Computational Modeling of Semiconductor Nanostructures for Optoelectronics

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Acknowledgements

- CEP Group University of Kassel
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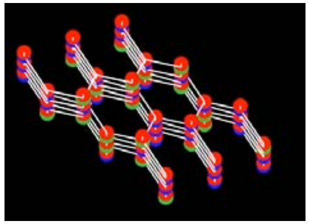
Computational Electronics and Photonics Group

Research:

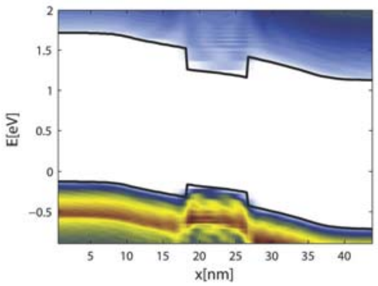
- Multi-Scale, Multi-Physics Computational Models for Design and Analysis of Electronic /Photonic (EP) Devices and Systems
- Research on Novel EP Concepts

GaN-Crystal



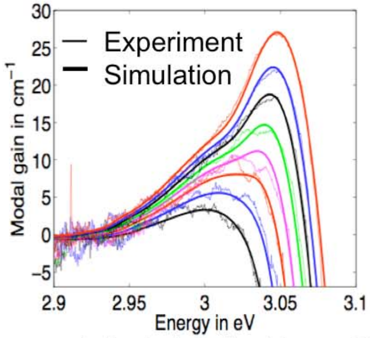
Materials Design

Quantum Transport



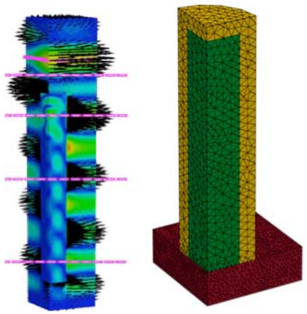
Nanoelectronics

GaN Laser Gain

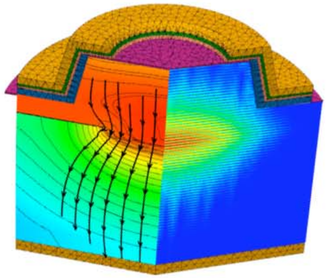


Light-Matter Coupling

Nanowire Solar Cell



Semiconductor Laser



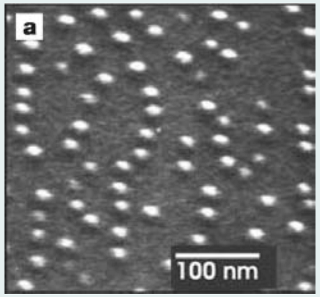
Device Physics

Applications:

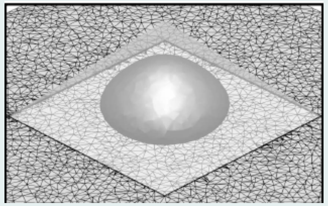
- Solid-State Lighting
- Information processing
- Photovoltaics
- Sensing

Nanostructures for Optoelectronics

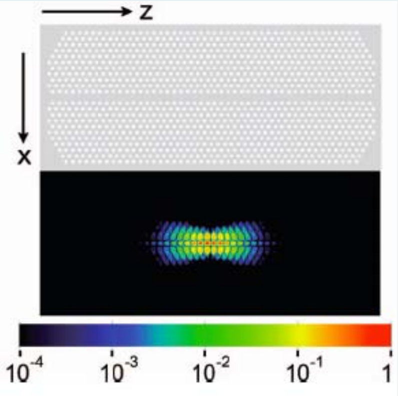
- Trends:
  - Nanowires
  - Nanoparticles
  - Nanostructured Materials
- Applications
  - Emitters
  - Detectors
- Features:
  - Quantization of Carriers
  - Optical Metamaterials
  - Strain Engineering



Reithmaier et al., Nature, 2004



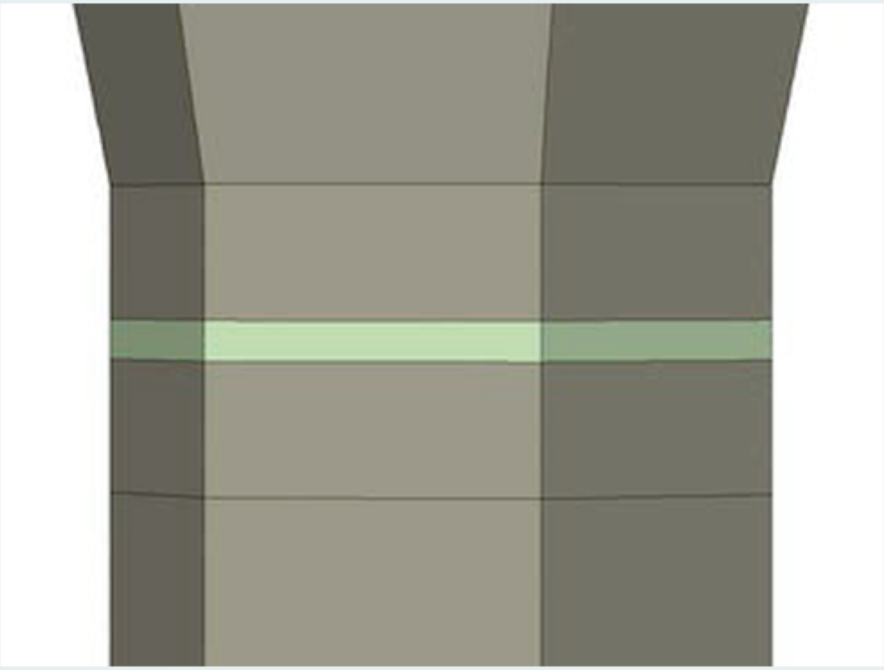
Witzigmann et al. JCSc., 2008

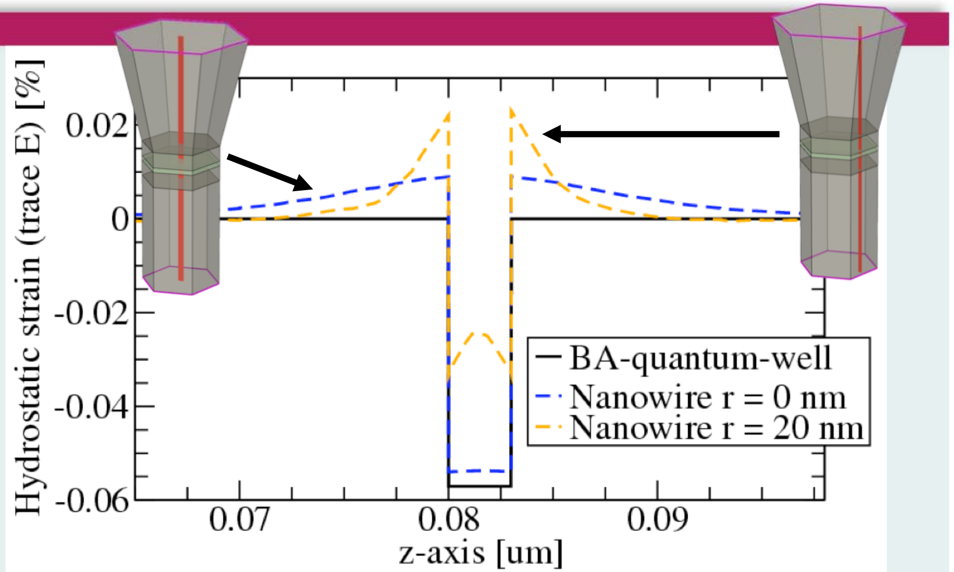


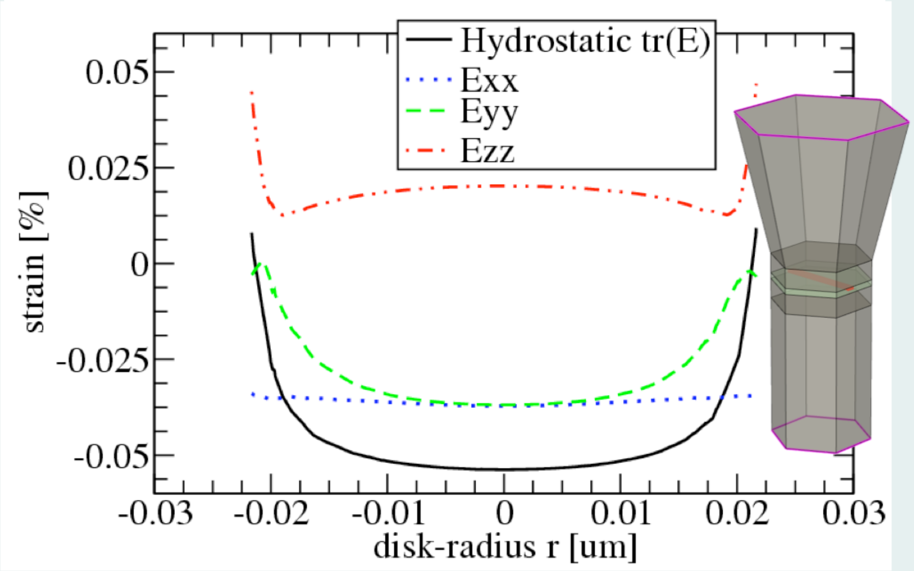
M. Notomi et al. APL, 2006

Nanowires

- Strain Engineering
  - Finite lateral extension allows in-plane relaxation



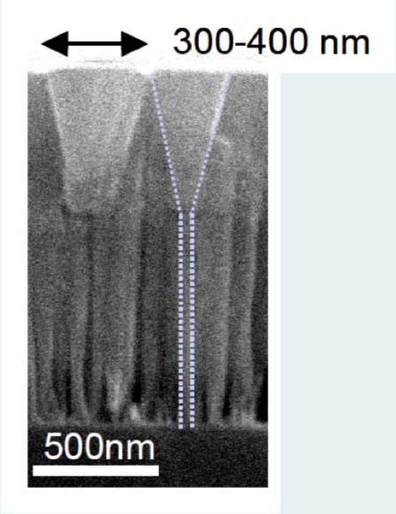




Nanowires

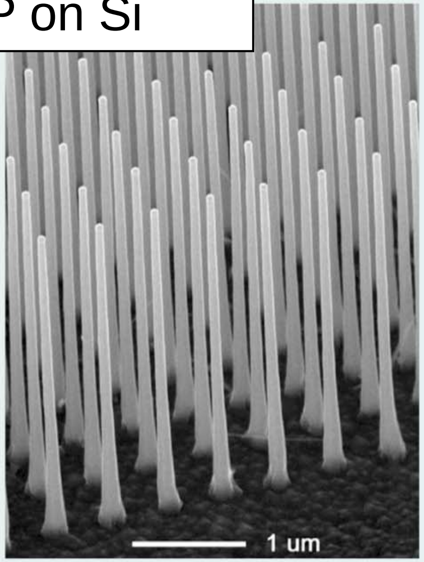
- Novel Material Combinations
  - Substrates
  - Device Hetero-Interfaces

GaN on Si



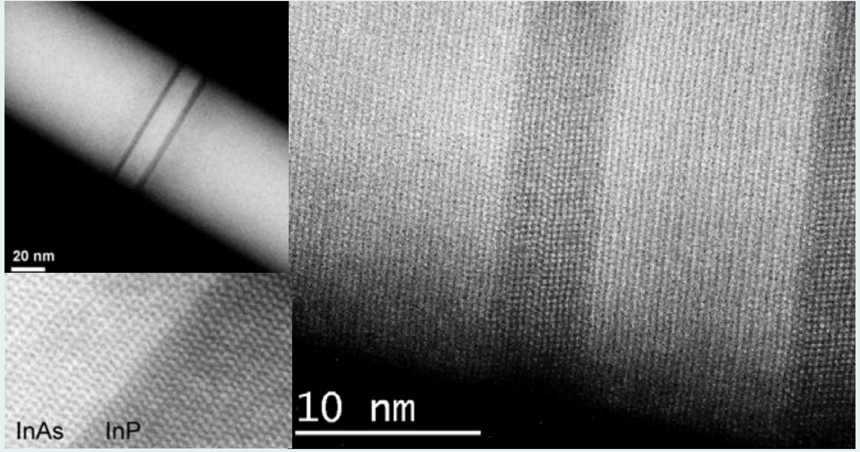
GaN nanowires on Si,
Kishino et al.

InP on Si



InP Nanowires on Si, University Lund

InP/InAs

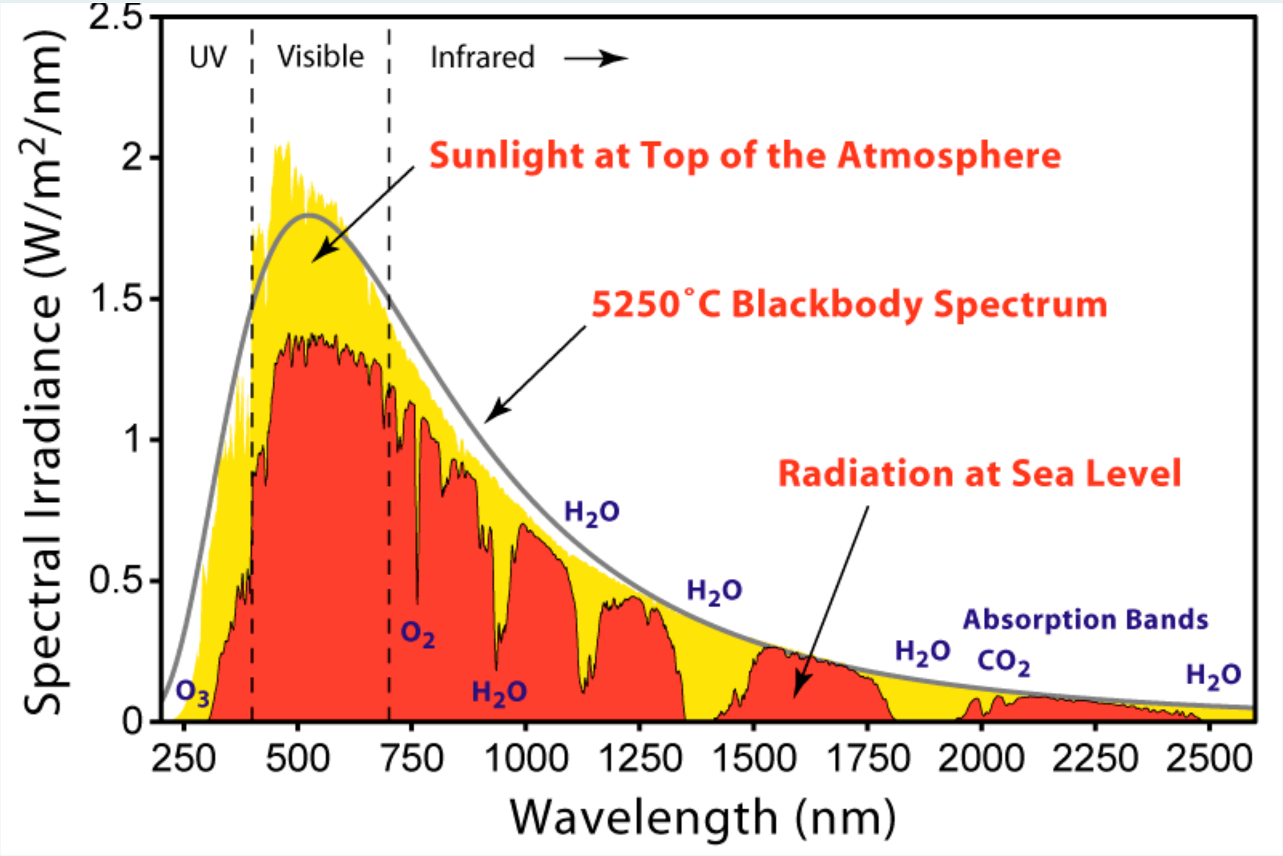


Photovoltaics

Funding: FP 7 AMON-RA: ‘Architectures, Materials, and One-dimensional Nanowires for Photovoltaics - Research and Application’

