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Modeling of Purely Strain-Induced CEO GaAs/$In_{0.16}Al_{0.84}As$ Quantum Wires

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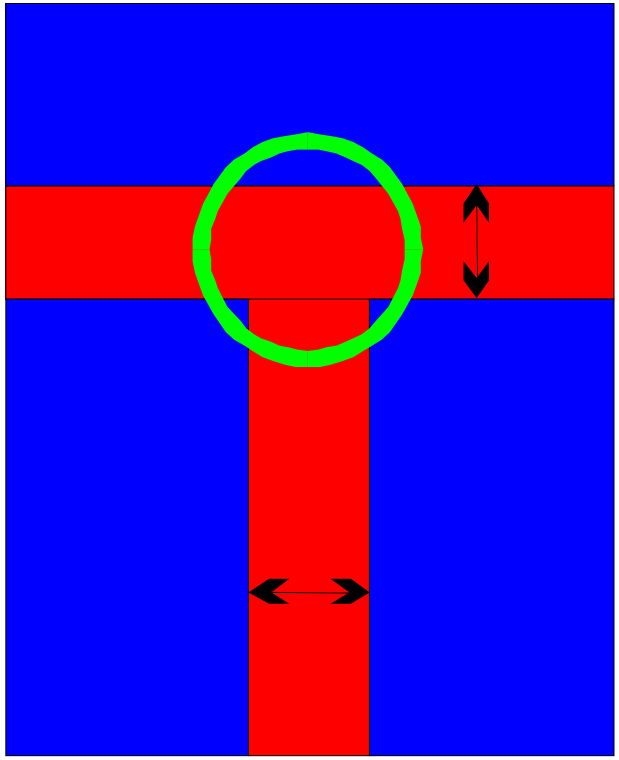
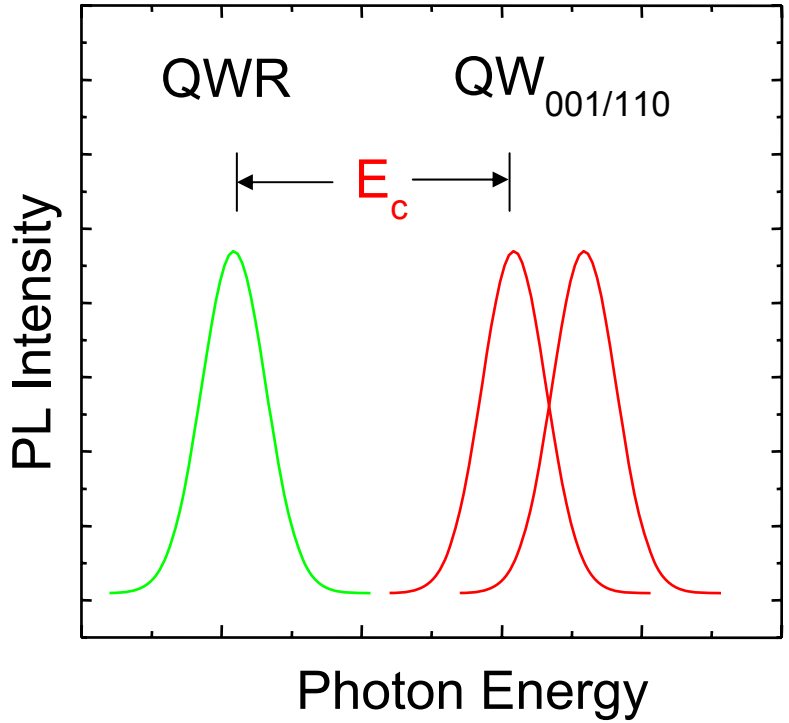
Sample layout

- T-shaped quantum wire at intersection of two QWs





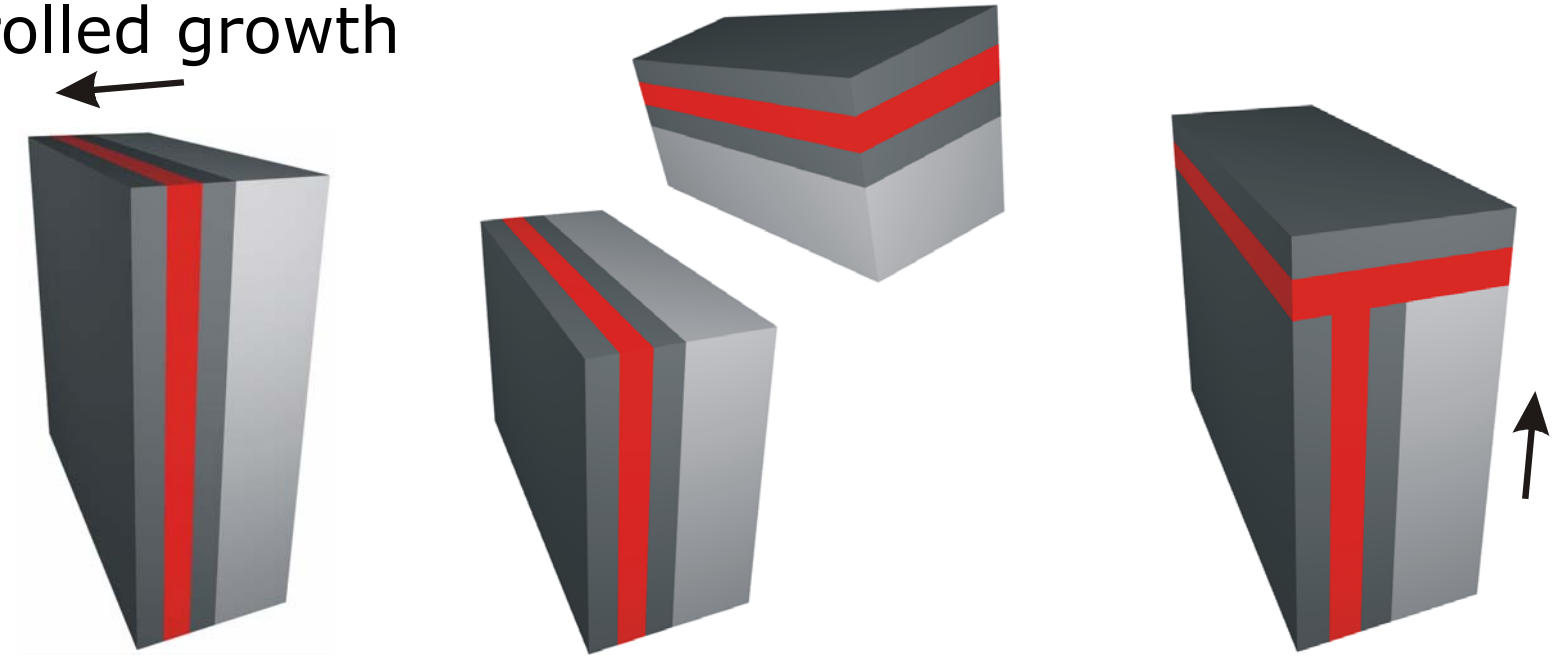
- Cleaved edge overgrowth

Enhance confinement energy E_c to achieve operation at 300 K

Cleaved edge overgrowth

pioneering work by
L. Pfeiffer et al.
*APL **56**, 1697 (1990)*

- Two growth steps
- Flexibility in crystal orientation
- Controlled growth
- MBE

