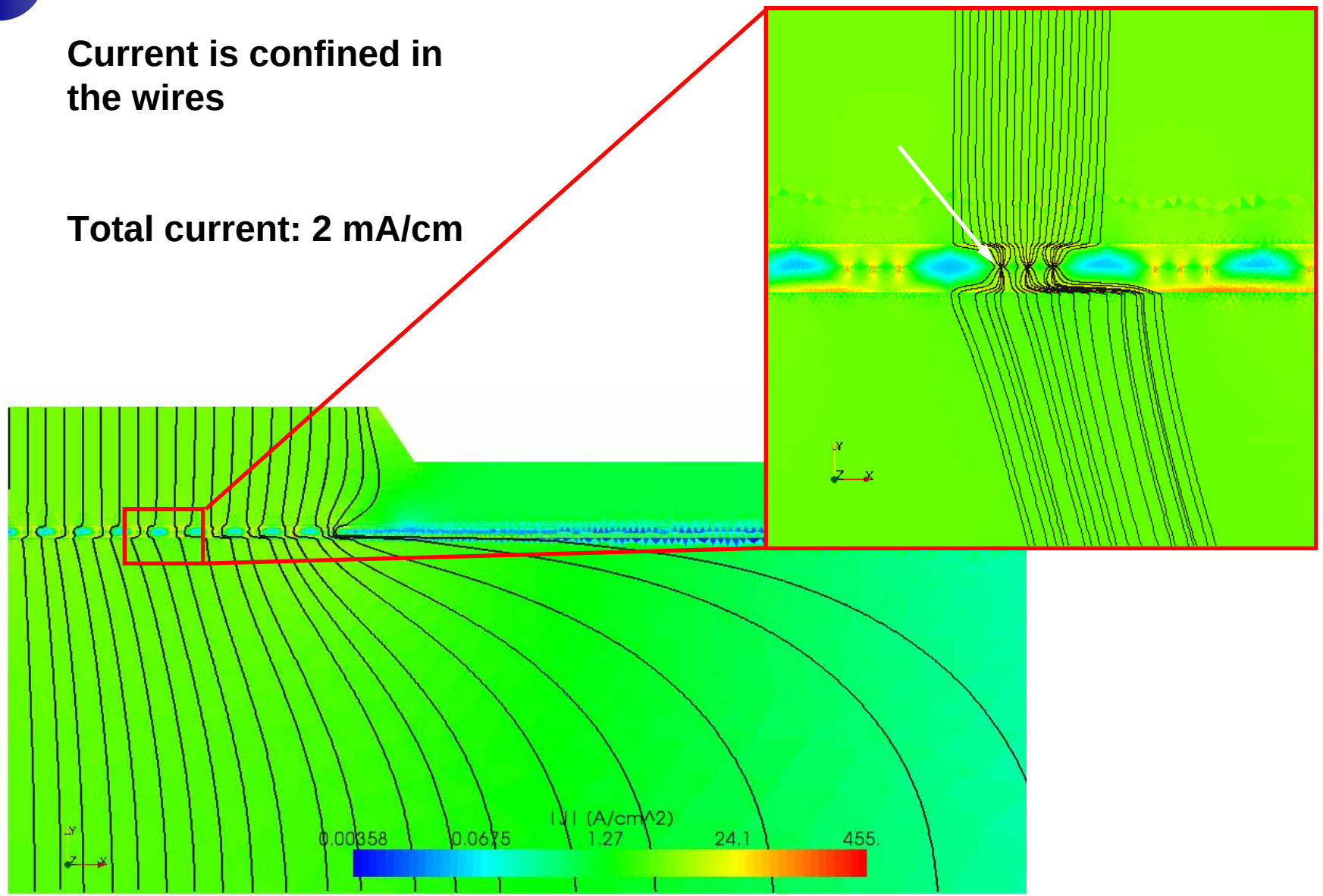
- We simulate wires instead of dots (2D simulation)