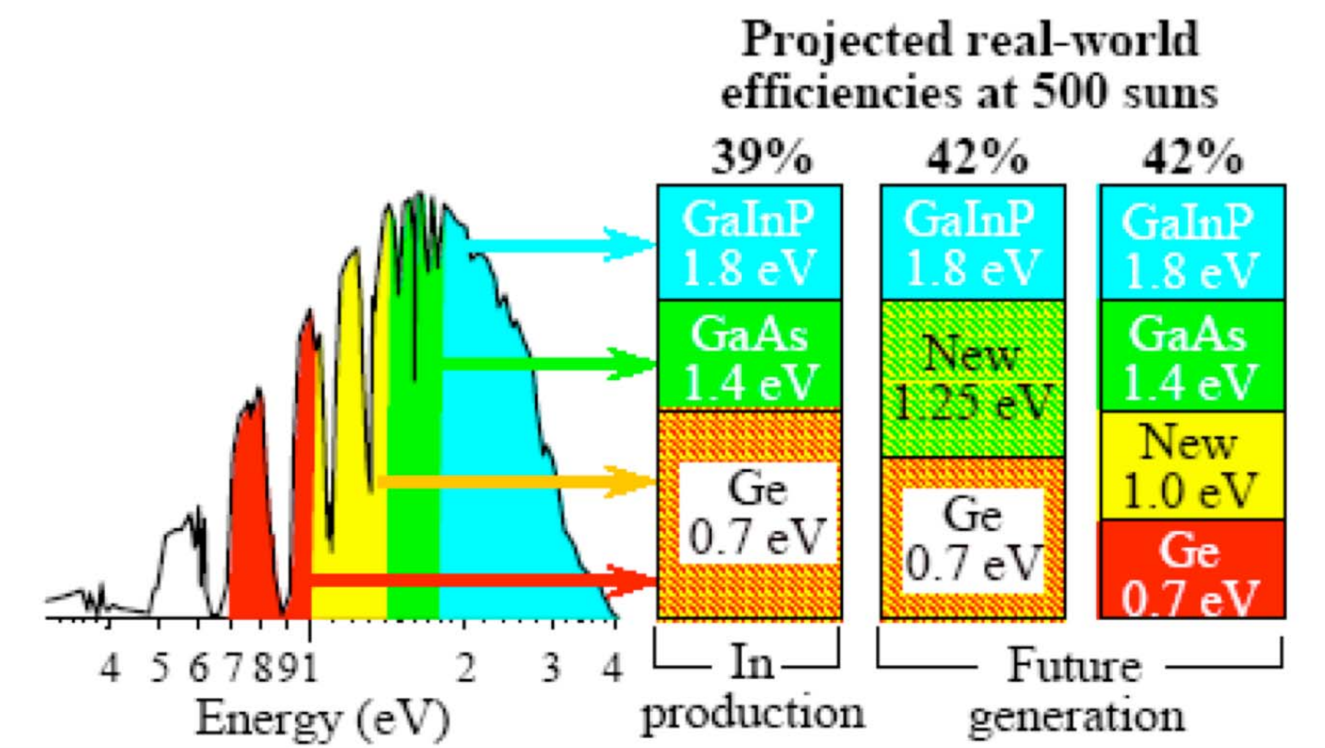
Solar Spectrum

Solar Energy on Earth Surface: 90’000 TW
Current Global Energy Consumption: 16 TW



High Efficiency Cells

- Idea: stack p-n junctions connected by tunnel-junctions
  - Bandgaps match solar spectrum
  - Theory: single junction 30%, infinite junctions 68%



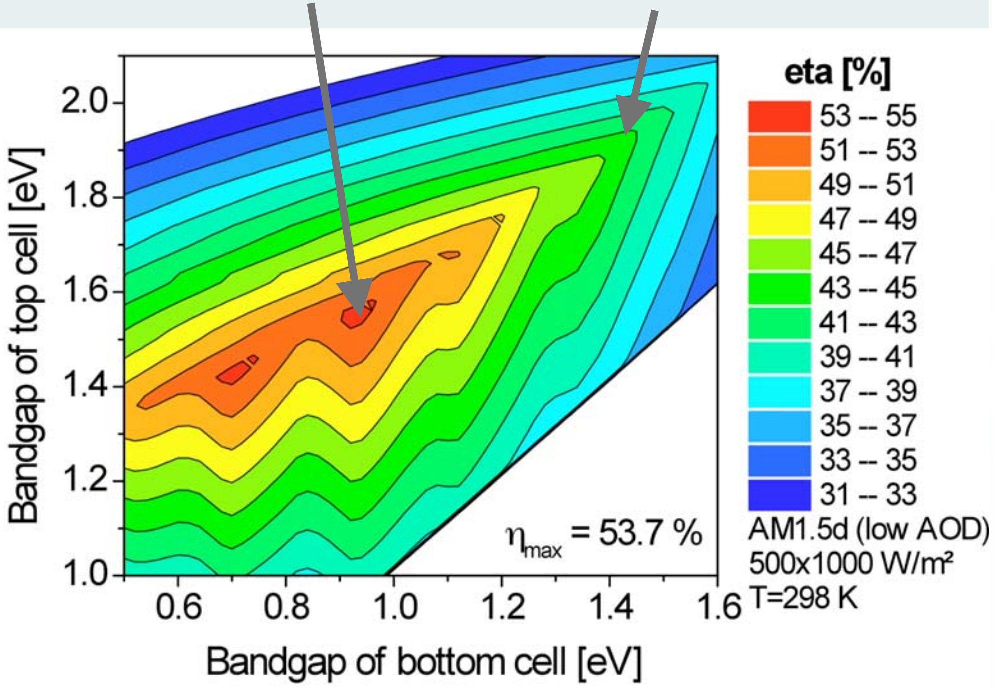
Photovoltaics

- Example: ideal dual-junction device

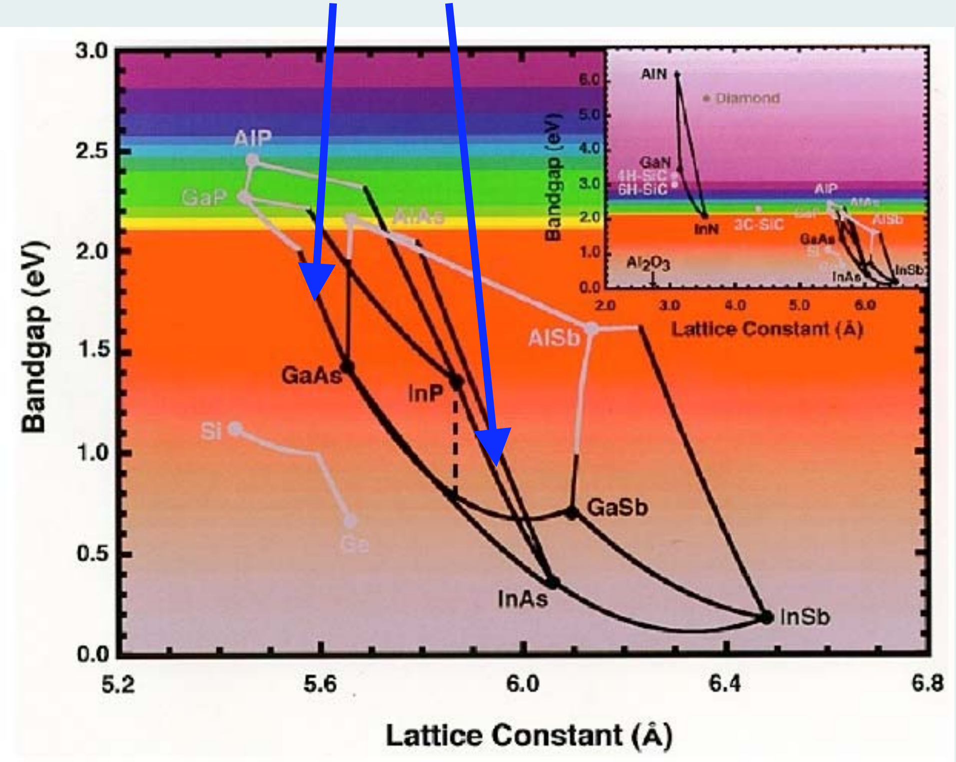
=> Efficiencies up to 55% achievable!

=> Nanowires can potentially have high strain!

GaAsP/InAsP GaAsP/GaAs



GaAsP/InAsP > 5% strain!



Nanowire Modeling: Electromagnetics

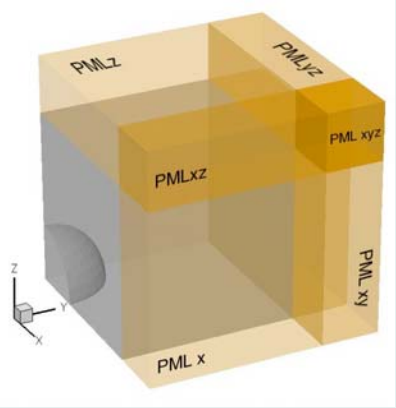
- However: Can a nanowire device capture as much light as a bulk semiconductor?

- Theoretical Investigation of the Optical Properties
  - Coupling of optical power flux into the Nanowire array
  - Wave Propagation in the Device

LUMI III – FEM Electromagnetics

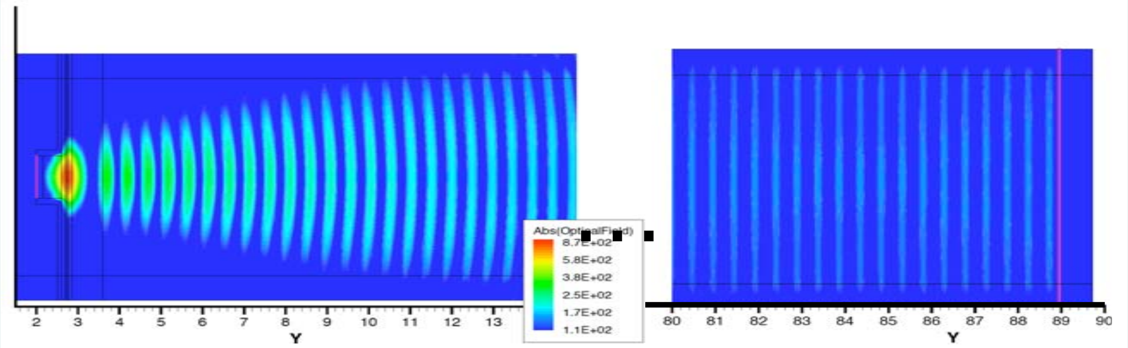
Homogeneous/Inh. Wave Equation: $\nabla \times (\overline{\overline{\mu}}_r^{-1} \nabla \times \mathbf{E}) - k^2 \overline{\overline{\epsilon}}_r \mathbf{E} = -jZ_0 k \mathbf{J}$

- – 2- /3- Dimensional
- – Complex, anisotropic refractive index
- – Boundaries: Neumann/Dirichlet/PML

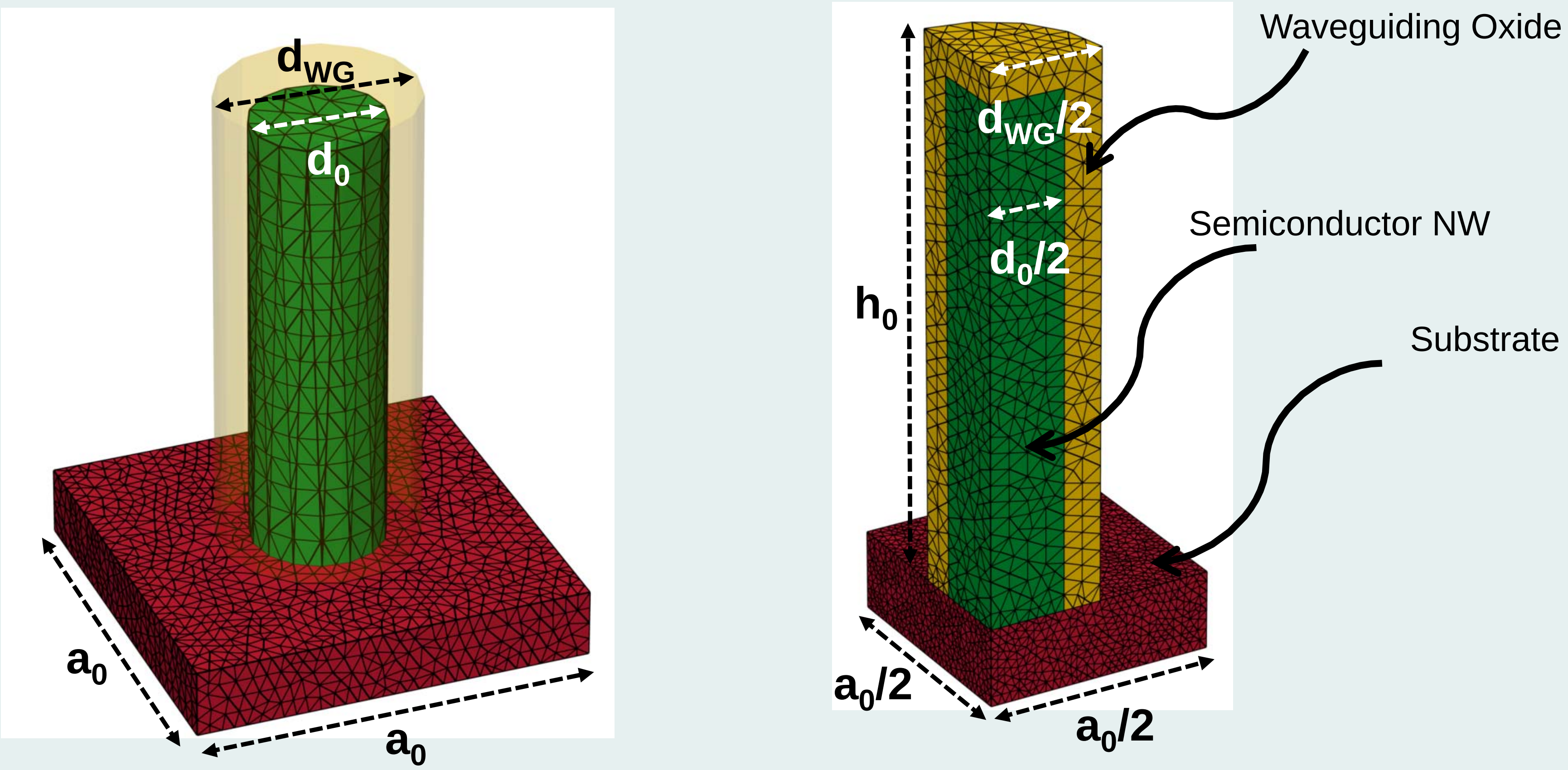


- Numerics:
  - – Nedelec Elements, first/second order
  - – Linear Solvers: Jacobi-Davidson, direct, iterative
- Postprocessing:
  - – Green’s Functions
  - – Power flux
  - – Iterative

    laser simulator



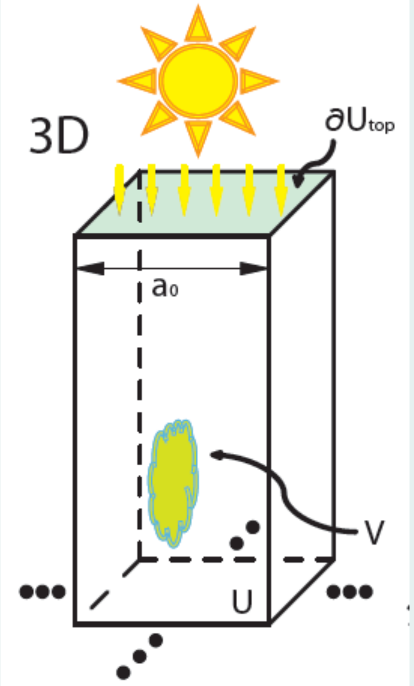
Structure Geometry



Geometry: infinite periodic array of cylindrical nanowires

Illustration of the unit cell (left) and quarter unit cell (right), all calculations were performed on the quarter unit cell.

