Carrier confining mechanisms in axial $In_xGa_{1-x}N/GaN$ nanowire heterostructures

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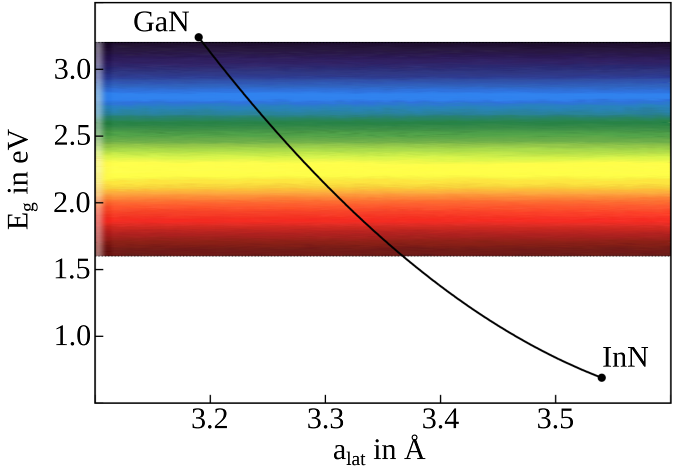
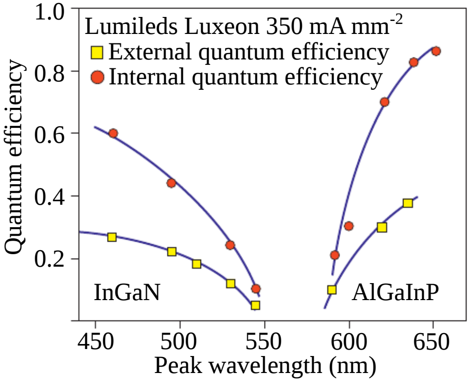
Light emission from $In_xGa_{1-x}N$

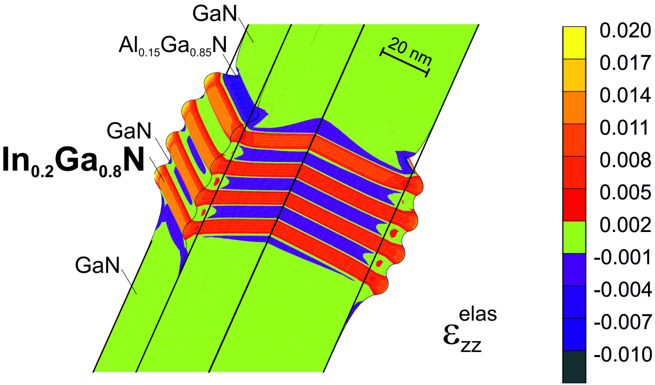


The bandgap of $In_xGa_{1-x}N$ spans the whole visible spectrum...
but crystal quality reduced due to large lattice mismatch!

Light emission: $In_xGa_{1-x}N$/GaN thin films



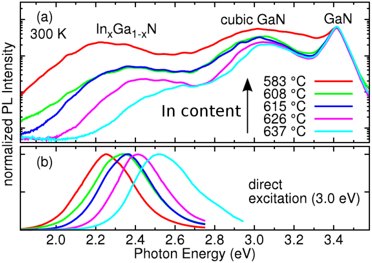
$In_xGa_{1-x}N$ films in GaN with high In content and high structural quality are hard to achieve, due to large lattice mismatch



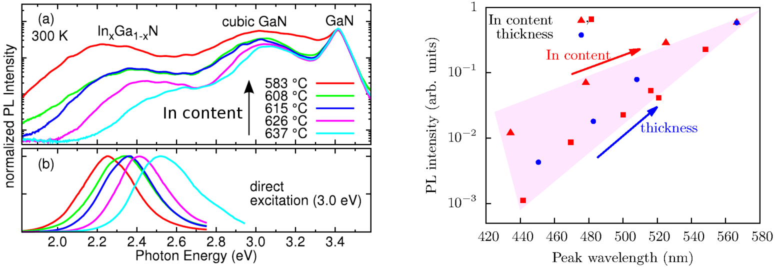
Axial $In_xGa_{1-x}N$ nanowire heterostructures facilitate elastic relaxation

Image courtesy of M. Hanke, PDI

Light emission: $In_xGa_{1-x}N$/GaN nanowires



1 Wölz et al., Nanotechnology **45**, 455203 (2012)



It is generally difficult to obtain blue emission from nanowires: Opposite trend compared to planar system!