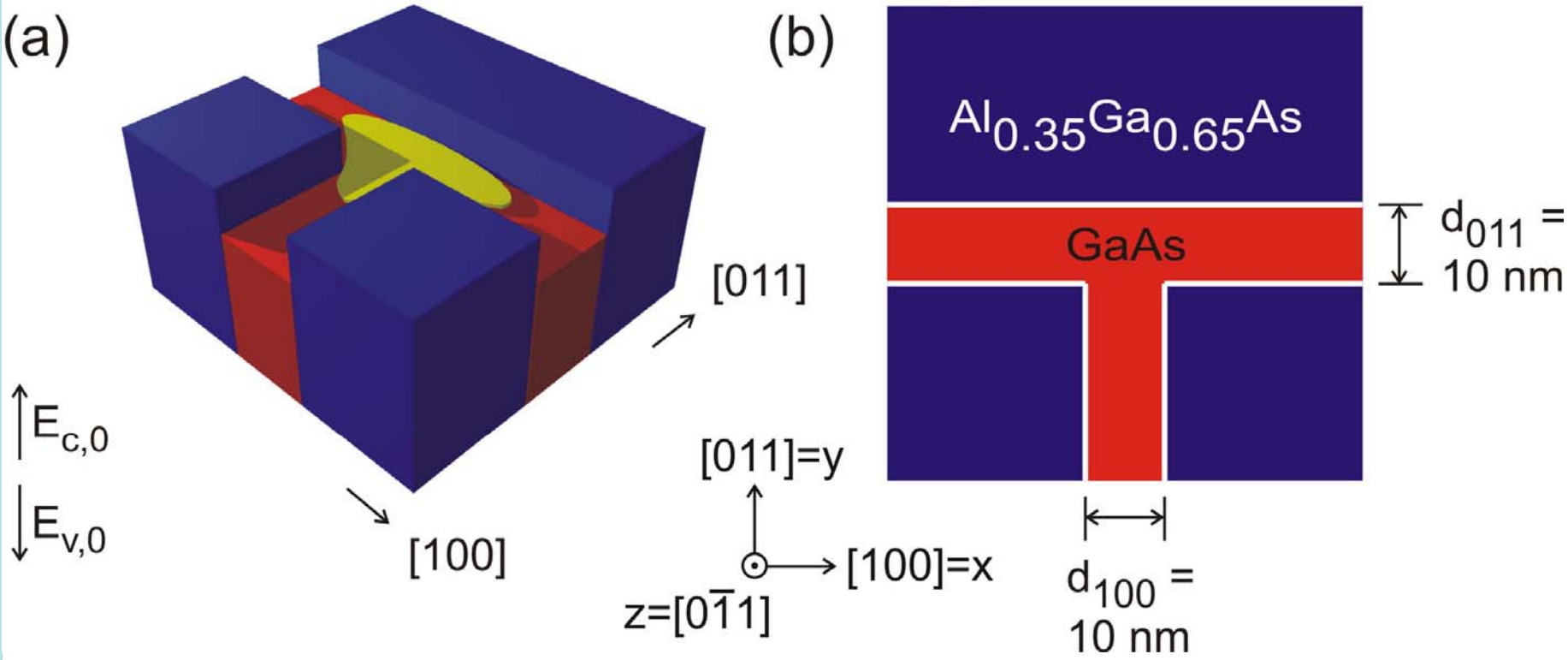


1st growth
[001]-direction

in-situ
cleavage

2nd growth
[110]-direction

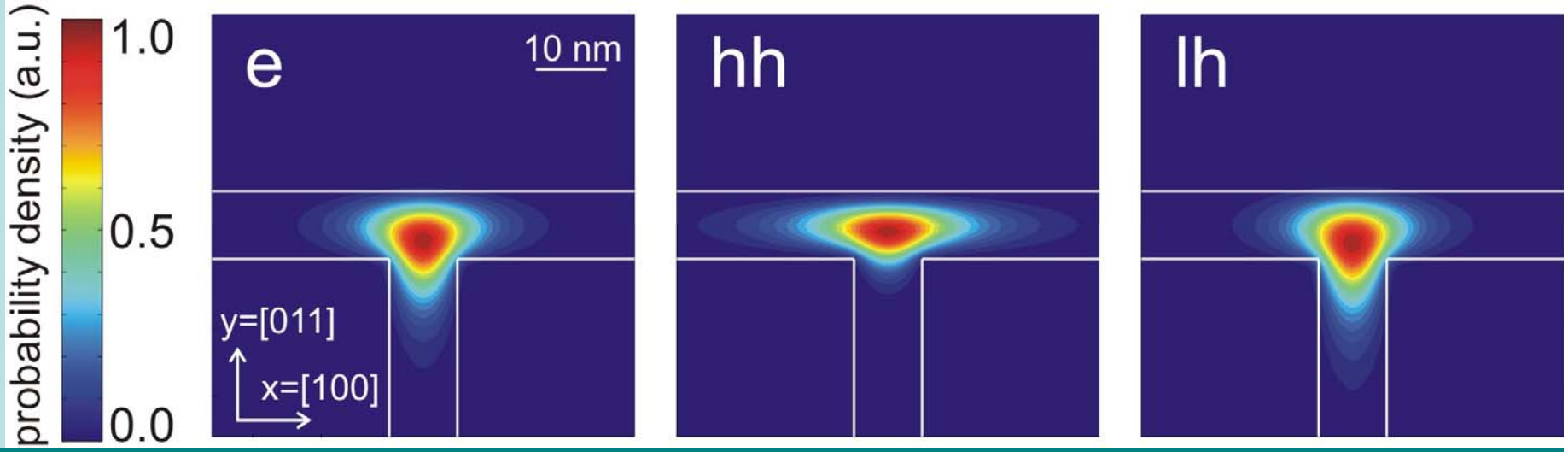
Unstrained quantum wire



Unstrained quantum wire

- electron mass: 0.067
- anisotropic effective mass tensor from Luttinger parameters γ_1, γ_2, γ_3

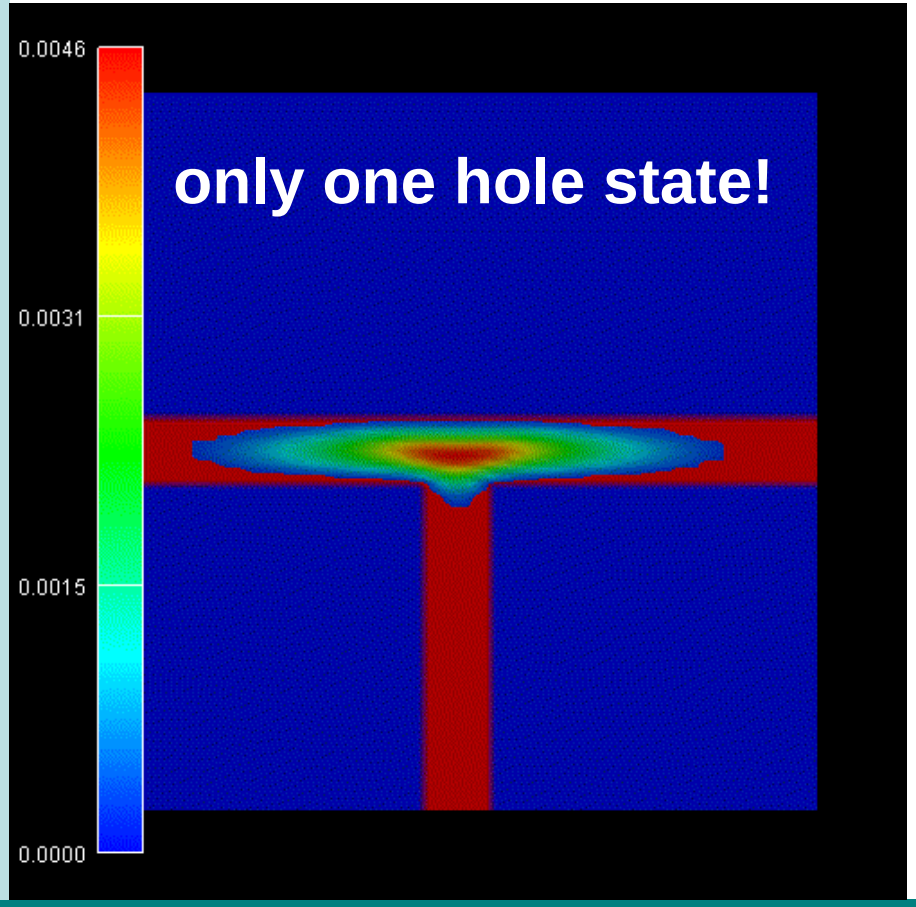
GaAs effective masses		**heavy hole**	**light hole**
along [100] direction	$1 / (\gamma_1 - 2\,\gamma_2)$	0.350	0.090
along [011] direction	$1 / (\gamma_1 - 1/2\,(\gamma_2 + 3\,\gamma_3))$	0.643	0.081
isotropic	$1 / (\gamma_1 \pm 0.8\,\gamma_2 \pm 1.2\,\gamma_3)$	0.551	0.082