Definition: Relative Power Absorption



Power dissipated (absorbed) within volume V

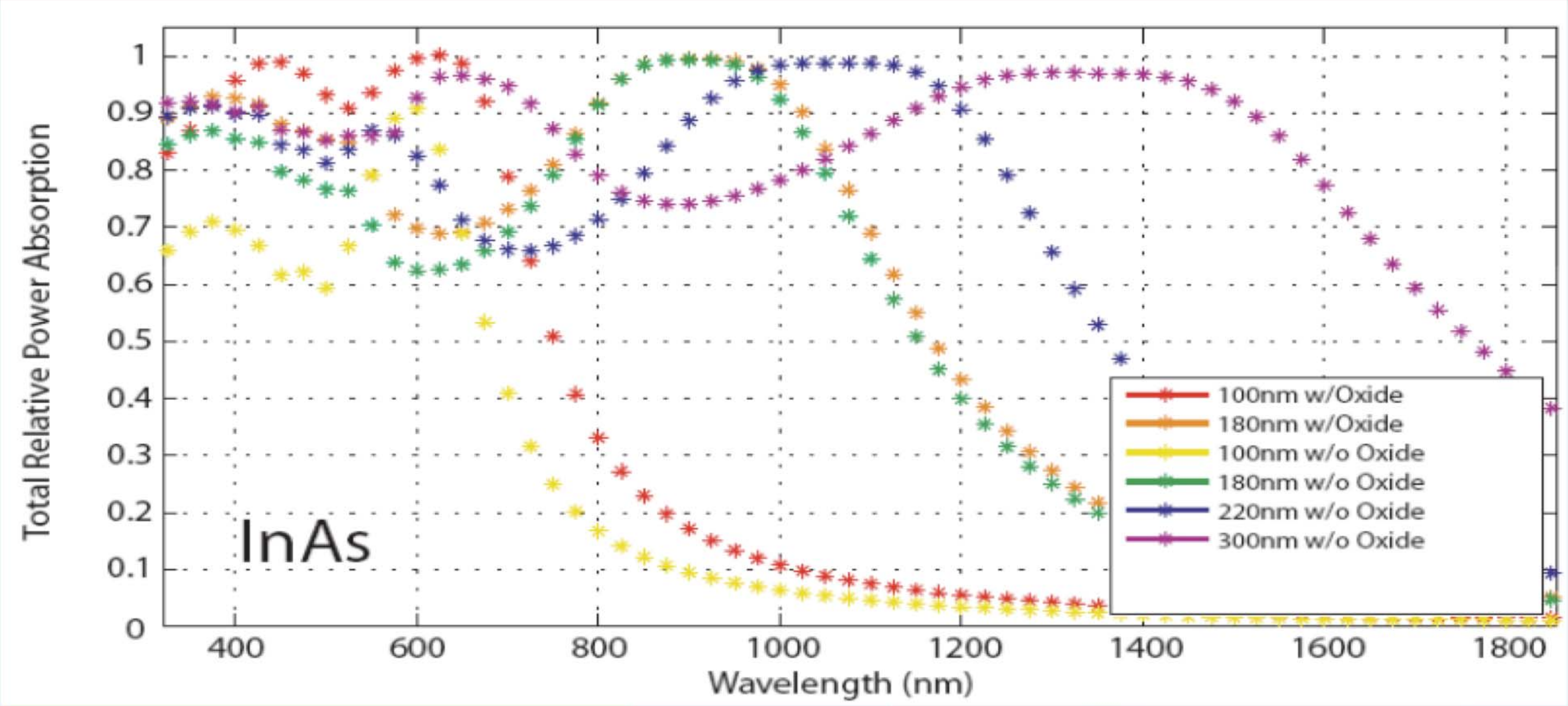
$$\eta_{\mathrm{p}}(V,\lambda_0)=\frac{\int_V p(\lambda_0)\,\mathrm{d}V}{\int_{\partial U_{top}}\Re\{\mathbf{S}_{\mathrm{inc}}\}\cdot\hat{\mathbf{z}}\,\mathrm{d}a}$$

Power radiated by the source into free space over an area of a_0^2 (= ideal coupling)

Two mechanisms decreasing relative power absorption

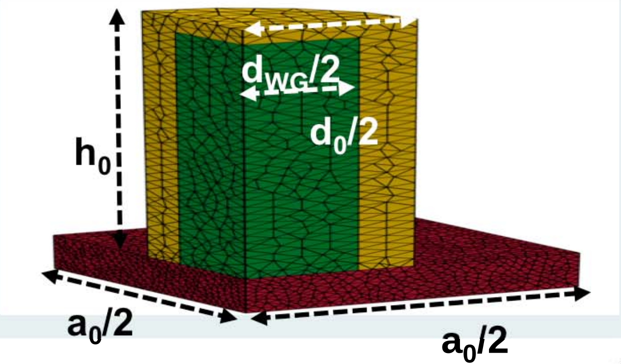
- Reflection of power at top interface: due to the dielectric interface, reflection occurs.
- Transmission through the nanowire array into the substrate

Total Relative Power Absorption



Geometry

- a_0 = 600 nm
- h_0 = 2000 nm
- d_{WG} = 200 nm (or 0 nm, see figure)
- d_0 see figure
- volume V: entire nanowire



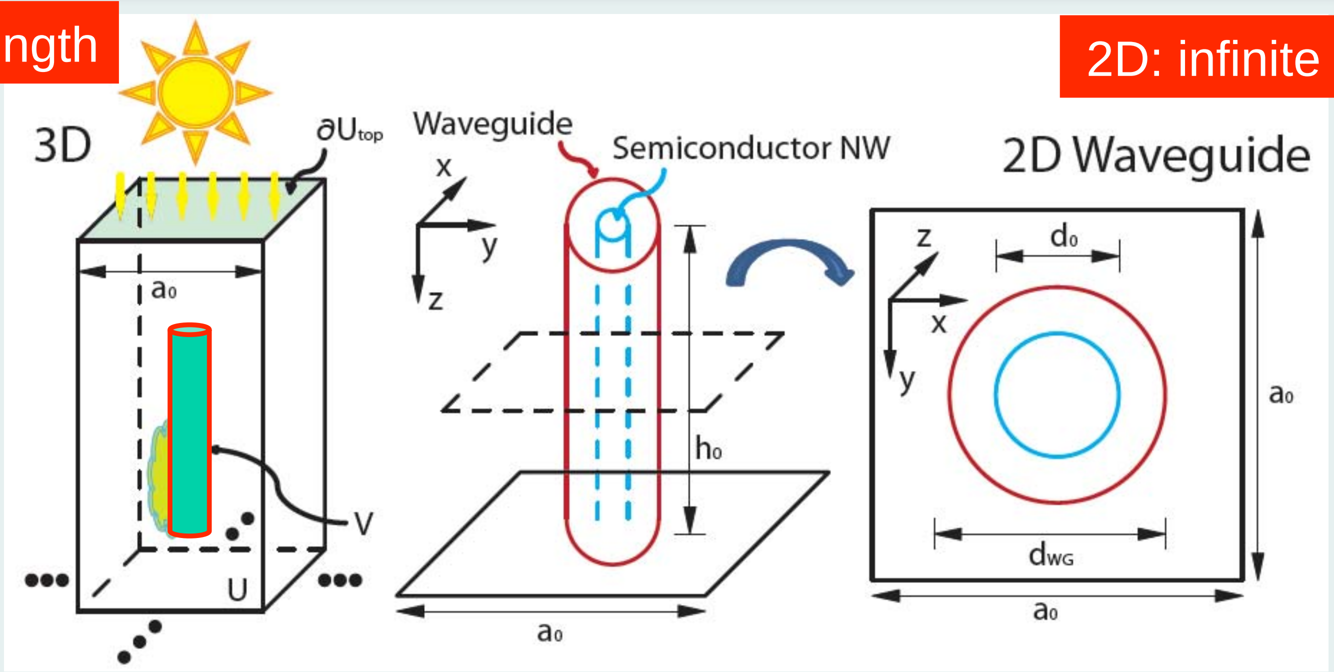
Questions arising from 3D EM

- What is the cause of the local maxima of the total relative power absorption?
- Which fraction is lost due to reflection and which due to transmission?
- What is the effect of increased nanowire length (resonance effects along the nanowire)?
- How can the total relative power absorption be increased?
- **Solution: Modal analysis of the nanowire solar cell.**

From 3D to 2D Modal Analysis

3D: finite NW length

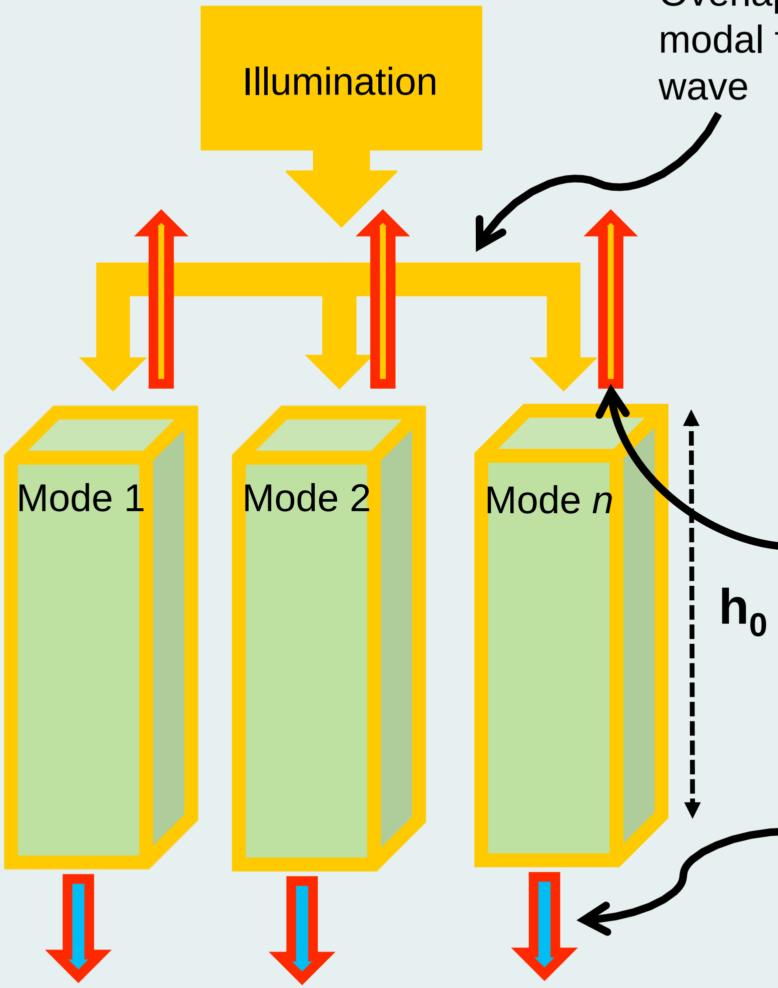
2D: infinite NW length



Idea

- Light propagates along the nanowires in the discrete modes of an infinite waveguide, no cross-talk between modes, power in each mode dissipates according to Beer-Lambert law
- In-coupling into modes is determined by the modal field distribution and the modal effective refractive index

2D Modal Analysis



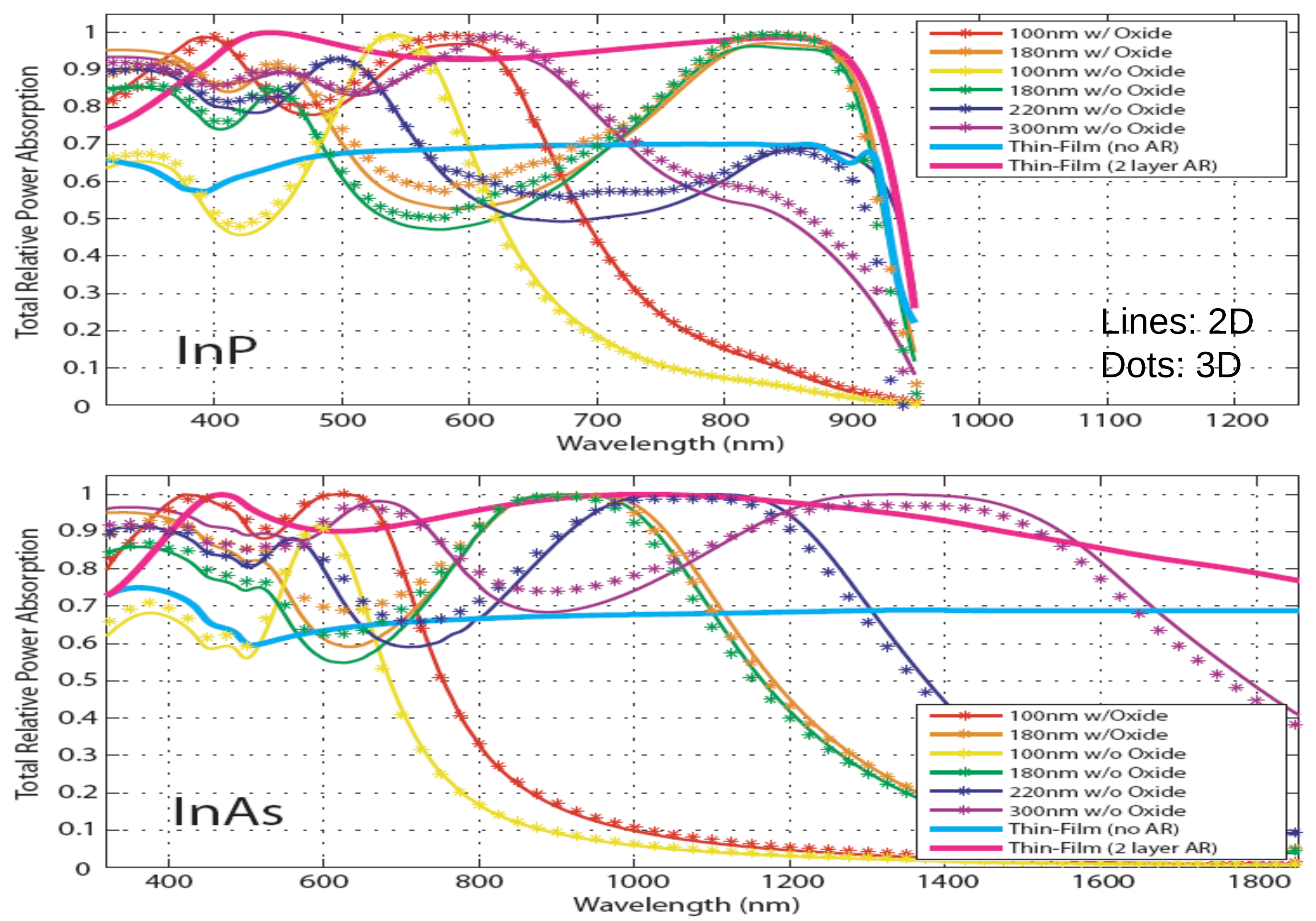
Overlap integral given by correlation of modal field profile and incident plane wave