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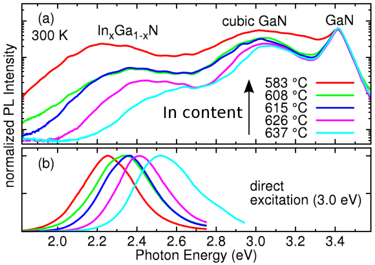
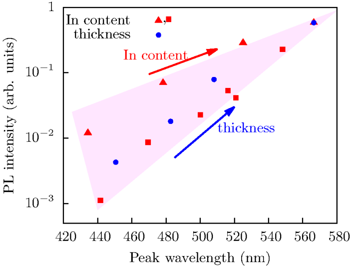
Light emission: $In_xGa_{1-x}N/GaN$ nanowires





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Opposite trend compared to planar system!
Theoretical description of nanowires required

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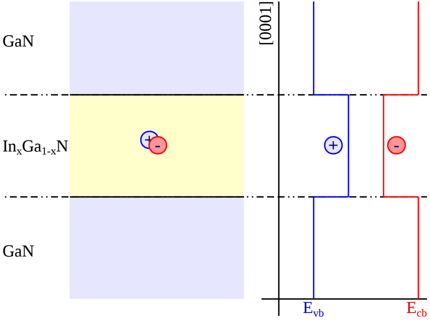
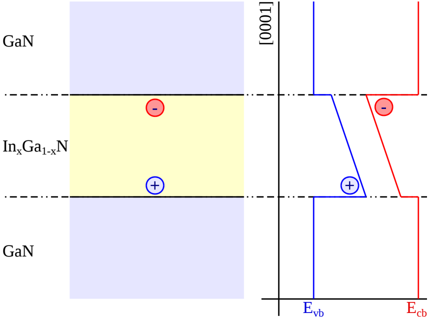


Planar layer

- Bulk band offsets

2 Böcklin et al., Phys. Rev. B **81**, 155306 (2010); Kaganer et al., Phys. Rev. B **85**, 125402 (2012)



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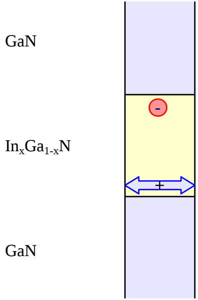

Nanowire

- Bulk band offsets
- Polarisation
- Elastic relaxation[2]
- Surface potentials: attractive for holes

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Atomistic model
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  Typical nanowire segment:
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Continuum approaches
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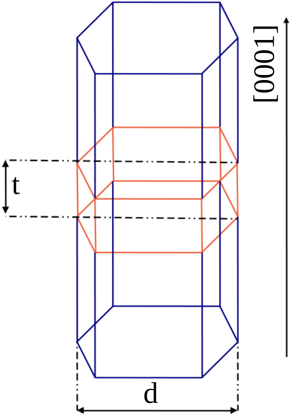
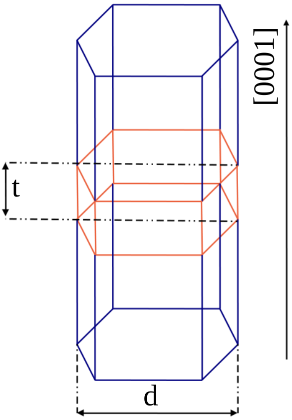
- Neglects atomistic character of the crystal
- Alloys described via average (local) composition
- Treatment of single atomistic effects difficult



- Hexagonal nanowire of diameter *d*
- $In_xGa_{1-x}N$ insertion of homogeneous In content *x* and thickness *t*
- Surface potential
  For homogeneous distribution of donor-related charge:
  $V_{\mathrm{surf}} \propto \varrho_{\mathrm{d}} \cdot d^2$.
  $\varrho_{\mathrm{d}} = 10^{17}\mathrm{cm}^{-3} \mathrel{\widehat{=}} \max(V_{\mathrm{surf}}) =$ 80 mV for a NW of d=80 nm
- Vary *x*, *t*, and *d*



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- Vary x, t, and d

$\longrightarrow$ Continuum approach favourable

Strain and polarisation
Continuum elasticity theory[3]

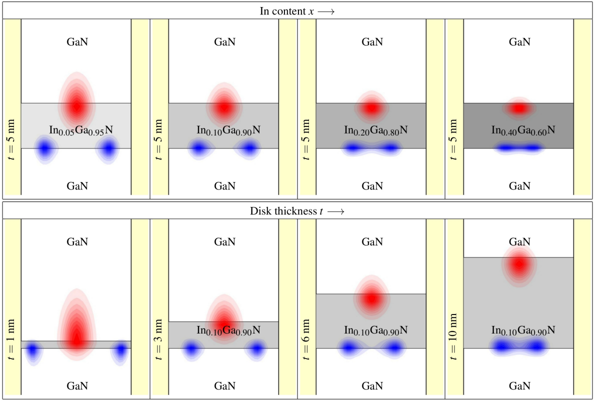
Single-particle electronic properties
eight-band $\mathbf{k} \cdot \mathbf{p}$ model for wurtzite semiconductors[4]