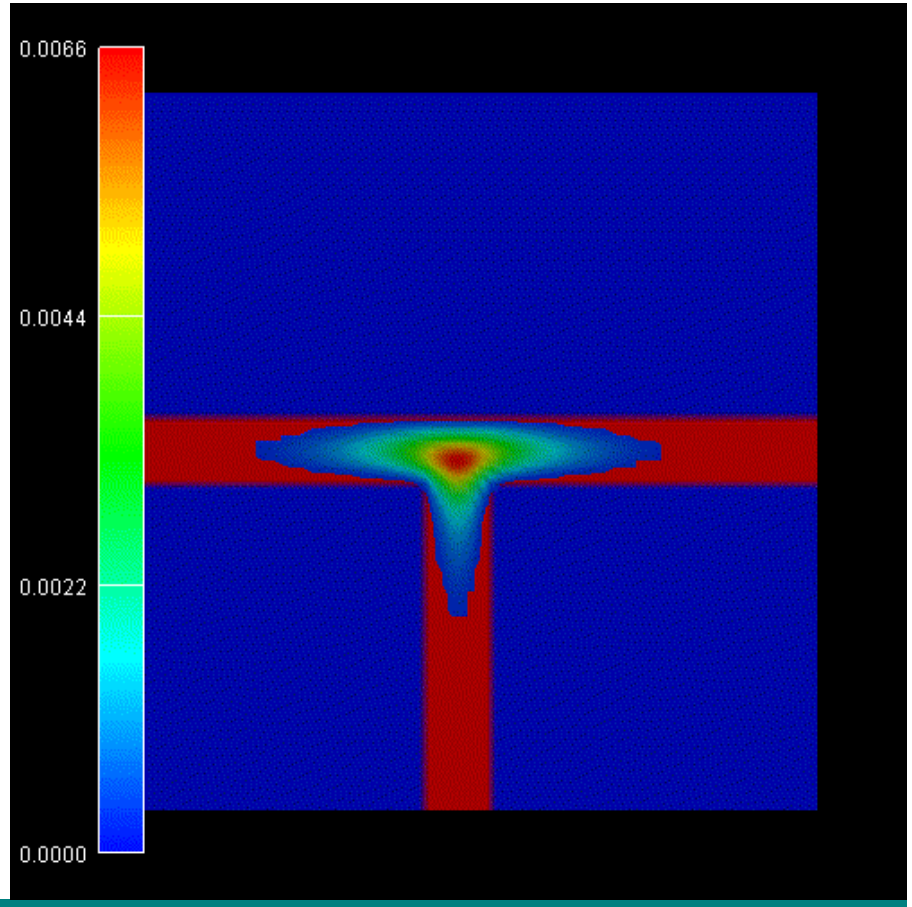


6x6 k.p (Luttinger parameters)

$\gamma_2 \neq \gamma_3$ => **anisotropic** masses

$\gamma_2 = \gamma_3$ => **isotropic** masses





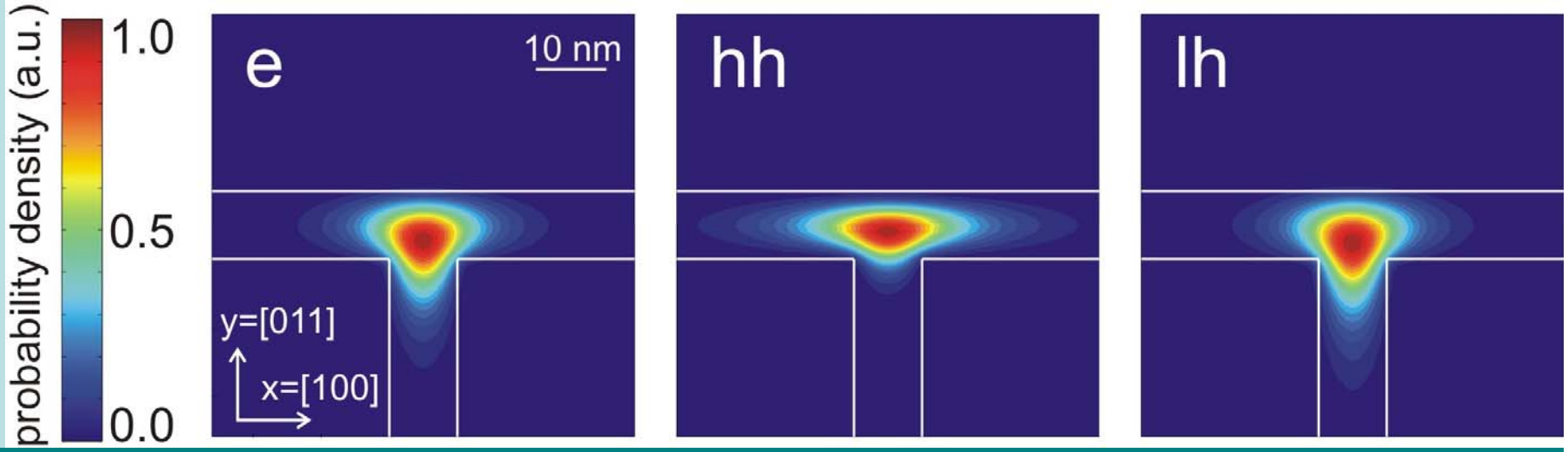
Interband transitions

- interband transitions

$$\left\langle \Psi_i \middle| \varepsilon \cdot \mathbf{p} \middle| \Psi_f \right\rangle \cong \sum_{l,m=1}^{8} \varepsilon \cdot \left\langle u_{f_l} \middle| \mathbf{p} \middle| u_{i_m} \right\rangle \int \psi_{f_l}^{*}(\mathbf{r}) \psi_{i_m}(\mathbf{r})$$

- spatial overlap integrals of envelope functions

electron / heavy hole:	**0.90**	**1.551 eV**
electron / light hole:	**0.99**	**1.567 eV**



Goal: Optimization of sample layout

- Geometry (2D)
- Material composition (huge!)
- Strain
- Piezoelectricity

=> to enhance confinement energies

- In principle, the physics is well understood.
- Individual solutions were demonstrated.
- Experimentalists need a general and easy to use tool to evaluate design.

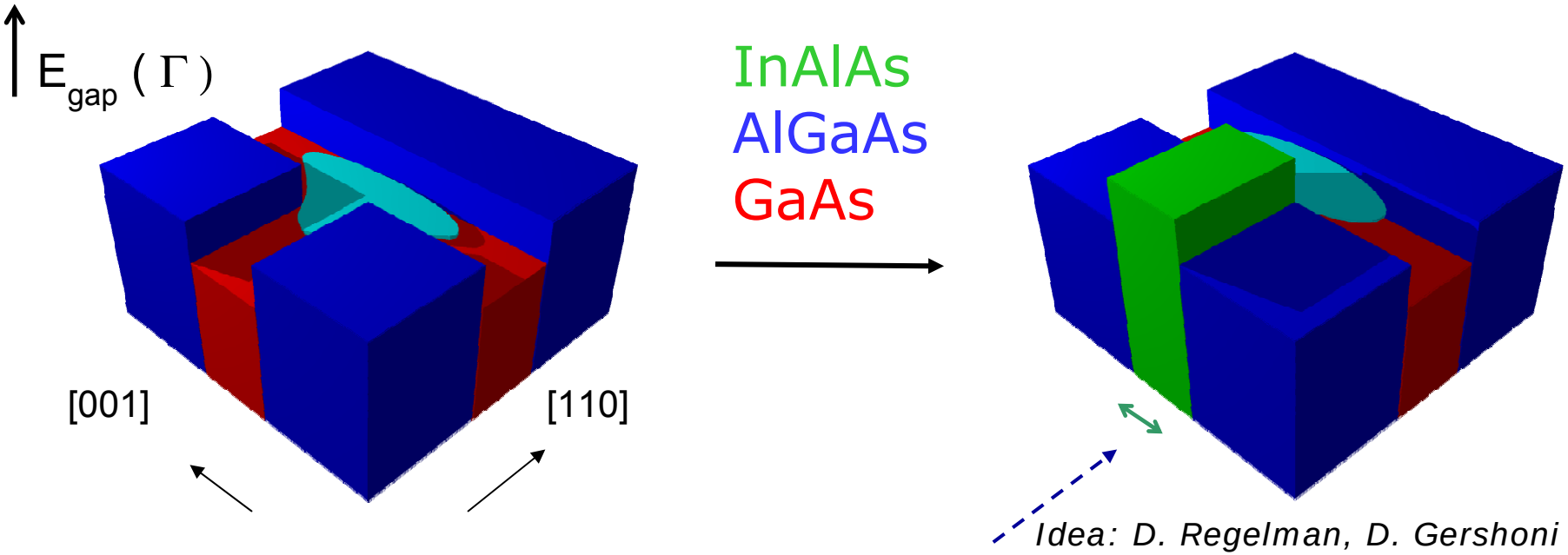
Physics contained in simulations

- strain (elasticity theory) & crystal orientation
- shift of bands (deformation potentials)
- piezoelectric charges (sign of constants)
- 2D Poisson equation
- 2D Schrödinger equation (single-band / **k**.**p**)
- Optical matrix elements (overlap)
- 2D Exciton correction