Absorption within each mode is governed by the Beer-Lambert law

Modal reflectivity given by Fresnel equation for modal effective refractive index

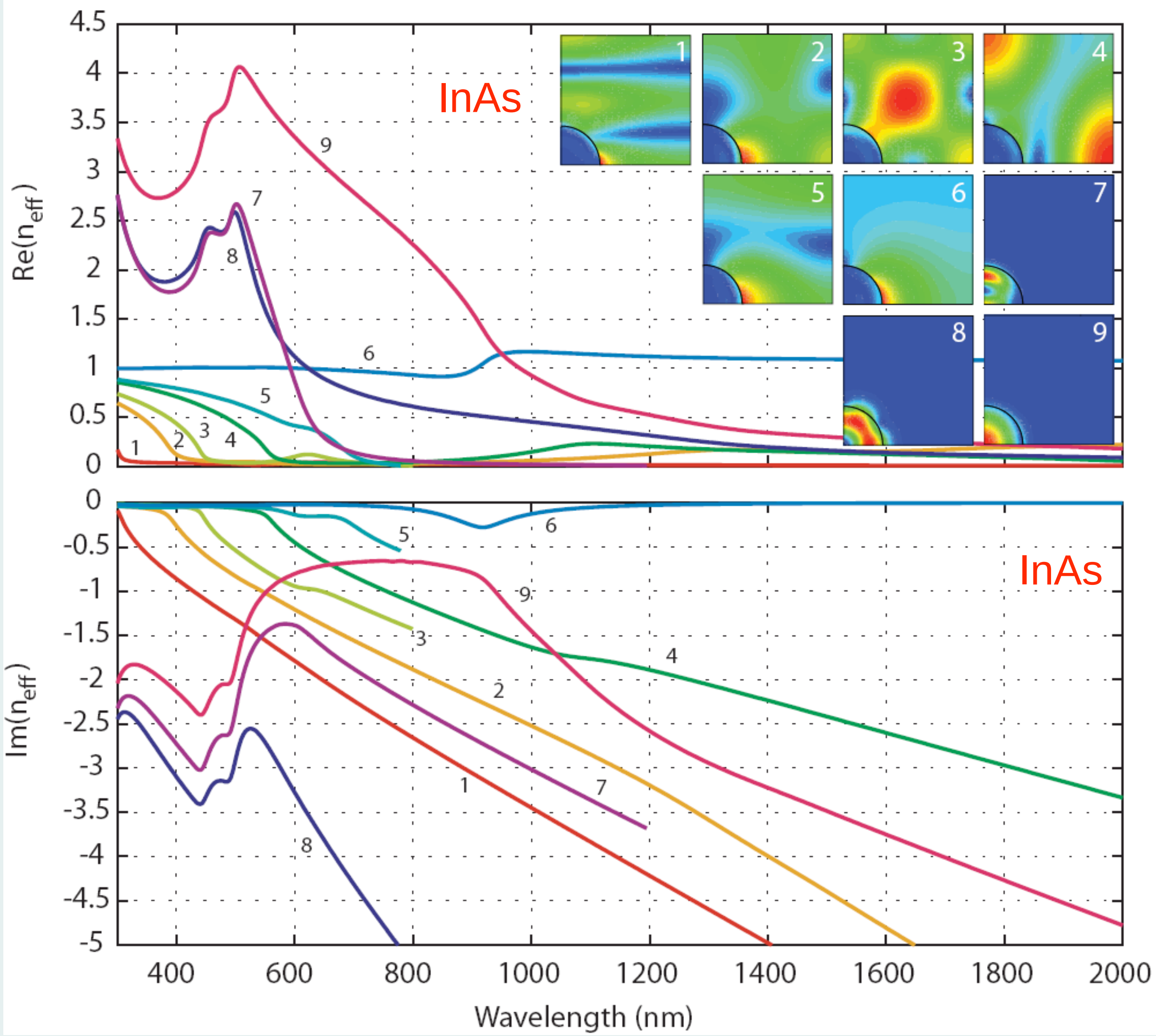
Transmission through nanowire array

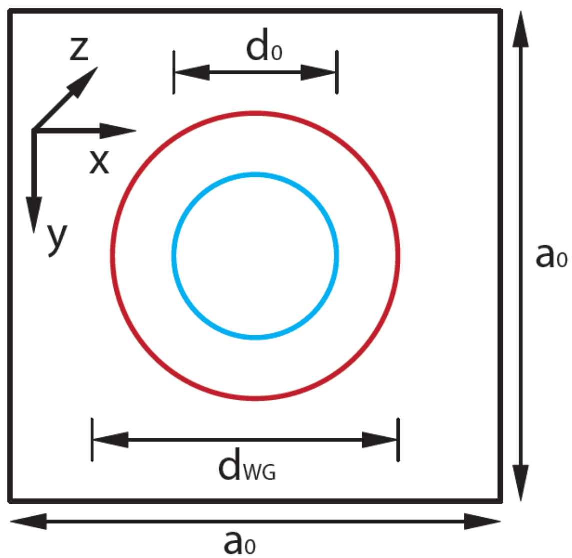
Comparison 3D and 2D Waveguide



Lines: 2D
Dots: 3D

Dispersion Relation of the NW Array





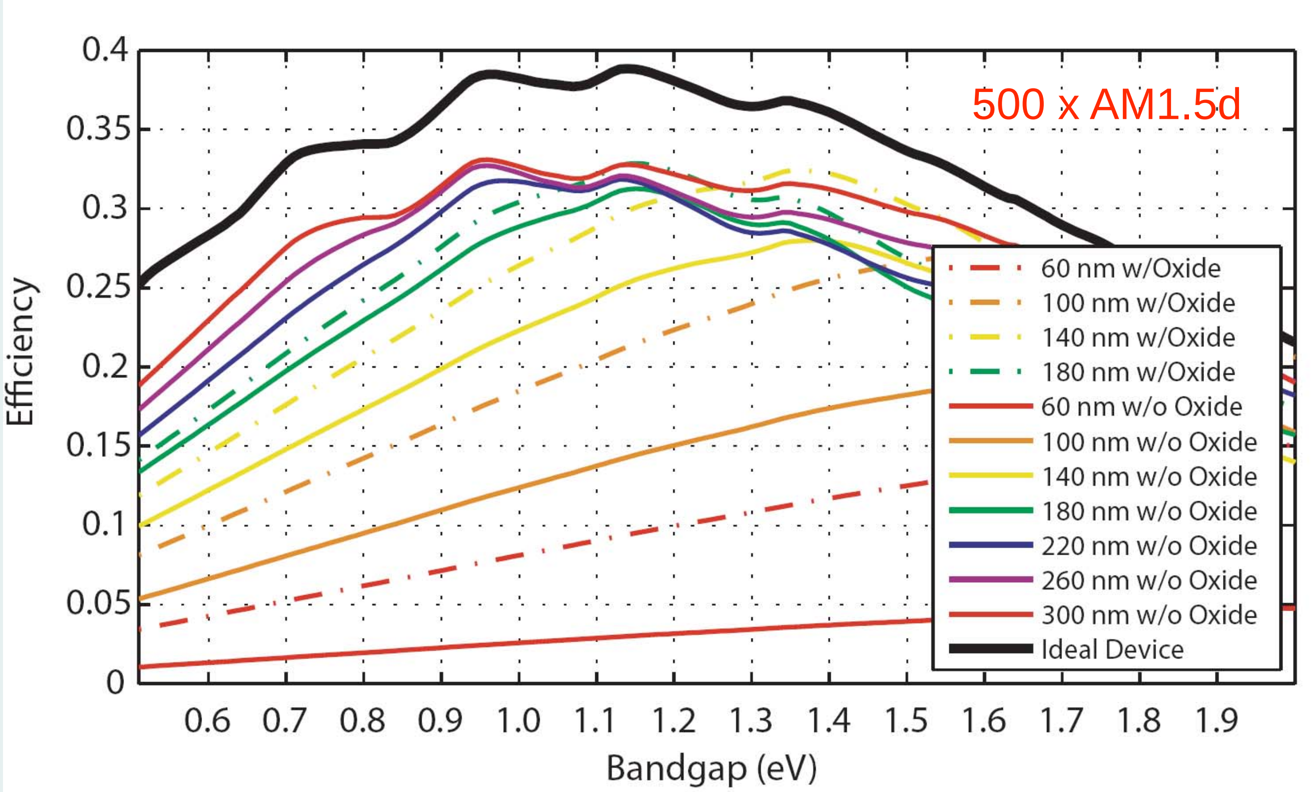
Geometry

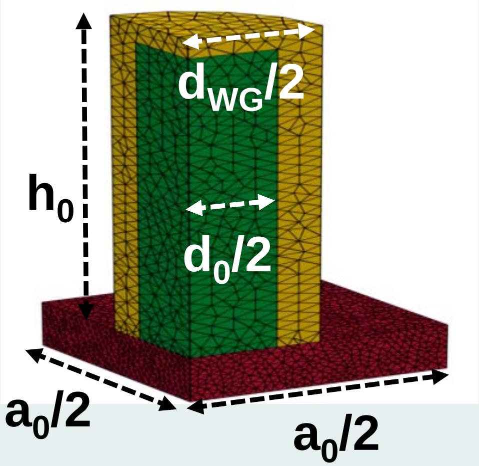
- a_0 = 600 nm
- d_0 = 90 nm
- waveguiding oxide not present

2D Waveguide and 3D EM Results

- 2D waveguide and 3D simulations are in good agreement even at moderate nanowire lengths.
- Local excursions of the total relative absorption are caused by transmission through the nanowire array, not by reflection.
- The reflectivity of the entire structure is very low due to the presence of a mode with n_{eff} approx. 1.
- Effect of increasing h_0 can be calculated using the Beer-Lambert law.
- Power absorption can be increased by improving coupling into lossy modes.
- The 2D modal analysis is far less computationally demanding allowing sweep over wide parameter space.

Efficiency: Single-Junction NW Array Solar Cell





Geometry & Illumination

- a_0 = 600 nm
- h_0 = 2000 nm
- Illumination: 500 x AM1.5d

Results

- Nanowire solar cells can reach efficiency similar to ideal thin film devices
- The presence of a non-active waveguide does improve absorption – however – only at a low absolute level

Summary

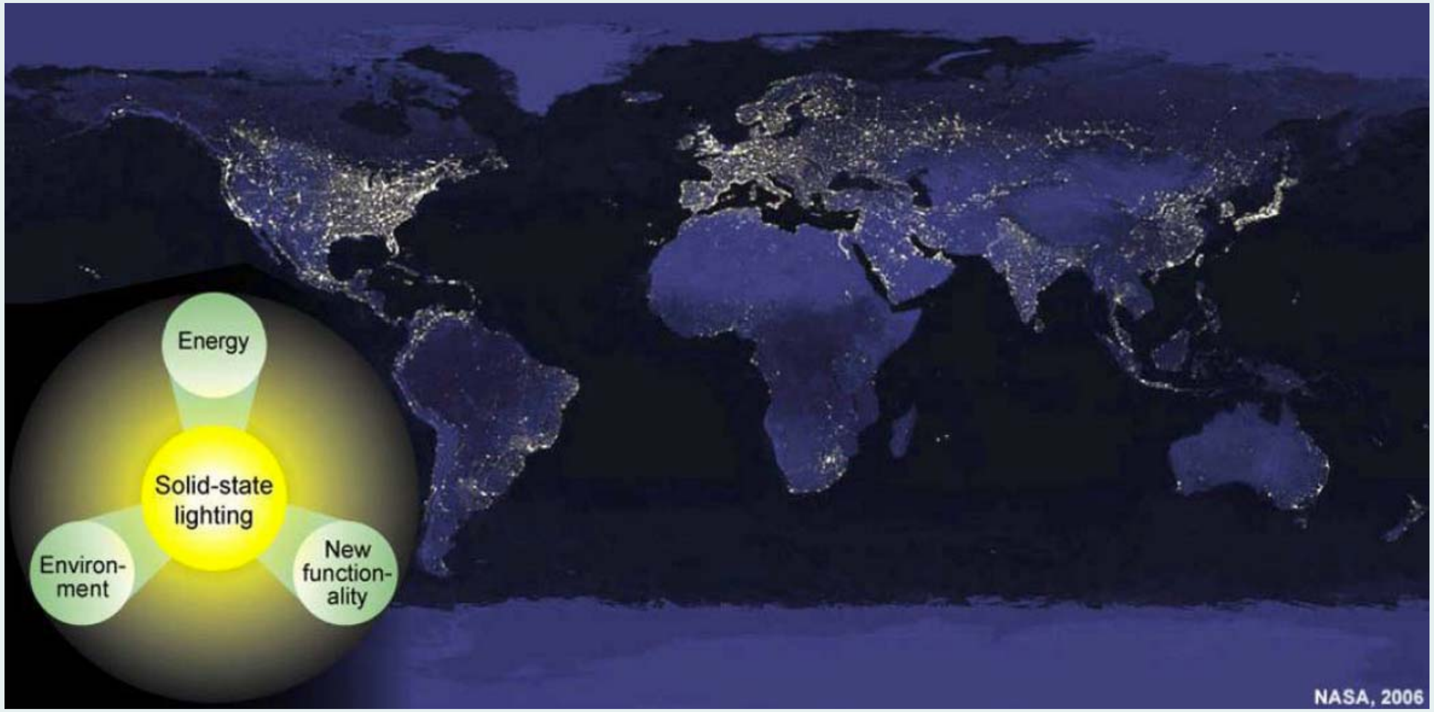
- 3D simulations related to 2D waveguide simulations show:
  - Structure has antireflective properties due to its dispersion characteristic.
  - The Beer-Lambert law is applicable predicting exponential power decay.
- The effect of the waveguiding oxide is limited
- Spatially and spectrally resolved detailed balance calculation illustrates:
  - Power absorption is higher than incident power weighted with area fill-factor due to micro-concentration.