Current density at 1 V

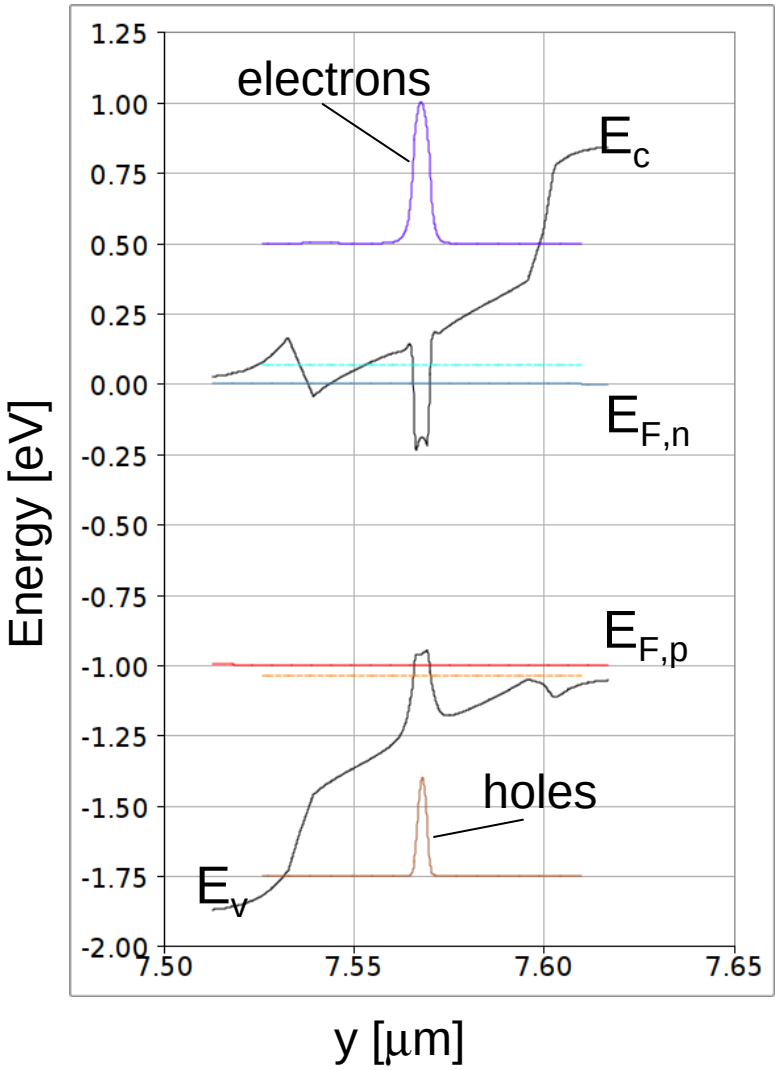
Current is confined in the wires

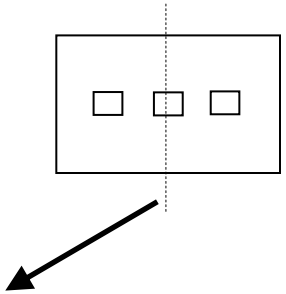
Total current: 2 mA/cm



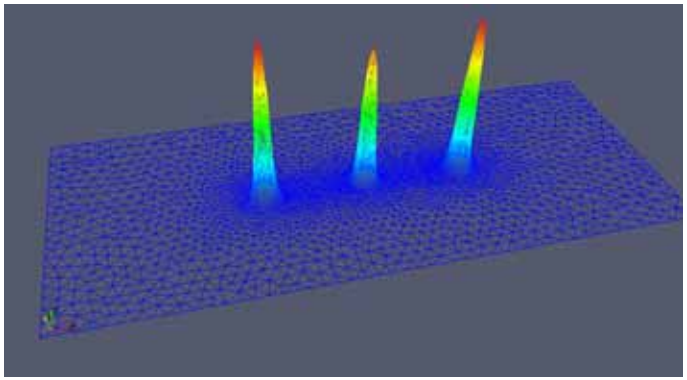
Emission spectra

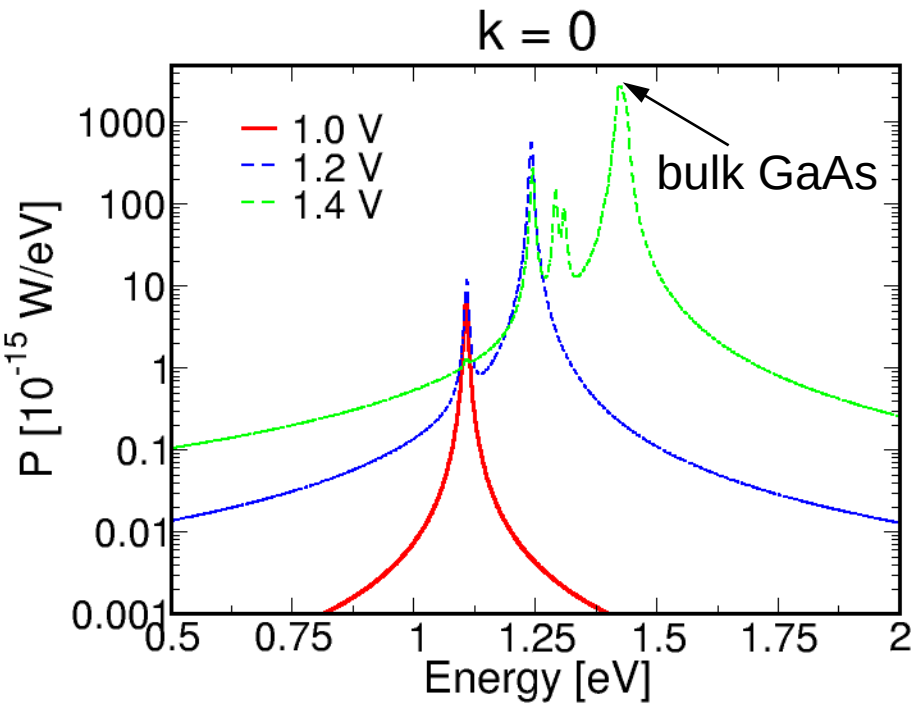
Band profile @ 1 V





Confined electron states





Conclusions and outlook

- Multiscale/multiphysics is requested in real modern electronic devices where electronics, optics, chemistry (and biology) are linked together
- TiberCAD is one of the first attempts to respond to this request
- Much effort is still needed to arrive at a true multiscale integration for transport simulations

Additional details on http://www.tibercad.org