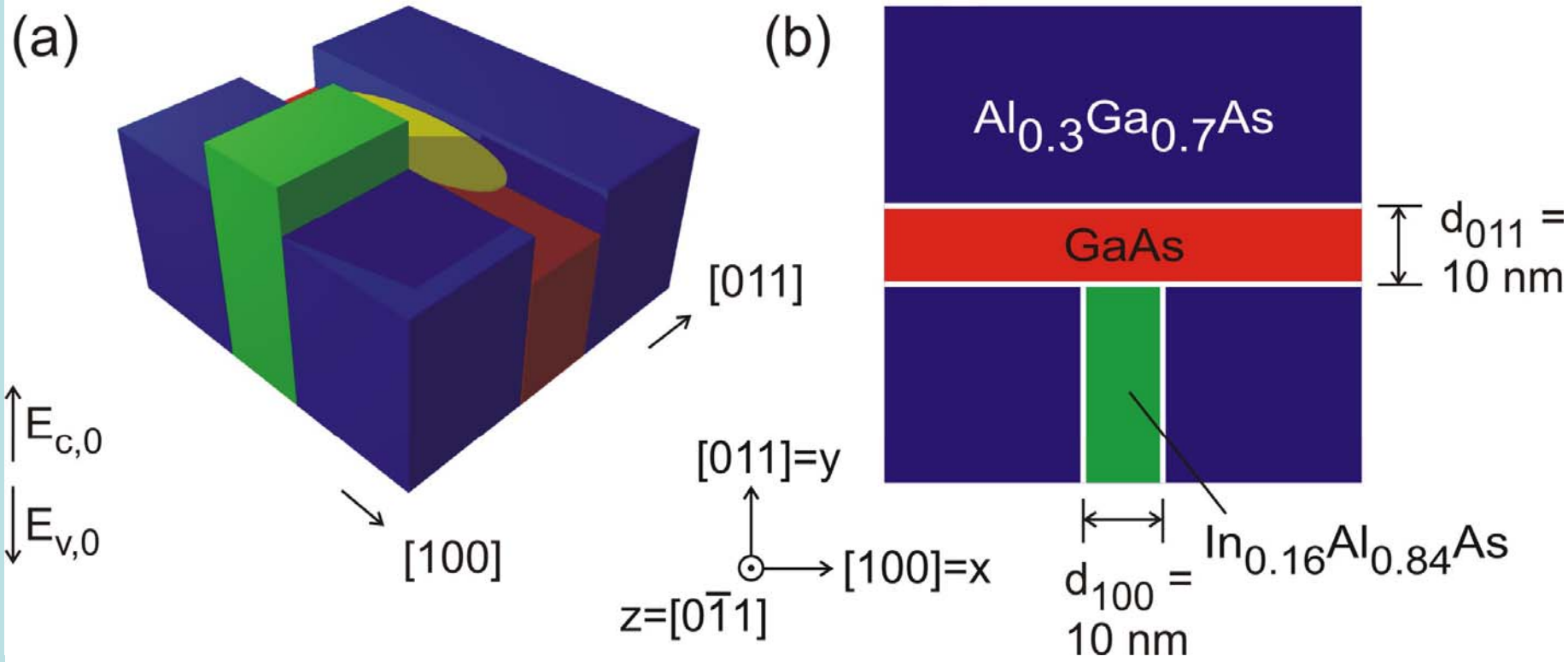
Sample layout (strained)

- GaAs (001) QW replaced by InAlAs stressor layer
- purely strain induced QWRs
- confinement energies of up to 90 meV predicted

M. Grundmann, O. Stier, A. Schliwa, D. Bimberg, Phys. Rev. B 61, 1744 (2000)



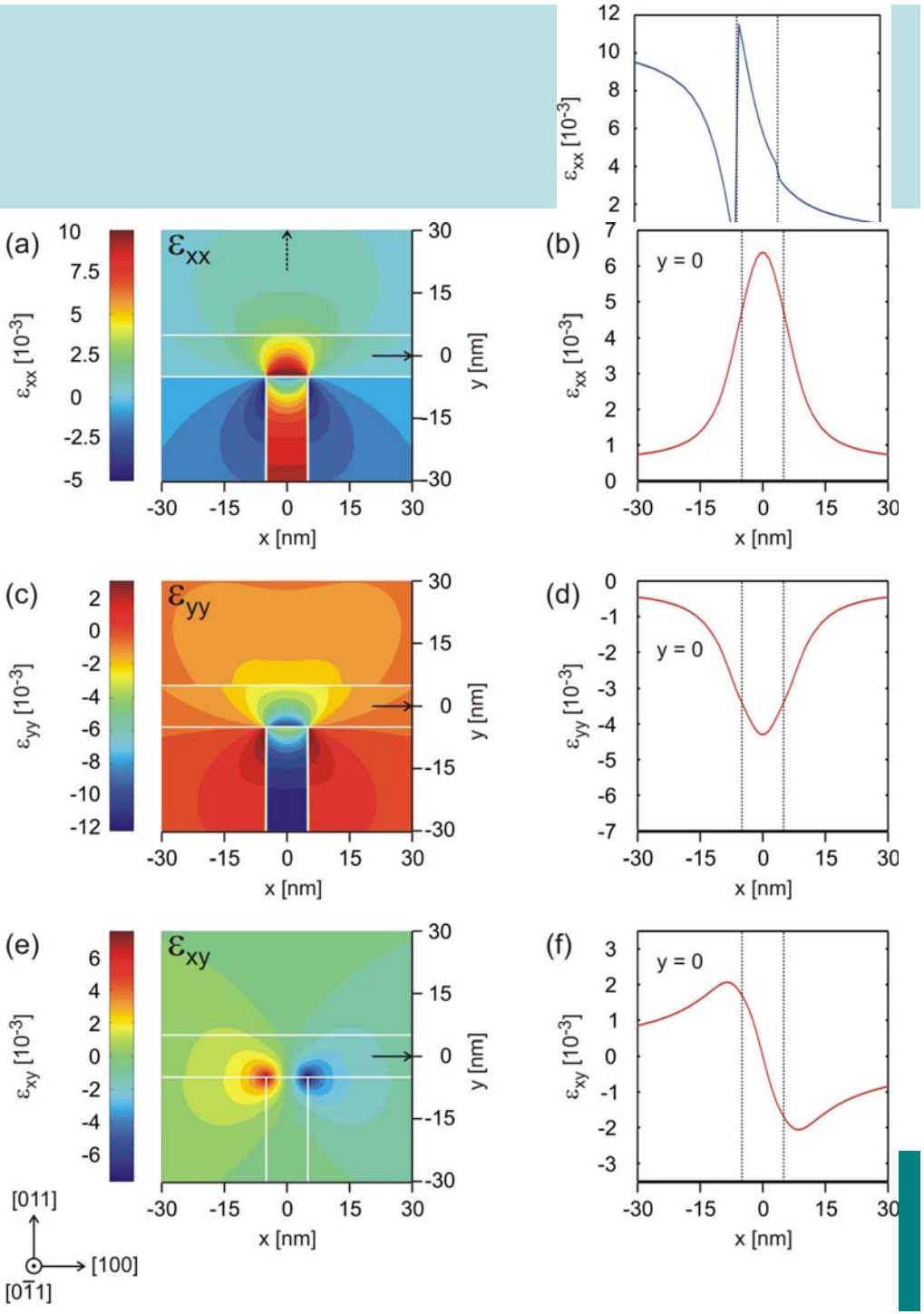
Sample layout (strained)