Nanowires for Solid State Lighting

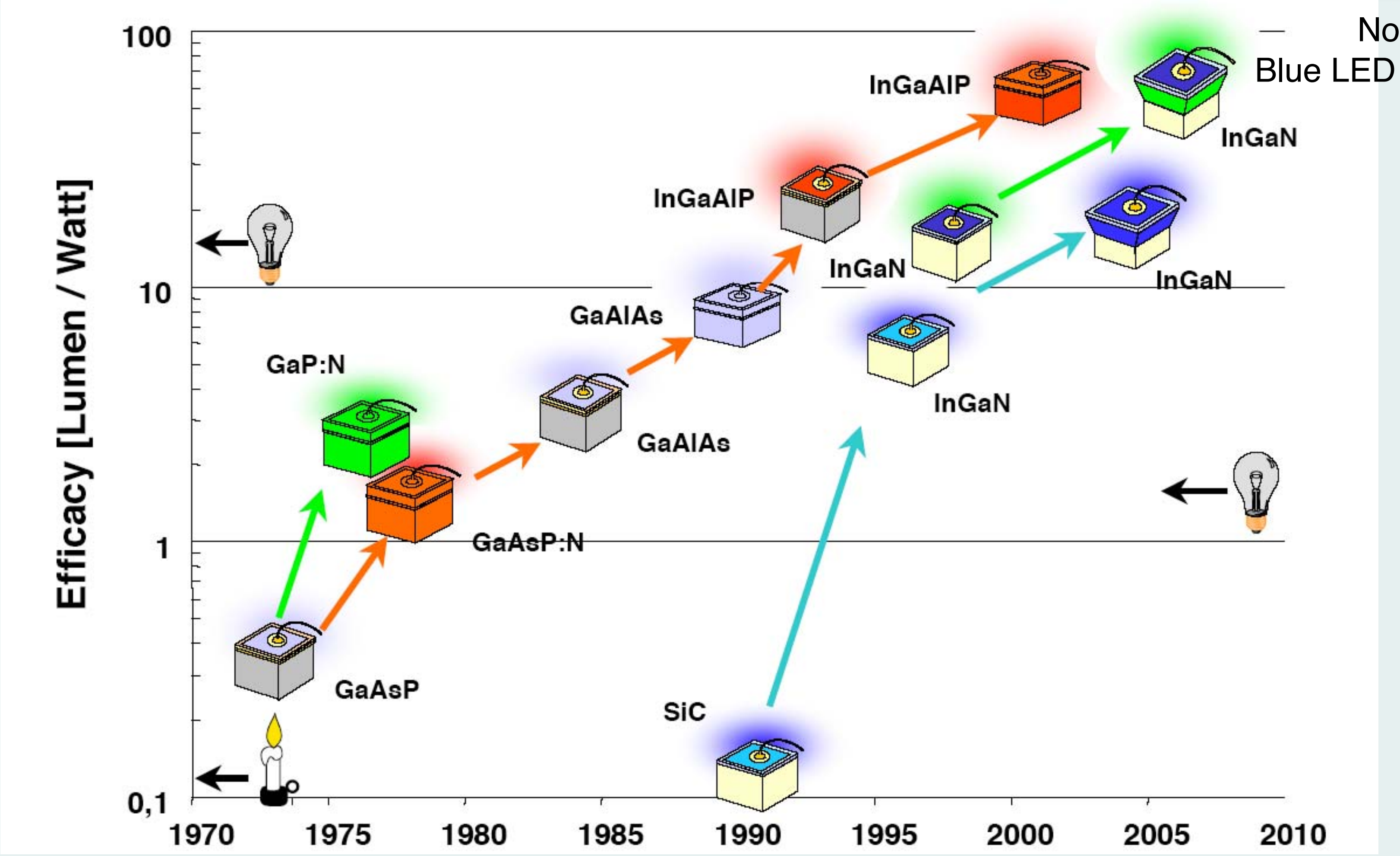
Funding: FP 7 SMASH: ’Smart Nanostructured Semiconductors for Energy-Saving Light Solutions’

Solid State Lighting: Motivation

- Energy benefits of Solid State Lighting
  - 22 % of electricity used for lighting
  - LED-based lighting can be 20x more efficient than incandescent and 5x more efficient than fluorescent lighting



LED: Luminous Source Efficiency



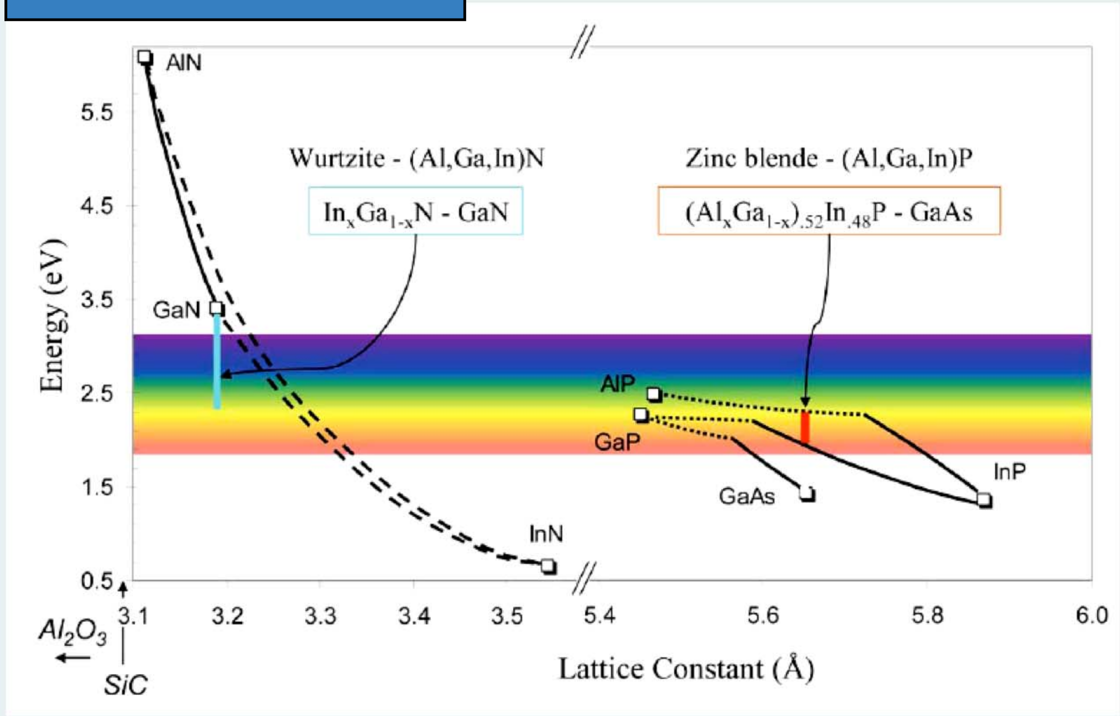
Nov 2008 (Cree):
Blue LED with 160 lm/W

Osram OS

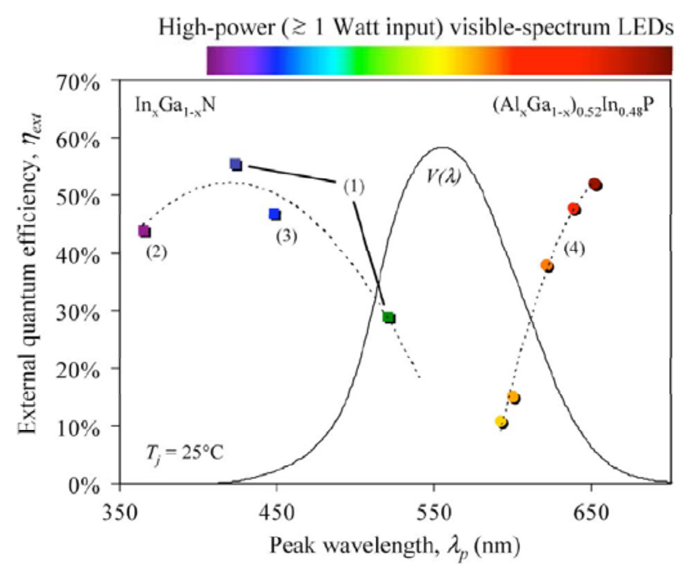
Maximum for white source: 100% CRI 240 lm/W
90% CRI 408 lm/W

White LEDs: GaN Material System

Material



Quantum Efficiency



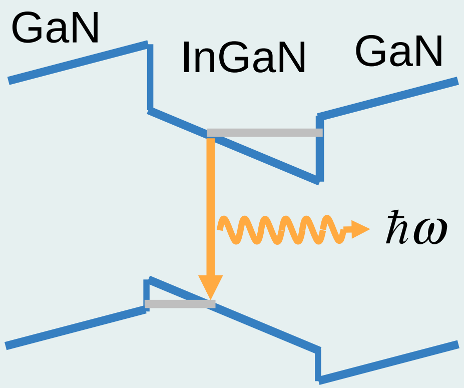
Krames et al. 2007

- InGaN LED / LD over entire visible spectra (trichromatic sources)
- High efficiency green emitters
- Cost efficient

GaN Material System

Technology

- InGaN allows LED / LD over entire visible spectra
- Violett, blue and green devices exist; red emission?
- High indium concentration reduces quantum efficiency



Science

- Variety of coupled physical effects:
  - strain (+ relaxation, defects)
  - piezo-electric fields
  - quantum confined stark effect
  - screening
- Inhomogenities (Immiscibility of InN in GaN), Dot-like states

GaN/InGaN thin films

Biaxial Strain

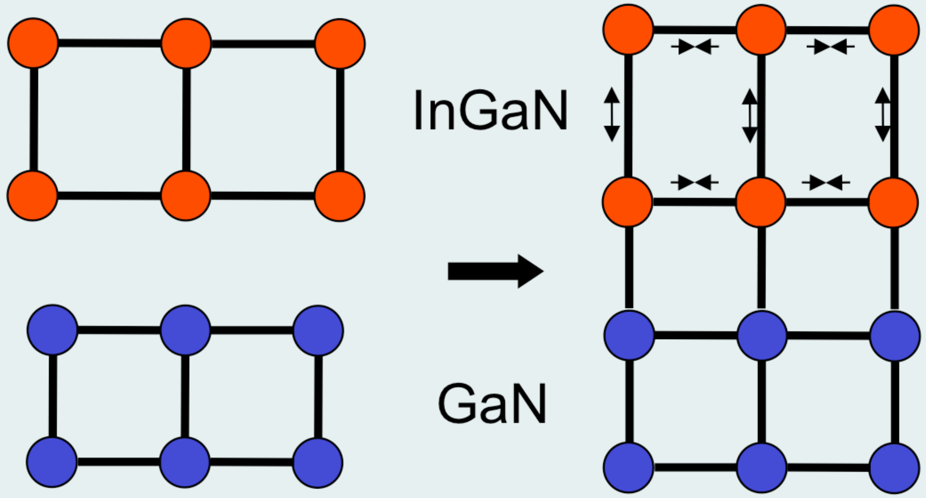
- InGaN on GaN: compressive strain in InGaN layer
- No in-plane relaxation due to infinite extension.

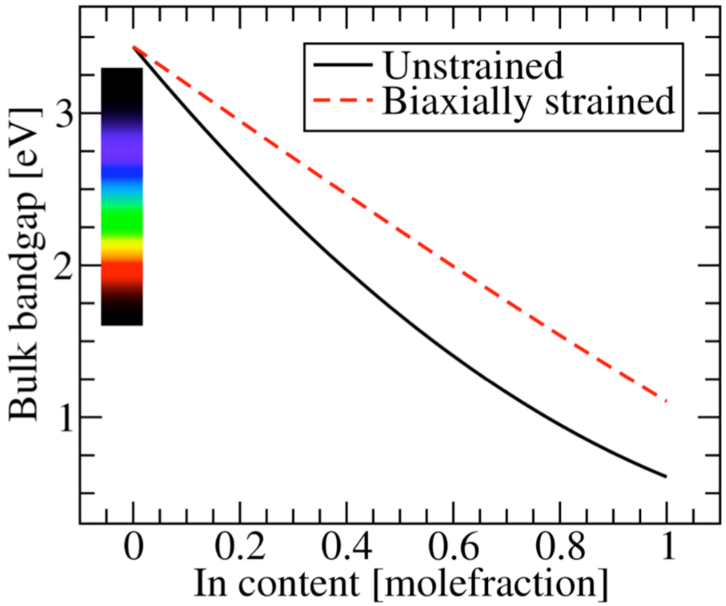
Bulk InGaN Band Gap

- increasing the indium content:

$$E_g(\mathrm{GaN}) - \Delta E(\mathrm{In}\,x) + \Delta E(\mathrm{Strain})$$

$$\Downarrow \qquad \Uparrow$$

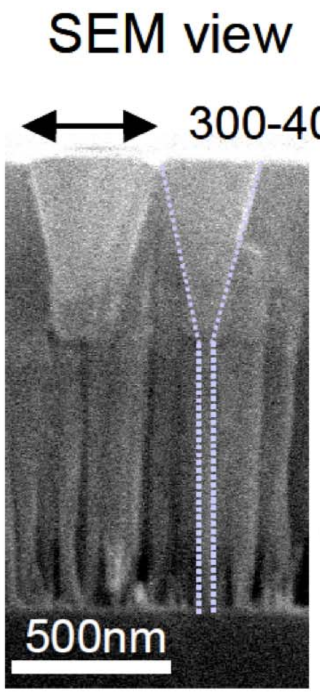


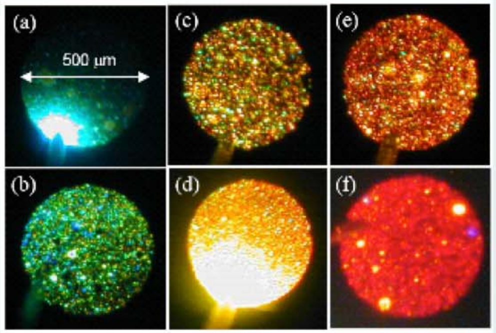


Nanocolumns [1]

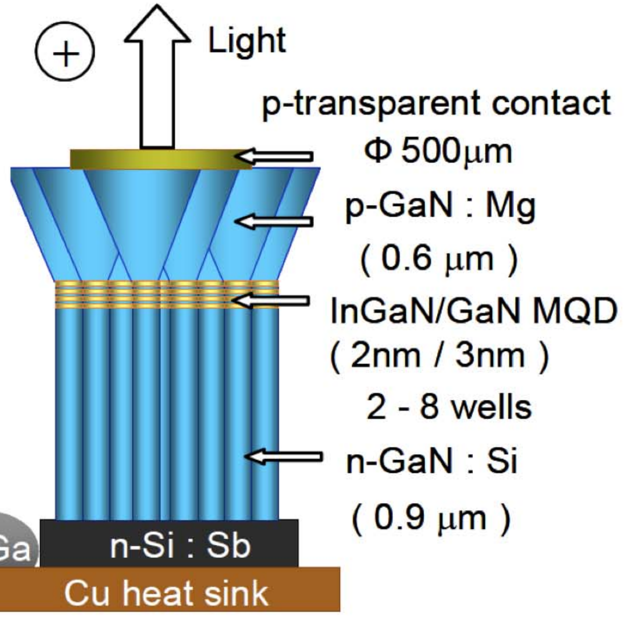
Nanocolumns

- Finite lateral extension allows in-plane relaxation
- GaN nanocolumns grown using rf-MBE on Si; low dislocation dens.
- InGaN quantum disks as active region, emits at 500-700 nm.
- Small blue shifts suggest low internal field (= small strains)