Electron-hole overlap

$$\mathcal{O} = \sum_{\mathbf{r}} \varrho_{\mathrm{el}}(\mathbf{r}) \varrho_{\mathrm{ho}}(\mathbf{r}) \tag{1}$$

Implementation within plane-wave framework[5]

3 Povolotskyi et al., Phys. Stat. Solidi (C) **2**, 3891 (2005).
4 Chuang et al., Phys. Rev. B **54**, 2491 (1999).
5 *www.sphinxlib.de*;
Boeck et al., Computer Phys. Commun **182**, 543 (2011);
Marquardt et al., Comp. Mat. Sci. **95**, 280 (2014).



Interplay between polarisation and surface potential – explains reduction of PL intensity with smaller In content or layer thickness

For a NW of 80 nm diameter and 20 nm segment length:
$\varrho_\mathrm{d}=10^{17}\mathrm{cm}^{-3}$ corresponds to 8.3 charges[7]!

7 Corfdir et al., Phys. Rev. B **90**, 205301 (2014).
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- Typical donors: Si, O represent **shallow donors** in $In_xGa_{1-x}N$
- Model individual donors via their Coulomb potential

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Electron and hole confinement

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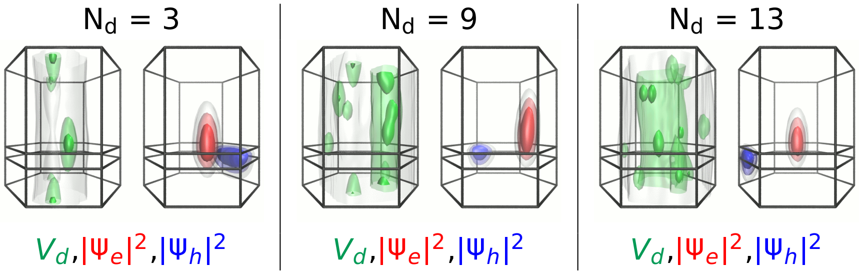

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Energies and electron-hole overlap

Model system configurations

x = 5%	x = 30%	x = 10%	x = 30%
t = 1 nm	t = 1 nm	t = 5 nm	t = 5 nm

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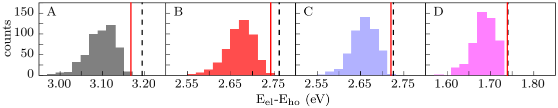

- Variation of emission wavelength unaffected by x and t
- Energies smaller than for homogeneous charge distribution and donor-free case

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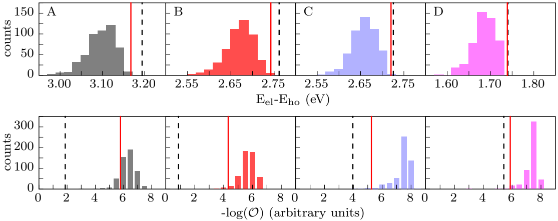

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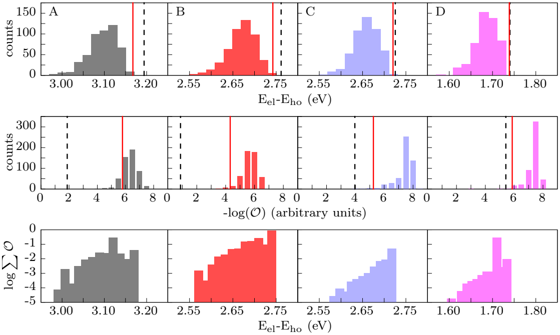
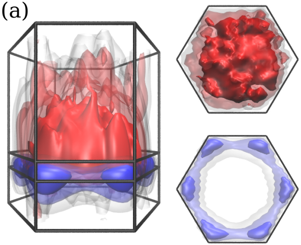
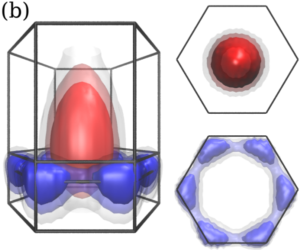


Ensemble average charge densities

ensemble average



homogeneous doping charge



- Average hole state confinement in good agreement with hole state in homogeneous doping charge model
- Electron localization governed by dopants – strong variations

Summary & next steps

- Continuum model to approach elastic, piezoelectric and electronic properties of semiconductor nanowires
- Generalised to arbitrary nanostructures and materials
- Multiband $\mathbf{k} \cdot \mathbf{p}$ model can be adjusted to computational demand and accuracy
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- Self-consistent simulations to consider excitonic effects
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Thank you for your kind attention!