Strain tensor

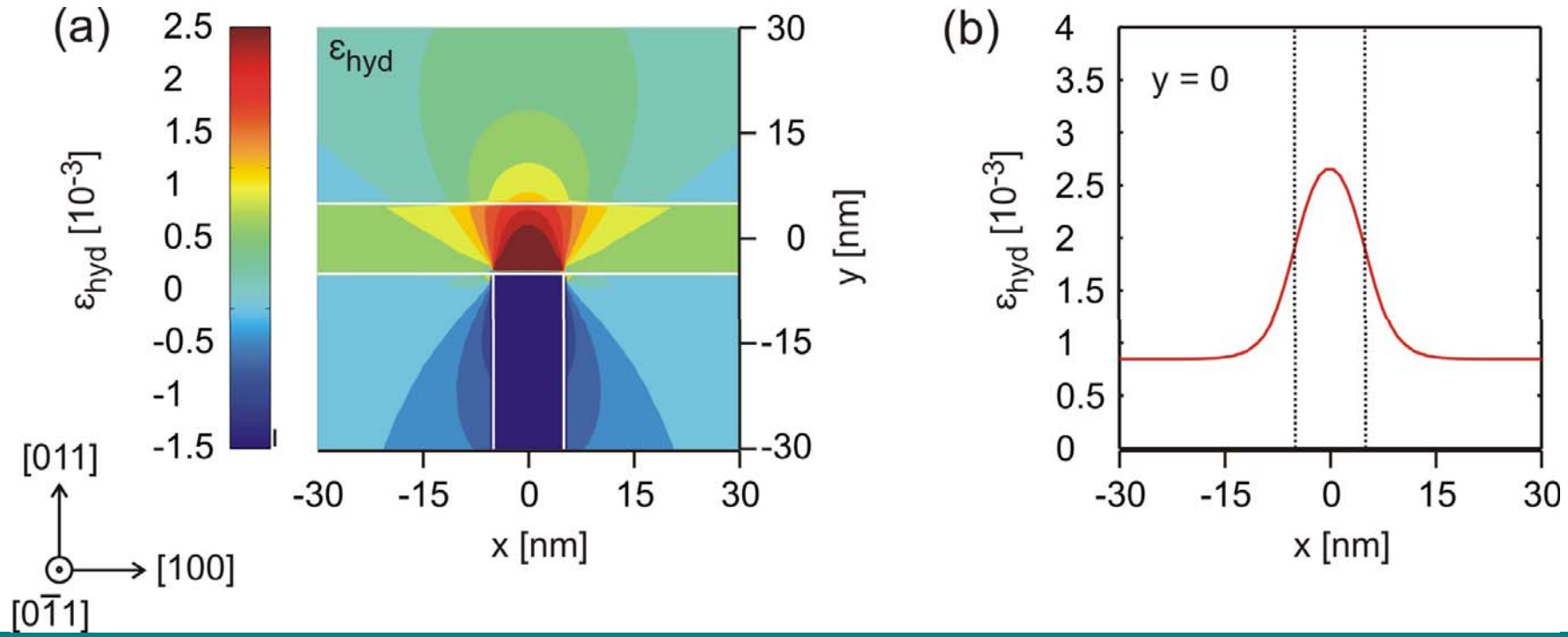
- off-diagonal components of strain tensor
- reduced symmetry

$$\sqrt{3}d\varepsilon_{xy}$$



Hydrostatic strain

- hydrostatic strain $Tr(e_{ij})$
- reduced band gap at intersection
- confinement purely due to strain



Deformation potentials

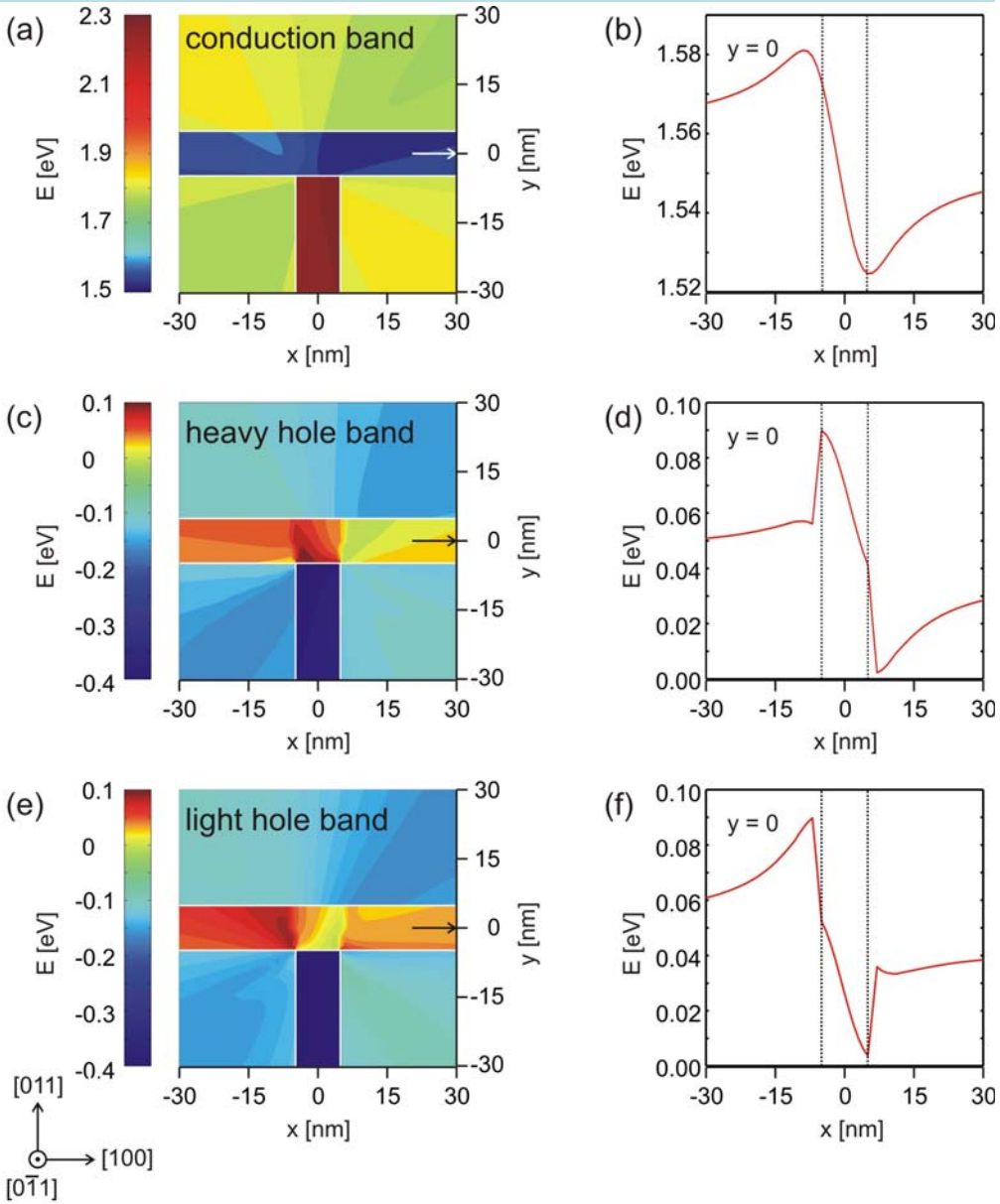
- absolute valence band def. potential
- absolute conduction band def. potential

$$E_c = E_{c,0} + a_{c,\Gamma}\, \varepsilon_{hydro}$$
$$E_{v,av} = E_{v,av,0} + a_v\, \varepsilon_{hydro}$$

- uniaxial / biaxial def. potentials
- obtain energy edges by diagonalizing 8x8 **k.p** Hamiltonian