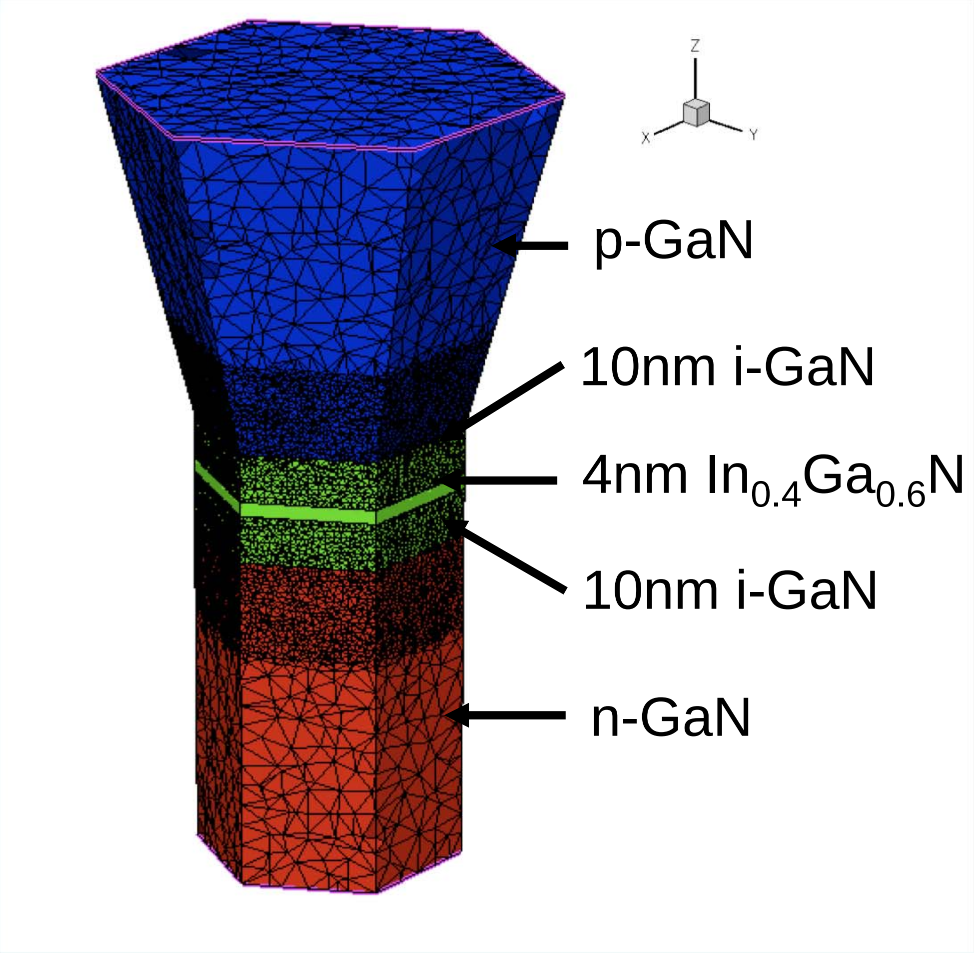


K. Kishino *et al.*, Proc. SPIE 64730T (2007)



[1] K. Kishino et al., Proc. Of SPIE Vol. 6473, 64730T (2007)

Modeling



Simulation Details

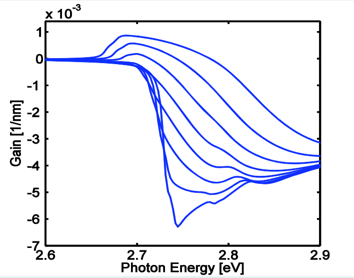
- Tool: tdkp/AQUA [2]
- Continuum-mechanics: FEM
- Displacement- / strain field from hexagonal strain equation
- Piezo-electric fields: surface charges at element faces
- Poisson’s equation: Nanocolumn is surrounded by air.
- Material parameters from [3]

[2] R.G. Veprek, S.Steiger and B.Witzigmann, Journal of Computational Electronics, in press (2008))
[3] I. Vurgaftman and J.R. Meyer, in J. Piprek, Nitride Semiconductor Devices (Wiley 2007)

tdkp/AQUA

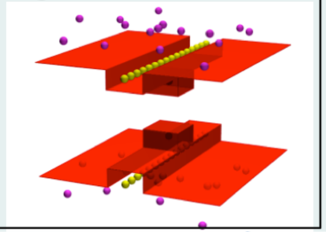
Luminescence: ***tdkp***

- 1D-3D strain calculation using continuum mechanics
- 1D-3D calculation of built-in fields
  from spont. and piezoelectric polarization
- 0D-3D Schrödinger solver
  - 4-, 6- or 8-band **kp** model
  - Zincblende, wurtzite
  - Including strain
- 0D-3D gain, spont. Emission
  - from *n*,*p* or E_{Fn},E_{Fp}
  - using free-carrier or screened HF



Transport: ***AQUA***

- 1D-3D drift-diffusion
- Partitioning of carriers into bound / unbound populations
- Bound carrier description:
  - Quantized directions:
    Full coherence → wave functions, $E_{n\mathbf{k}}$
  - Remaining directions:
    No coherence → DD transport
- Recombination:
  - Nonradiative (SRH, Auger)
  - Radiative: spatially and spectrally resolved spont. emission
- Coupling of populations:
  - Capture
  - Electrostatic potential



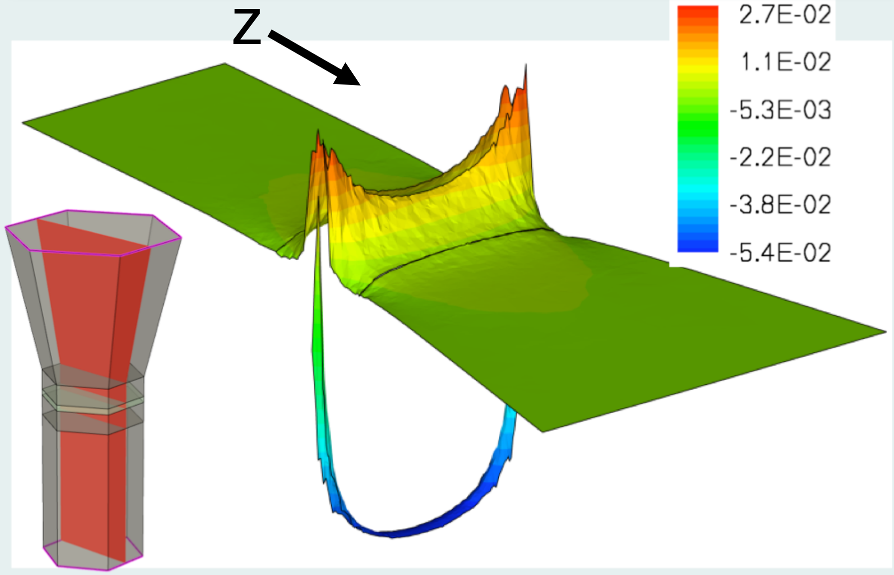
Strain Distribution $In_{0.4}GaN$ 3nm QW

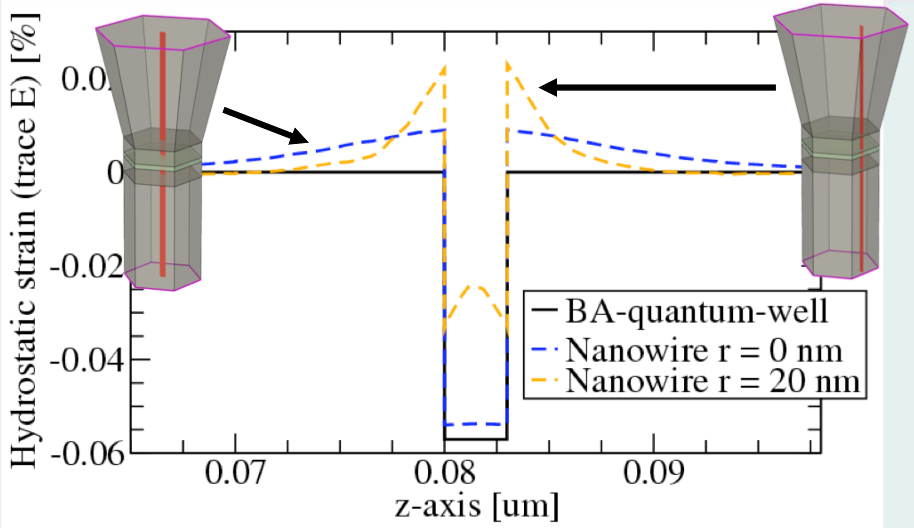
Hydrostatic Strain

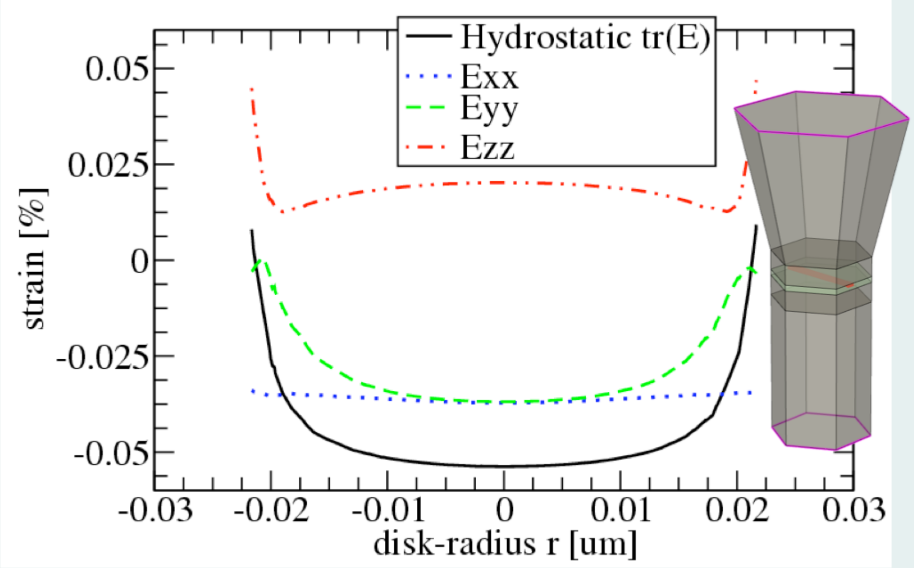
- Bandgap change (**first approx.**):

$$E_g(\varepsilon) = E_g + a_g\,\mathrm{Tr}(\varepsilon)$$

- Strain potential InN/GaN: a_g between - 9.9 and - 4.2 [eV]



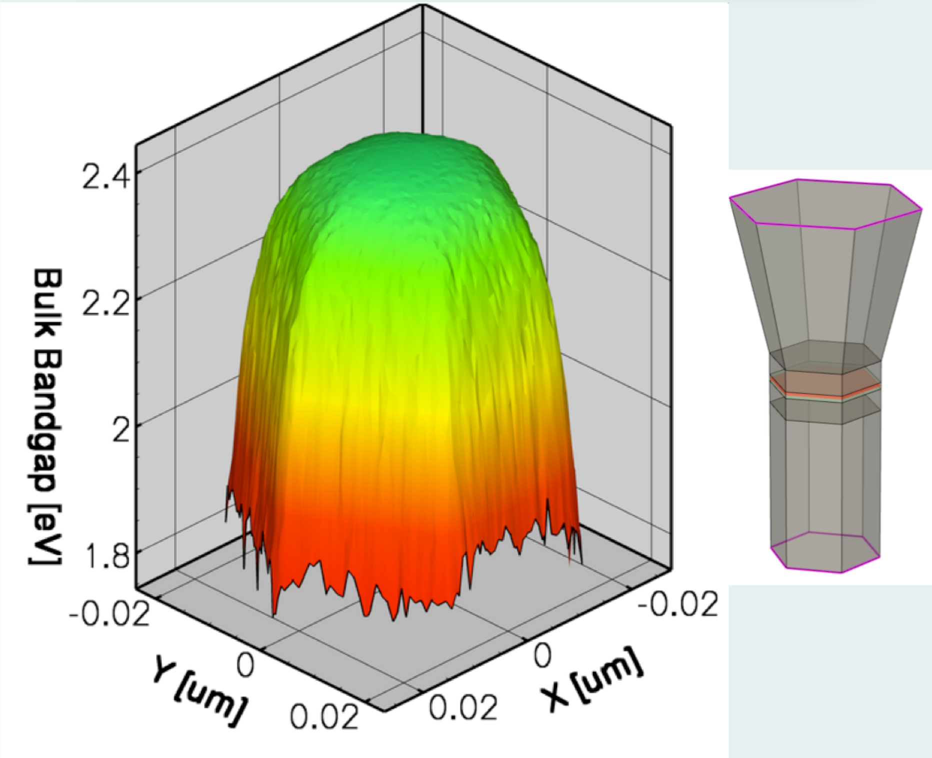




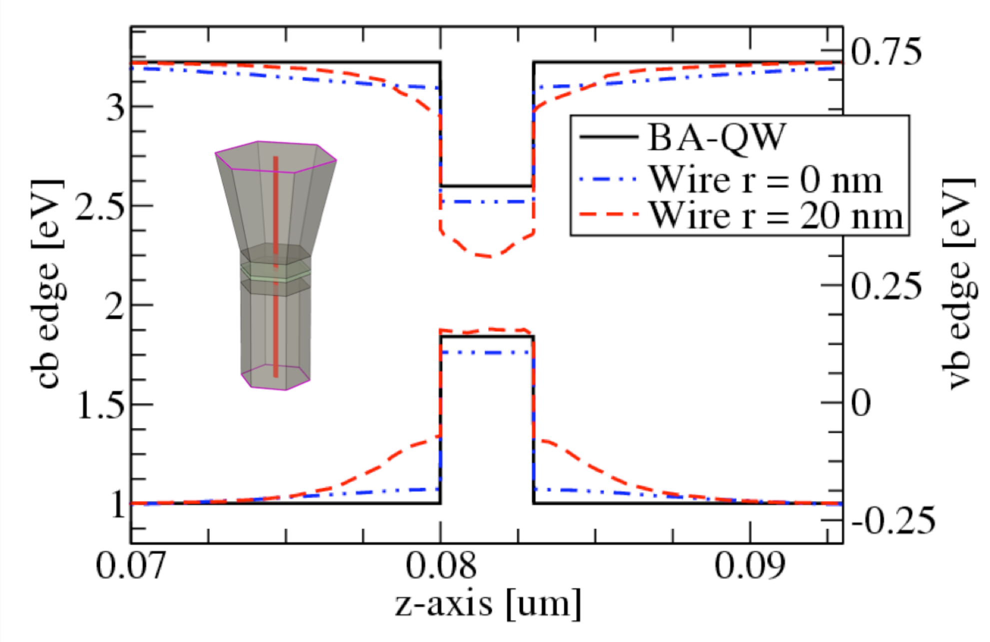
Bulk Band Gap and Band Edge

Bulk Band Gap

- **k·p** matrix at k = 0



Bulk Band Edges



Note: no quantization or Piezoelectric effects included

Impact of Strain and Piezoelectricity

Strain

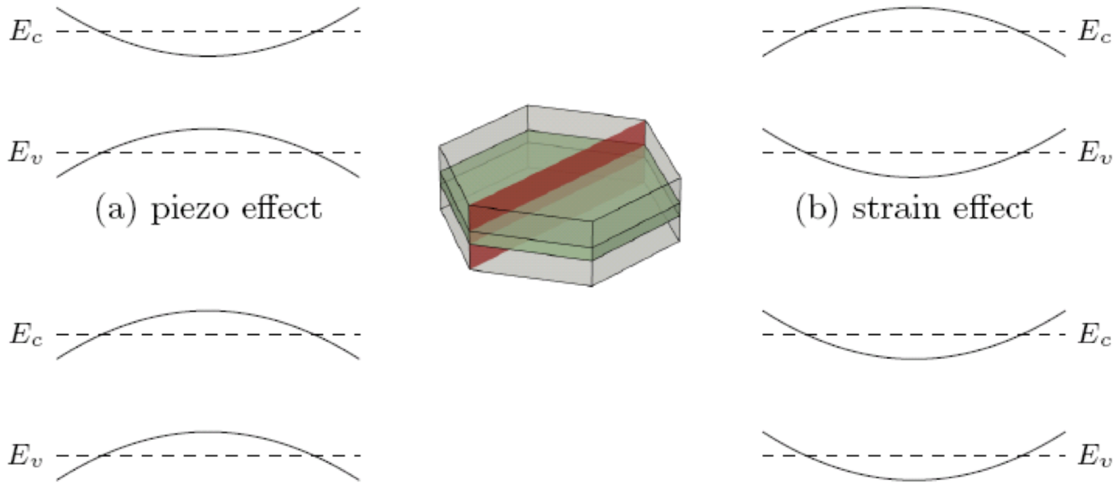
- Strain ($a_g<0$, $\mathrm{Tr}(e)<0$)

$$E_g(\varepsilon) = E_g + a_g \,\mathrm{Tr}(\varepsilon)$$

Piezo

- Strain ($e_{ijk}>0$, $e_{jk}<0$)

$$P_i(x) = \sum e_{ijk}\varepsilon_{jk} + P_{i,spont.}(x)$$



(a) piezo effect

(b) strain effect

(c,d) piezo and strain effects mixed

Figure 5.13: Piezoelectric and strain effects on the bandstructure in the lateral well direction.

