Modeling of Purely Strain-Induced CEO GaAs/In$_{0.16}$Al$_{0.84}$As Quantum Wires

Stefan Birner$^1$, Robert Schuster$^2$, Michael Povolotskyi$^3$, Peter Vogl$^1$

$^1$ nextnano$^3$ & Walter Schottky Institute, TU Munich
$^2$ University of Regensburg
$^3$ University of Rome “Tor Vergata”
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

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

1\textsuperscript{st} growth [001]-direction
in-situ cleavage
2\textsuperscript{nd} growth [110]-direction

Pioneering work by L. Pfeiffer et al.
APL 56, 1697 (1990)
Unstrained quantum wire
Unstrained quantum wire

- electron mass: 0.067
- anisotropic effective mass tensor from Luttinger parameters $\gamma_1, \gamma_2, \gamma_3$

<table>
<thead>
<tr>
<th>GaAs effective masses</th>
<th>heavy hole</th>
<th>light hole</th>
</tr>
</thead>
<tbody>
<tr>
<td>along [100] direction</td>
<td>$1 / (\gamma_1 - 2 \gamma_2)$</td>
<td>0.350</td>
</tr>
<tr>
<td>along [011] direction</td>
<td>$1 / (\gamma_1 - 1/2 (\gamma_2 + 3 \gamma_3))$</td>
<td>0.643</td>
</tr>
<tr>
<td>isotropic</td>
<td>$1 / (\gamma_1 \pm 0.8 \gamma_2 \pm 1.2 \gamma_3)$</td>
<td>0.551</td>
</tr>
</tbody>
</table>
$\gamma_2 \neq \gamma_3 \Rightarrow \text{anisotropic masses}$

$\gamma_2 = \gamma_3 \Rightarrow \text{isotropic masses}$

only one hole state!
**Interband transitions**

- **interband transitions**

\[ \langle \Psi_i | \varepsilon \cdot p | \Psi_f \rangle \cong \sum_{l,m=1}^{8} \varepsilon \cdot \langle u_{f_{l}} | p | u_{i_{m}} \rangle \int \psi_{f_{l}}^{*} (r) \psi_{i_{m}} (r) \]

- **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 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 / $k \cdot p$)
- 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


InAlAs AlGaAs GaAs

$E_{gap\ (\Gamma)}$

[001] [110]

Idea: D. Regelman, D. Gershoni
Sample layout (strained)

- $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$
- $\text{GaAs}$
- $\text{In}_{0.16}\text{Al}_{0.84}\text{As}$

Dimensions:
- $d_{011} = 10\ \text{nm}$
- $d_{100} = 10\ \text{nm}$
Strain tensor

- off-diagonal components of strain tensor
- reduced symmetry

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

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

![Diagram showing hydrostatic strain distribution with contours and axes for x and y in nanometers.](image)
Deformation potentials

- absolute valence band def. potential
  \[ E_c = E_{c,0} + a_{c,\Gamma} \varepsilon_{\text{hydro}} \]
- absolute conduction band def. potential
  \[ E_{v,av} = E_{v,av,0} + a_v \varepsilon_{\text{hydro}} \]
- uniaxial / biaxial def. potentials
- obtain energy edges by diagonalizing 8x8 \textbf{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

![Graph and images showing wavefunctions with and without piezoeffect]
Piezoeffect: Crystal vs. sim. system

\[
P_{pz} = e_{14} \begin{pmatrix} 2\varepsilon_{yz} \\ 2\varepsilon_{xz} \\ 2\varepsilon_{xy} \end{pmatrix}
\]

\[
\rho_{pz} = -\nabla \cdot P^{pz}
\]
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

<table>
<thead>
<tr>
<th>d_{011}</th>
<th>exp. th.</th>
</tr>
</thead>
<tbody>
<tr>
<td>A 7 nm</td>
<td>▲</td>
</tr>
<tr>
<td>B 10 nm</td>
<td>▰</td>
</tr>
</tbody>
</table>

Experimental data (● ▲)

Calculation including piezo effect
Calculation without piezo effect

Stefan Birner
Experiments

- Confinement energy vs. layer thickness
  strong confinement $\sim 51.5$ meV
- Trend is well reproduced
- Piezo effect is good for confinement energies but bad for overlap
- Suggestion: $\text{In}_{0.16}\text{Al}_{0.84-x}\text{Ga}_x\text{As}$
  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 $\text{In}_{0.16}\text{Al}_{0.14}\text{Ga}_{0.70}\text{As}$
- enhanced overlap
Suggestion: CEO Quantum Dots

- controlled growth of QDs (!)

Diagram:

- [100] quantum wire
- [011] quantum wire
- first cleavage
- quantum dot (in GaAs quantum well)

Materials:
- GaAs
- AlGaAs
- InAlAs
Outlook

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

- Kwan Lee’s talk on InGaN quantum dots (Oxford)
- nextnano³ 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**: $\text{GaAs}_N / \text{InGaAs}_N$
  $\Rightarrow$ conduction band energy
- **QDs**: Variation of capping material

- **QWs**: Use absorption spectra to extract band offsets

*Infineon Technologies, CPR Photonics Group

Stefan Birner