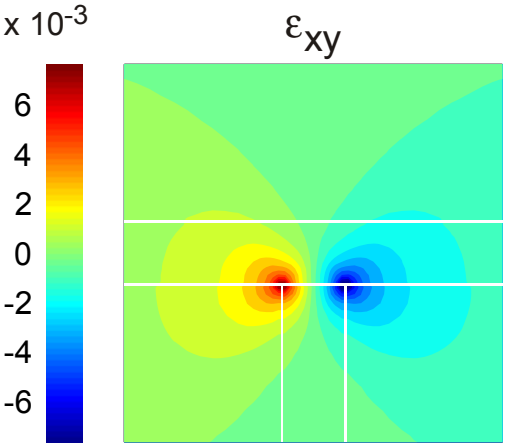
Conduction and valence band edges

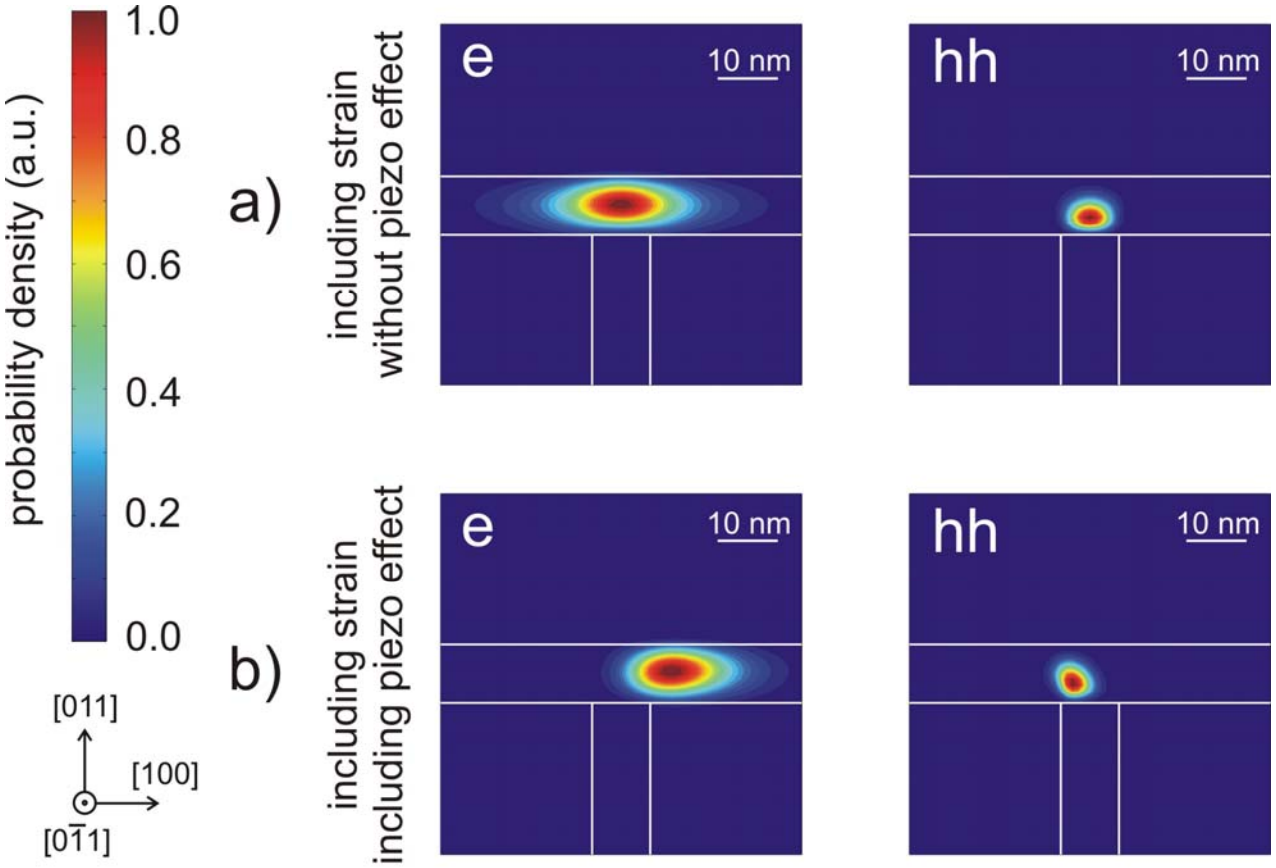
- Band profile due to
  - strain
  - piezo charges
- Minimum of conduction and valence bands spatially separated
- HH very different from LH



Wavefunctions (Piezoeffect!)

- separation of electron & hole
- reduced overlap
- reduced symmetry

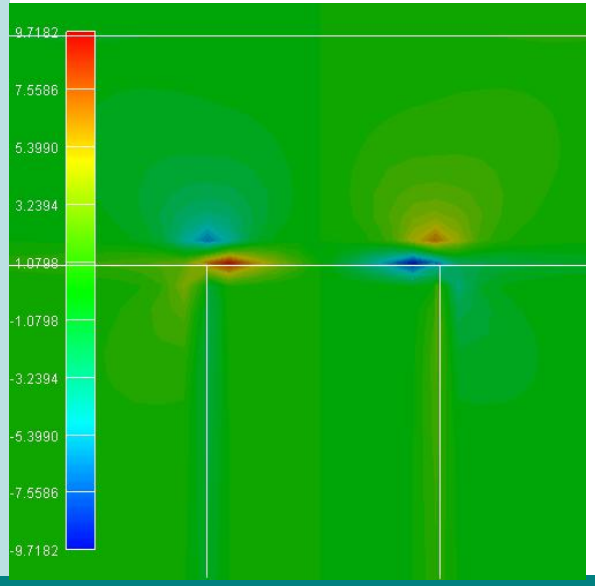


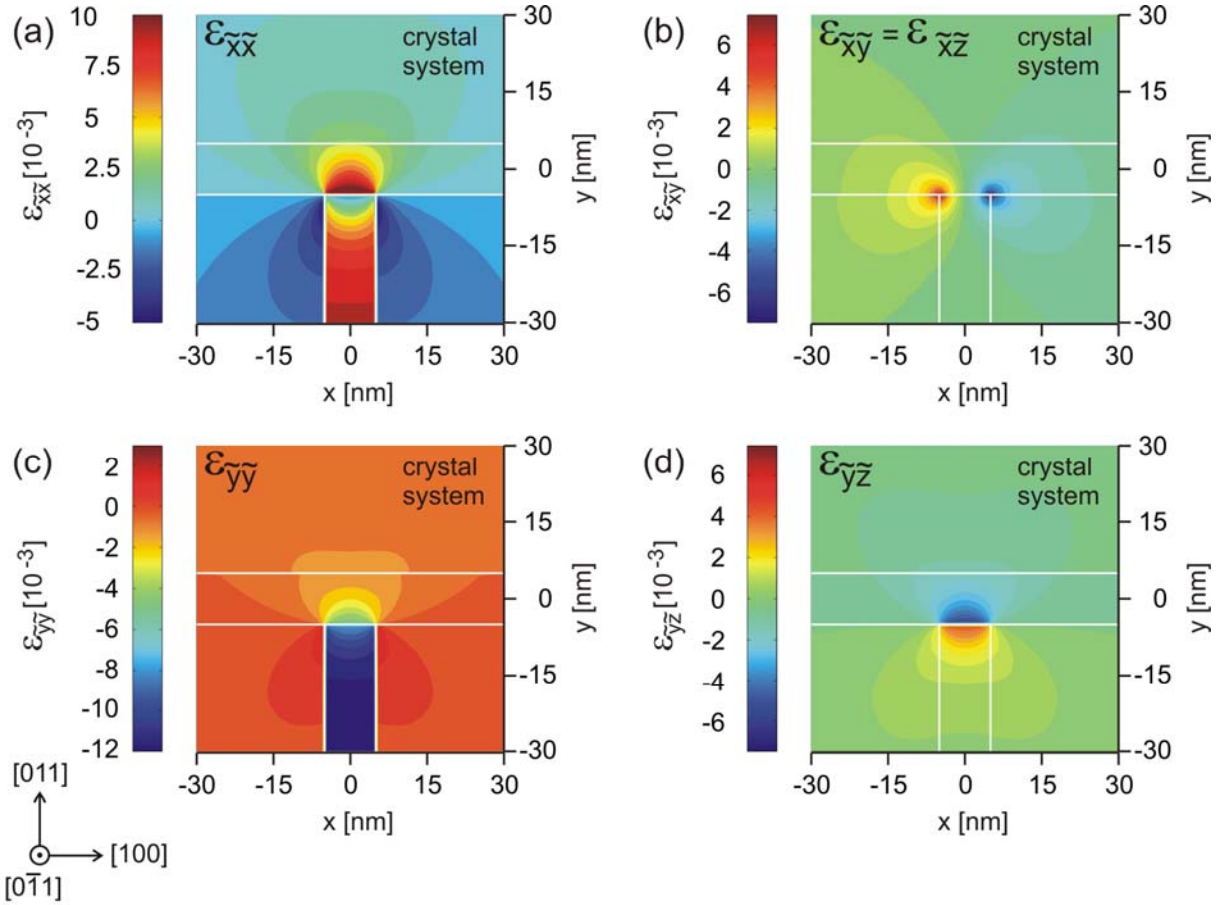


Piezoeffect: Crystal vs. sim. system

$$\mathbf{P}_{pz} = e_{14}\begin{pmatrix} 2\varepsilon_{yz} \\ 2\varepsilon_{xz} \\ 2\varepsilon_{xy} \end{pmatrix}$$

$$\rho_{pz} = -\nabla \cdot \mathbf{P}^{pz}$$





Several effects have to be considered

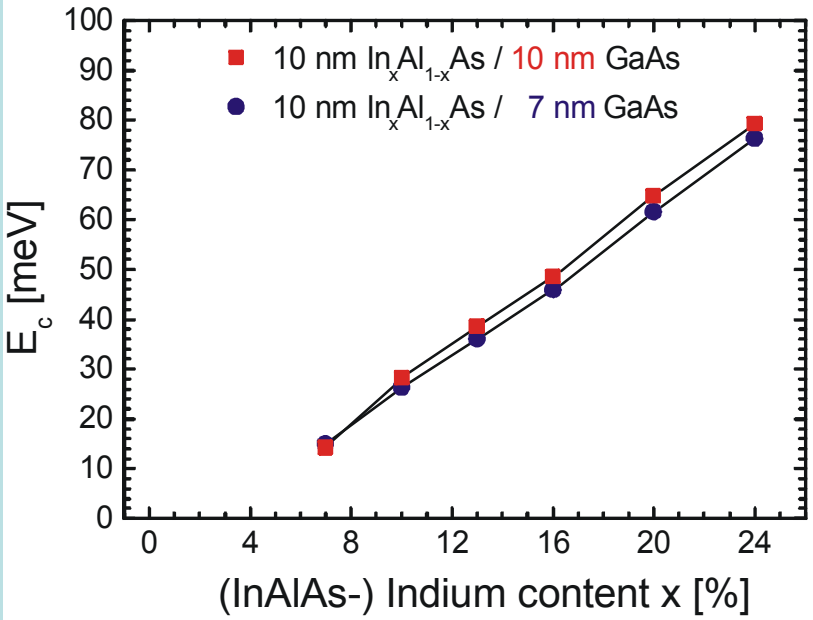
Conduction and valence band edges are influenced by