Strained Band Edges

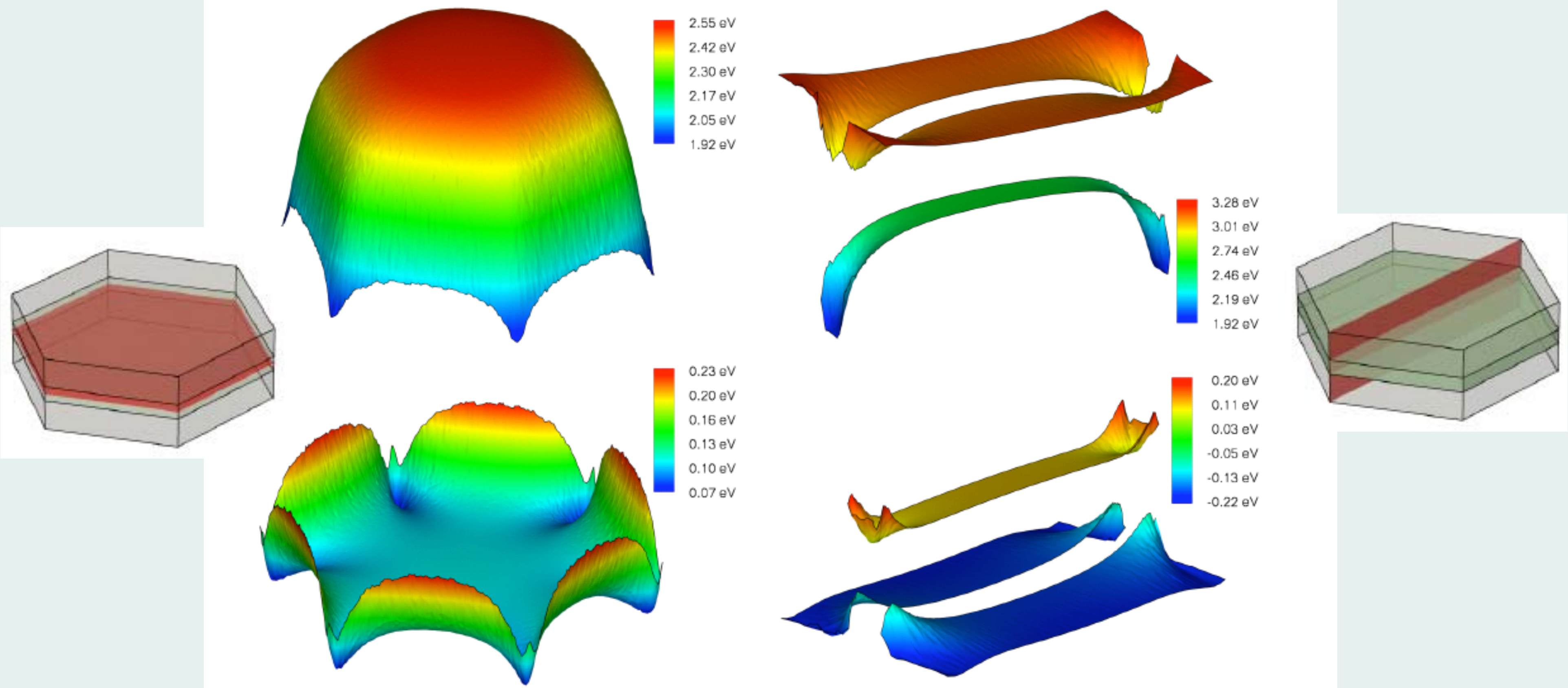


Figure 5.6: Bandedges with strain effect taken into account.

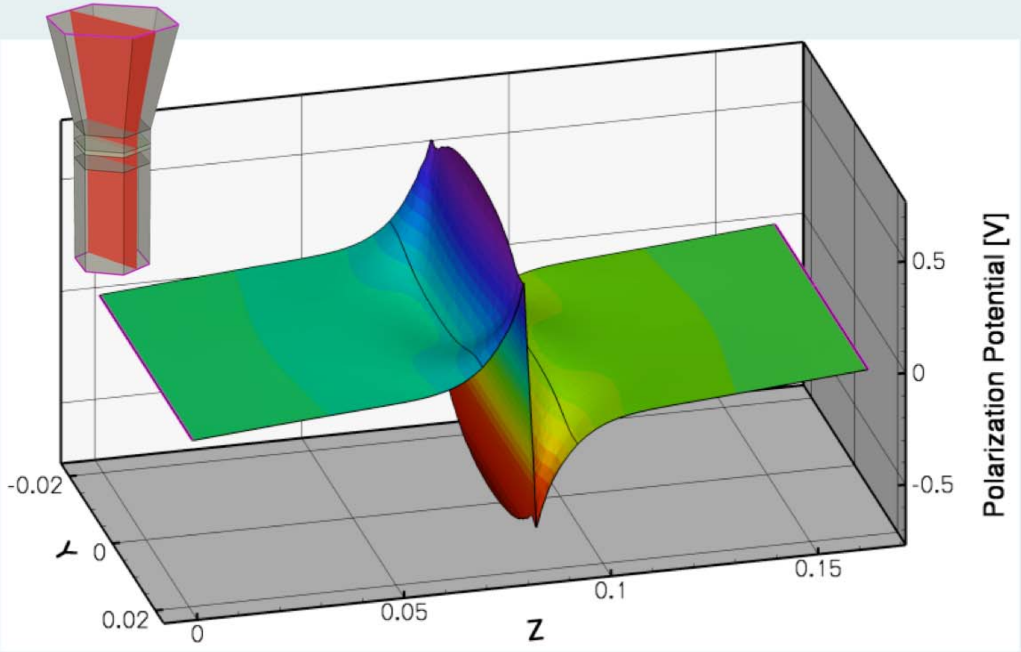
Piezoelectric Potential

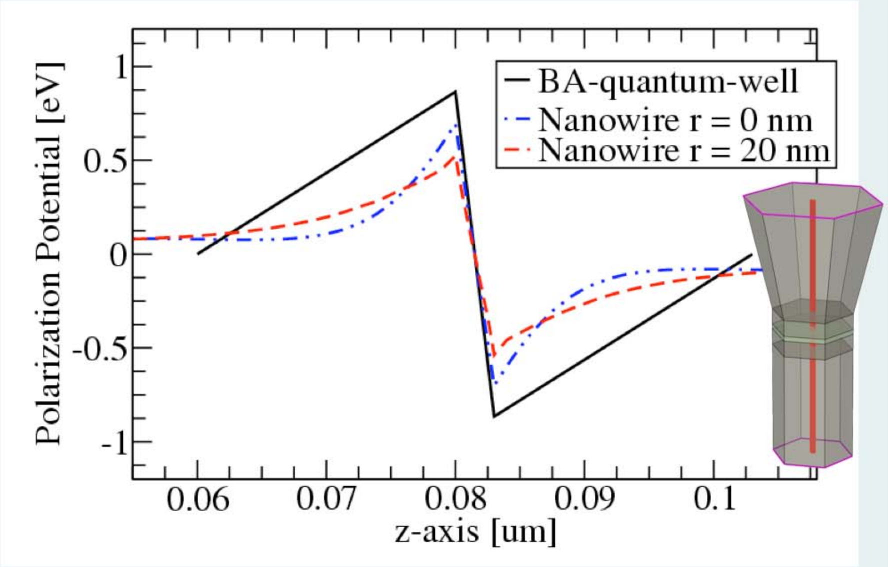
Built-in Field in Nanocolumn

$$P_i(x) = \sum e_{ijk}\varepsilon_{jk} + P_{i,spont.}(x)$$

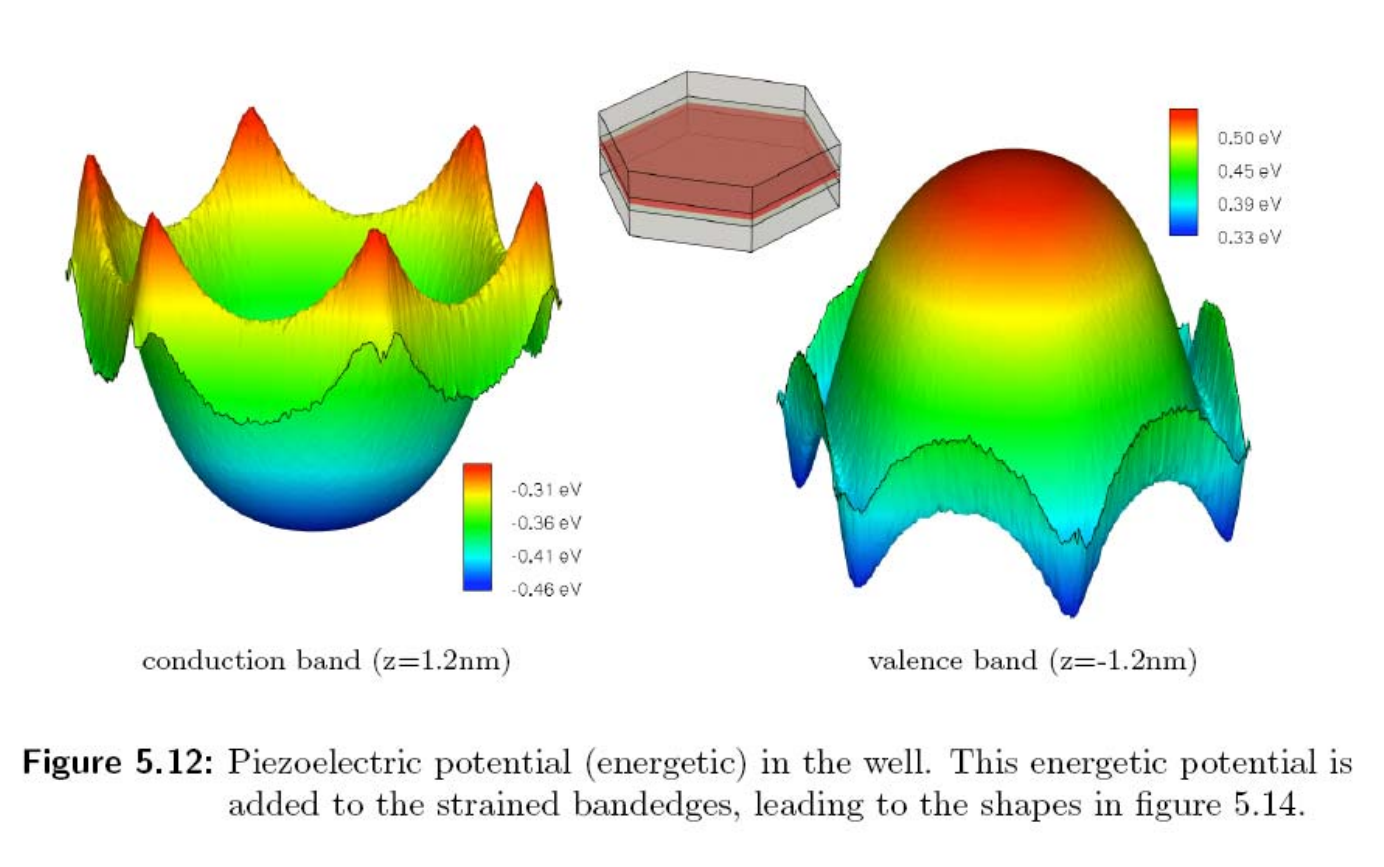
$$\rho = -\nabla \cdot \mathbf{P}$$

Comparison with Biaxial BA Quantum Well





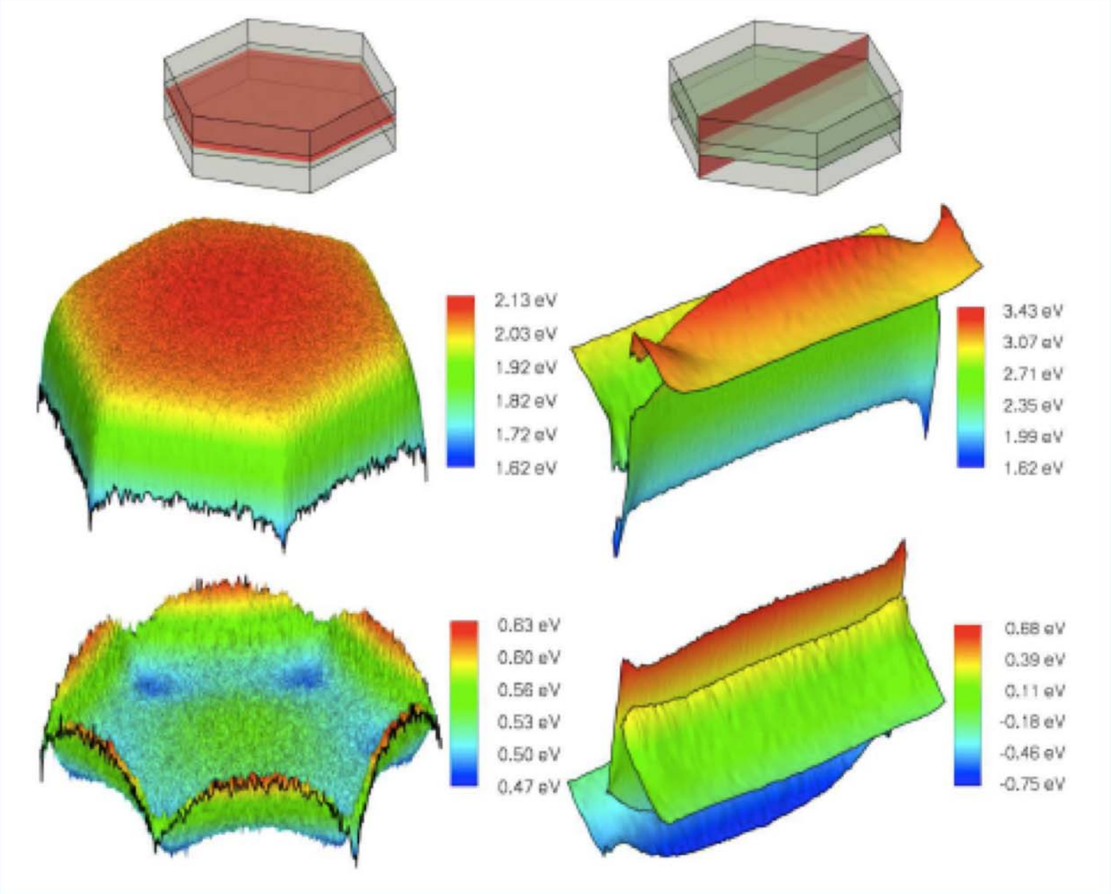
Piezoelectric Potential



conduction band (z=1.2nm) valence band (z=-1.2nm)

Figure 5.12: Piezoelectric potential (energetic) in the well. This energetic potential is added to the strained bandedges, leading to the shapes in figure 5.14.