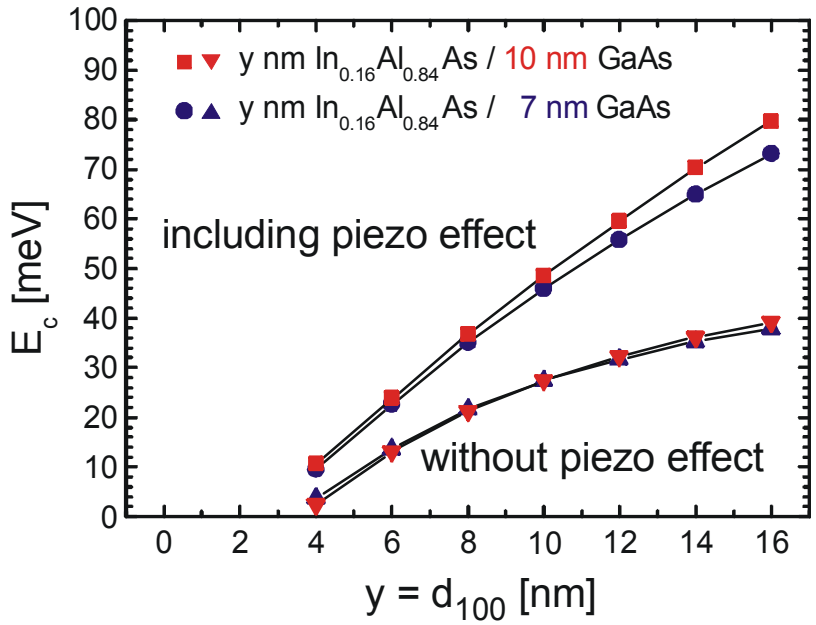
- Strain (including off-diagonal strain components)
- Piezoelectric charge -> Poisson equation

In 2D/3D simulations, the resulting band edges can only be obtained by numerical computations.

Simulation results

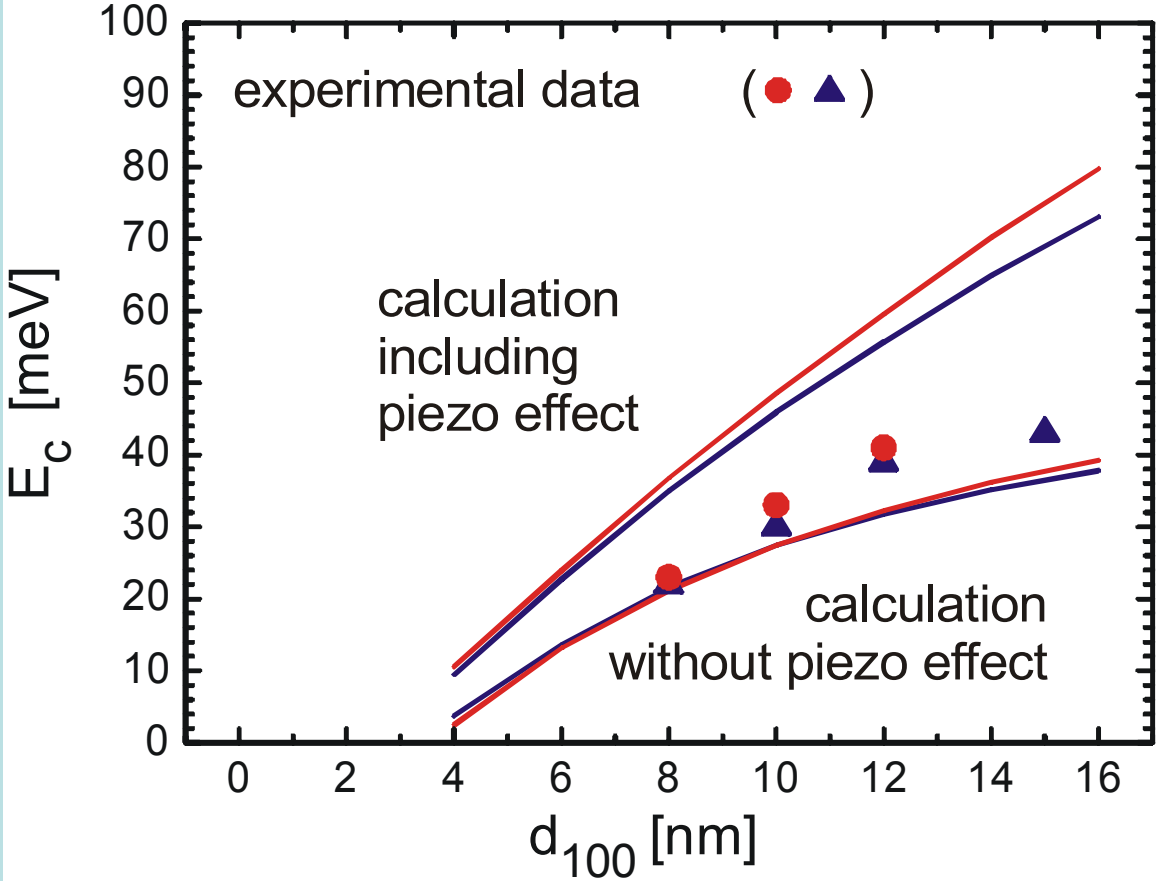
- variation of In content (InAlAs strain)
- variation of GaAs QW thickness
- variation of InAlAs thickness





Simulation vs. experiment

- the trends are well reproduced



	d_{011}	exp.	th.
A	7 nm	▲	—
B	10 nm	●	—

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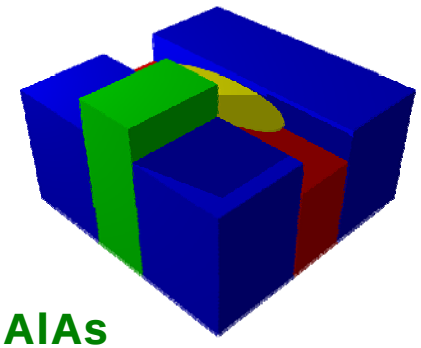
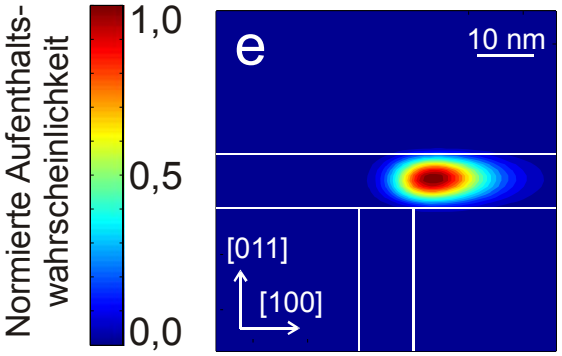
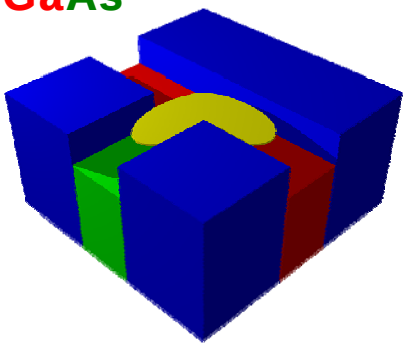
Experiments

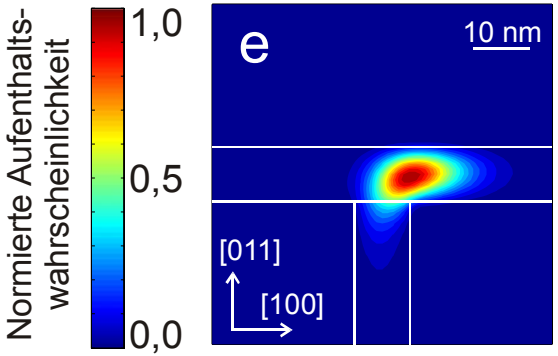
- Confinement energy vs. layer thickness
  strong confinement ~51.5 meV
- Trend is well reproduced
- Piezo effect is good for confinement energies
  but bad for overlap
- Suggestion: $In_{0.16}Al_{0.84-x}Ga_xAs$
  increasing x: band gap gets smaller, strain unaffected, for x=0.7 electron close to center
- Promising concept for quantum wires at RT

Suggestion





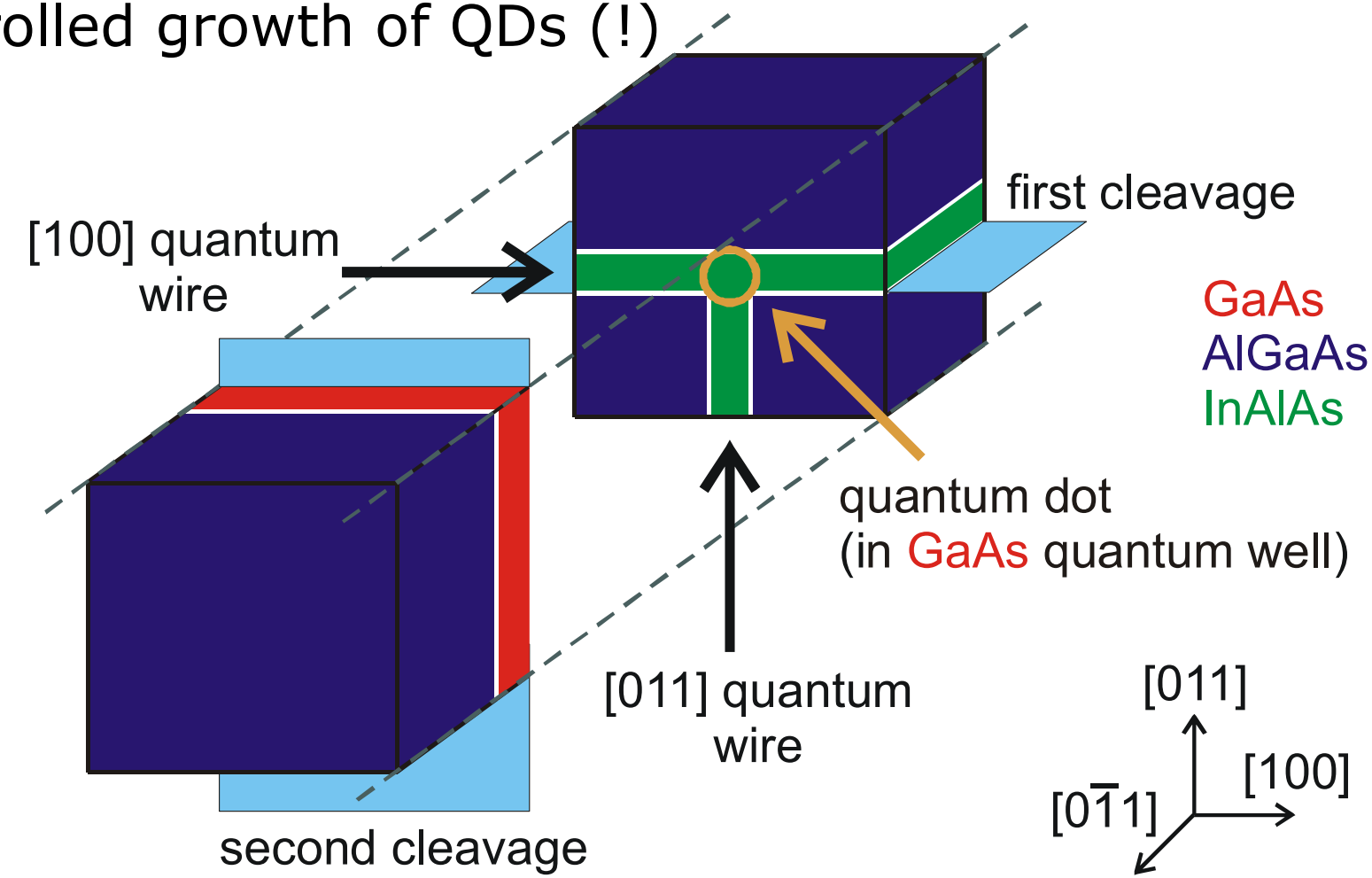




- use quaternary material $In_{0.16}Al_{0.14}\mathbf{Ga}_{0.70}As$
- enhanced overlap

Suggestion: CEO Quantum Dots

- controlled growth of QDs (!)



Outlook

- 2D exciton correction demonstrated (not implemented yet)
- $k_{||}=k_z\neq 0$ dispersion
- Oscillator strength / optical transitions (interband matrix elements)
- single-band vs. 8x8 **k.p**

- Kwan Lee's talk on InGaN quantum dots (Oxford)
- next**nano**^{3} workshop on Friday, 13:30-17:00

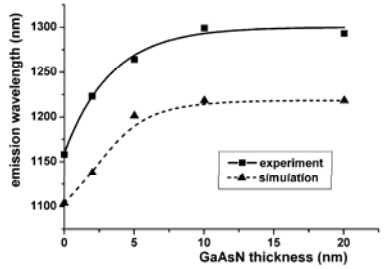
Conclusion

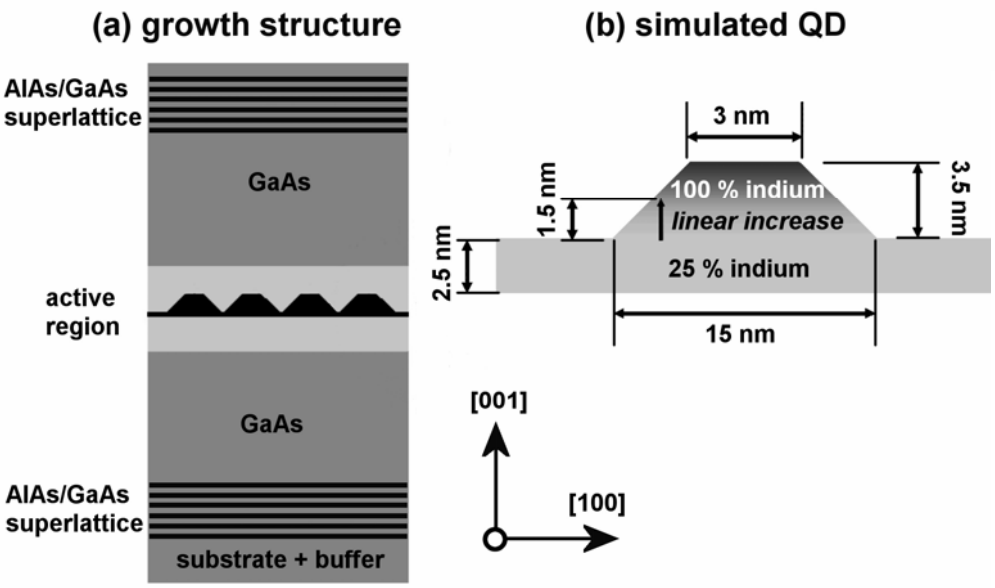
- InAlAs layer in a CEO structure leads to purely strain induced QWR
- Variation of layer thickness in simulation and experiment

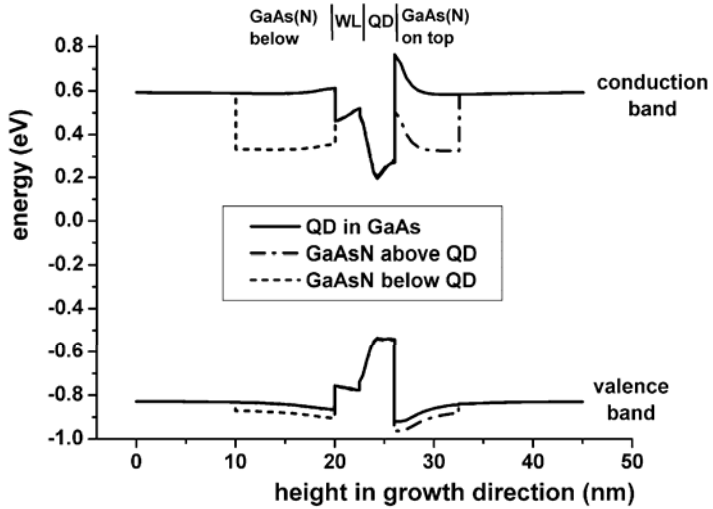
  -> Trends of confinement energies can be reproduced
- Structure shows a strong charge carrier confinement
- Predictions to improve performance

Further work on optics*

- Diluted nitrides: GaAs**N** / InGaAs**N**
  => conduction band energy
- QDs: Variation of capping material







- QWs: Use absorption spectra to extract band offsets

*Infineon Technologies, CPR Photonics Group