Total Potential



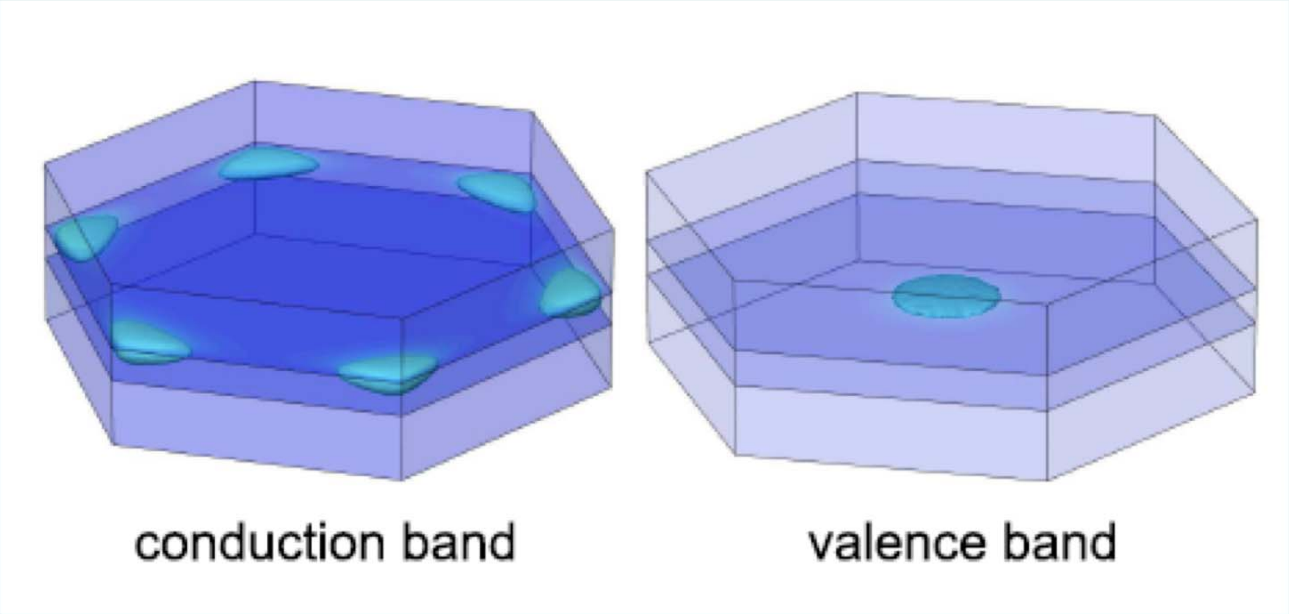
Strain and Piezoelectricity

- Conduction Band: Strain effect dominates
- Valence Band: Piezoelectric Potential dominates

3D Electron-Hole Wavefunctions

Electrons E1

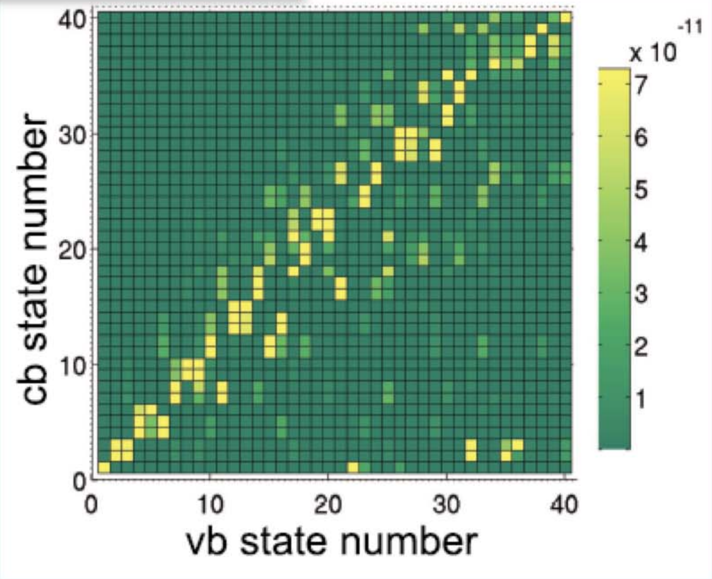
Holes H1



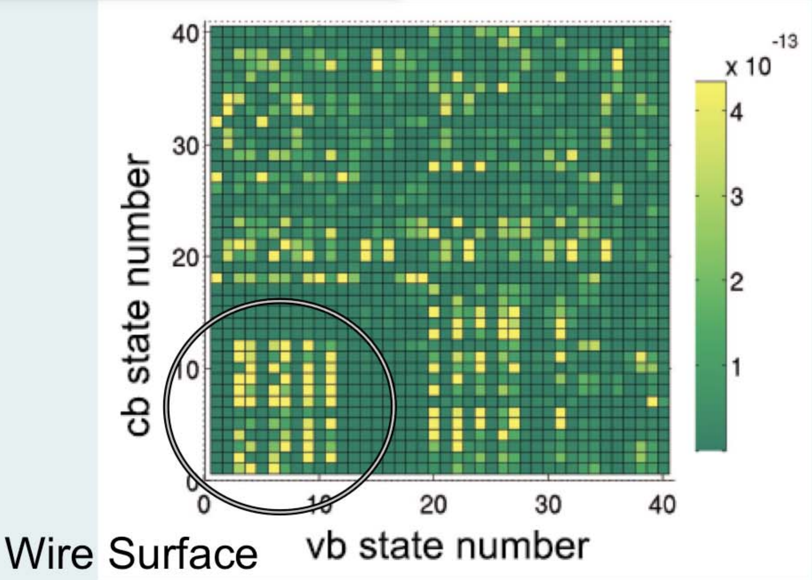
=> Small Wavefunction Overlap for Radiative Recombination

Optical Transition Strength

Unstrained, No Polarization

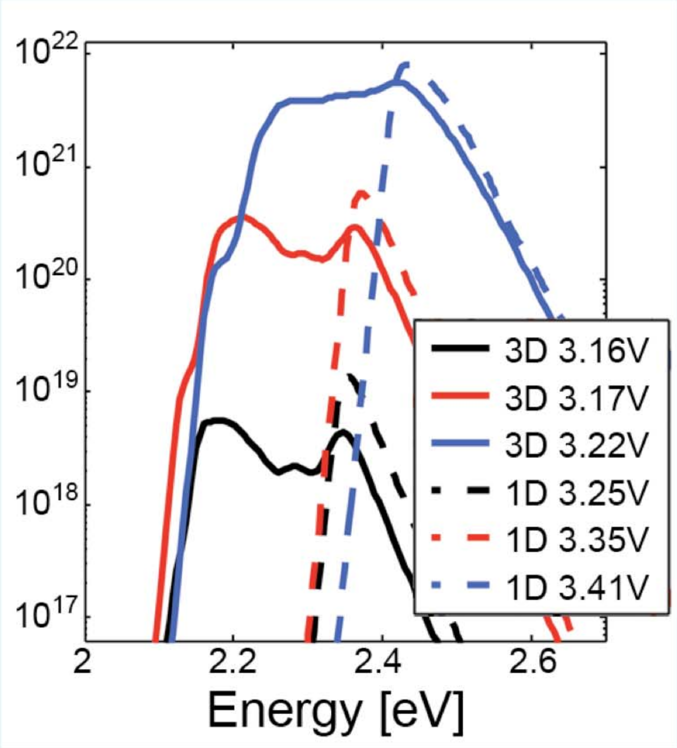


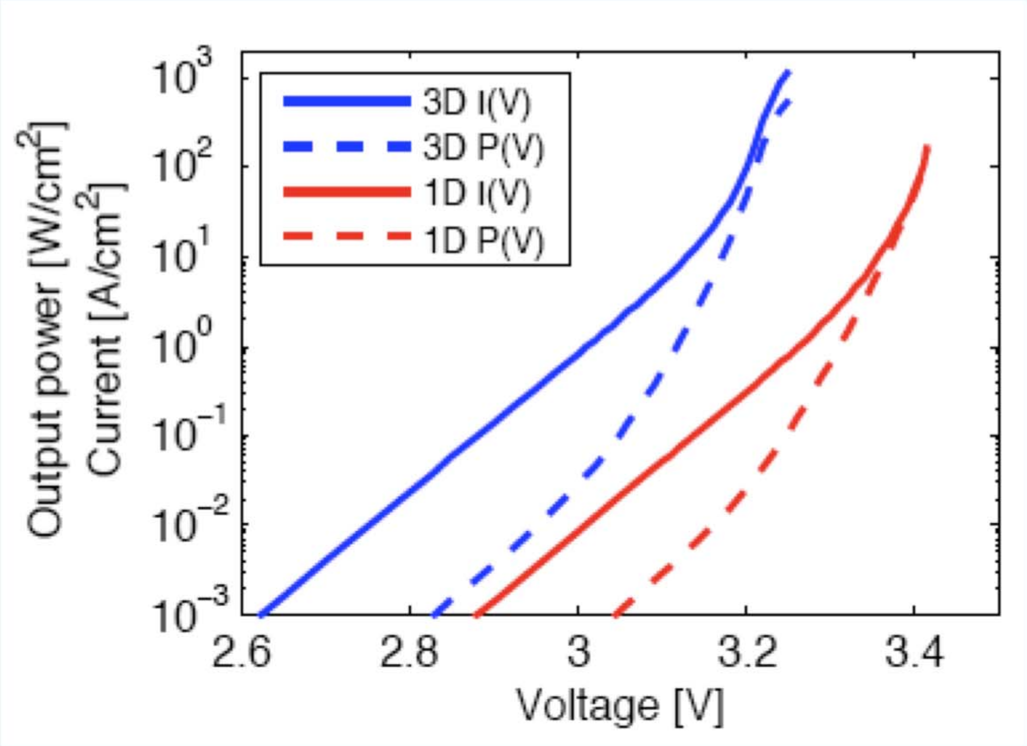
Strained, With Polarization



Strong Transitions occur mainly for states close to the nanocolumn surface

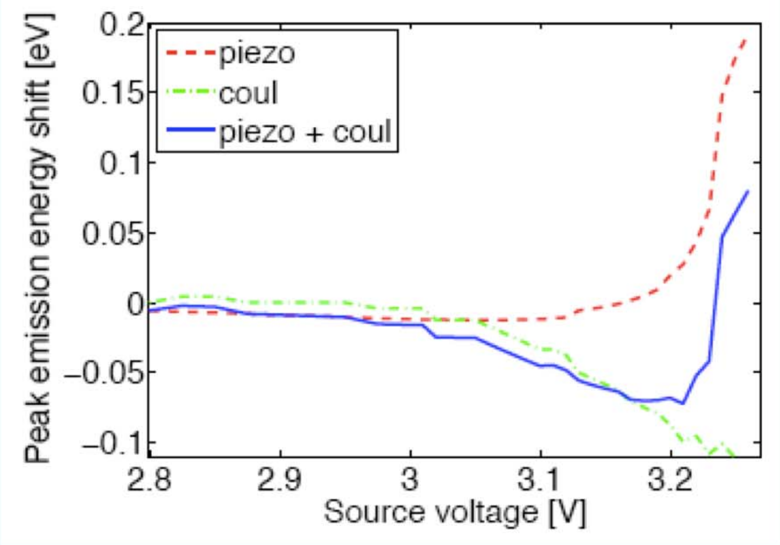
Output Power and Spectrum

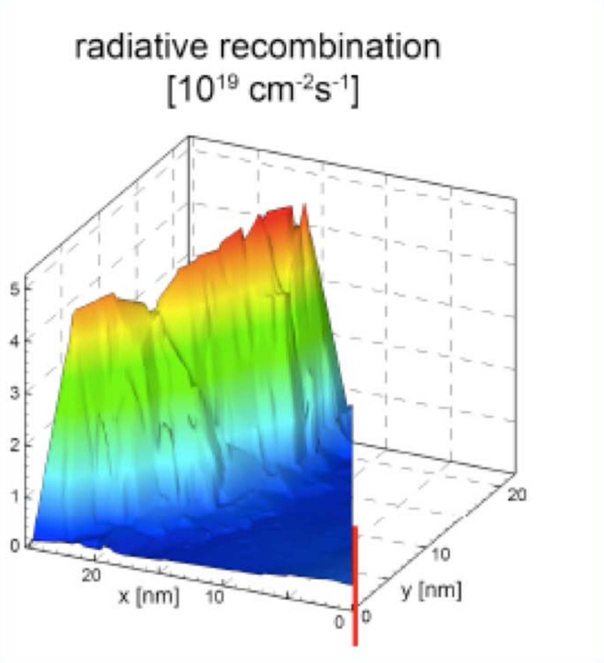


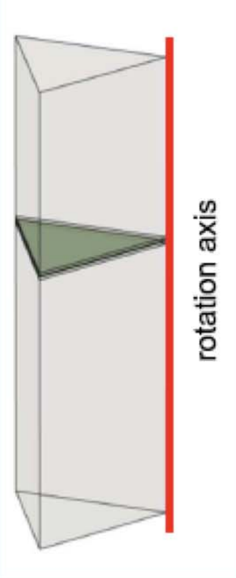


- Comparison of Thin film (‘1D’) and Nanowire (‘3D’) case
- Nanowire shows green/yellow emission (not red…)

Analysis







- Emission mainly from nanowire surface
- Emission energy shift from piezo screening and coulomb renormalization

Open questions

- Indium distribution in Disk
- Wire Surface: Topology and Models
- Nonlinear Piezo effects
- Root cause for red emission

Conclusion

- Nanostructures (still) offer tremendous possibilities for Optoelectronics
- Physics-based Modeling is paramount for Analysis and Design
- Multi-Scale, Multi-Physics Models with various Degrees of Coupling

Thank you for your Attention!