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für Höchstfrequenztechnik

Accurate Modeling of InGaN QWs

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Outline

- motivation
- theoretical model
- numerical results
  - TQW vs. SQW
    (exp.: mostly TQW, theoret.: mostly SQW, no direct comparison)
  - influence of polarization fields and doping (screening)

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Motivation

- wurtzite InGaN quantum wells – active region of violet, blue and green light emitting diodes and laser diodes
- spontaneous and piezoelectric polarisation fields $\Longrightarrow$ self–consistent solution of Poisson and Schrödinger equations necessary for computation of luminescence and gain spectra
- several shortcomings of published models
  - parabolic band approximation
  - only fundamental electron and hole states taken into account
  - excess carrier density acts as input parameter
  - boundary conditions for electro-static or Hartree potential and chemical potentials remain unclear

Energy bands and wave functions

Schrödinger equation: 8×8 $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian taking into account 3 uppermost valence bands and lowest conduction band, doubly degenerated

$$\mathbf{H}\left(E_c^*, E_v^*, \boldsymbol{k}_{||}, \frac{d}{dz},\right)\Psi_n(\boldsymbol{k}_{||}, z) = E_n(\boldsymbol{k}_{||})\Psi_n(\boldsymbol{k}_{||}, z)$$

renormalization of bulk band edges

$$E_c^* = E_c - e\phi_{\mathrm{H}} - \frac{1}{2}V_{\mathrm{xc}}\left(\frac{n+p}{2}\right)$$

$$E_v^* = E_v - e\phi_{\mathrm{H}} + \frac{1}{2}V_{\mathrm{xc}}\left(\frac{n+p}{2}\right)$$

V_{xc} exchange–correlation potential in local density approximation

ϕ_{H} Hartree potential from Maxwell's equation

Hartree potential

Poisson equation
$$\mathrm{div}\,\boldsymbol{D} = e(p - n + N_{\mathrm{D}}^{+} - N_{\mathrm{A}}^{-}) - \mathrm{div}\,\boldsymbol{P}$$
$$\boldsymbol{D} = -\varepsilon_0 \varepsilon_{\mathrm{r}}\,\mathrm{grad}\,\phi_{\mathrm{H}}$$

electron and hole densities
$$n = n^{\mathrm{2D}} + n^{\mathrm{3D}}, \quad p = p^{\mathrm{2D}} + p^{\mathrm{3D}}$$

quantum electron density
$$n^{\mathrm{2D}} = \sum_{n_{\mathrm{c}}} \frac{1}{4\pi^2} \int |\Psi_{n_{\mathrm{c}}}(\boldsymbol{k}_{||})|^2 f\Big(\frac{E_{n_{\mathrm{c}}}(\boldsymbol{k}_{||}) - e\phi_n}{k_{\mathrm{B}}T}\Big)\, d^2\boldsymbol{k}_{||}$$

free electron density
$$n^{\mathrm{3D}} = N_c \mathrm{F}_{1/2}\Big(\frac{\max(E_{n_{\mathrm{c}}}(0), E_{\mathrm{c}}^{*}) - e\phi_n}{k_{\mathrm{B}}T}\Big)$$

similar for p^{2D} and p^{3D}

macroscopic polarization
$$\boldsymbol{P} = \boldsymbol{P}_{\mathrm{spont}} + \boldsymbol{P}_{\mathrm{piezo}}$$

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Boundary conditions

- wavefunction

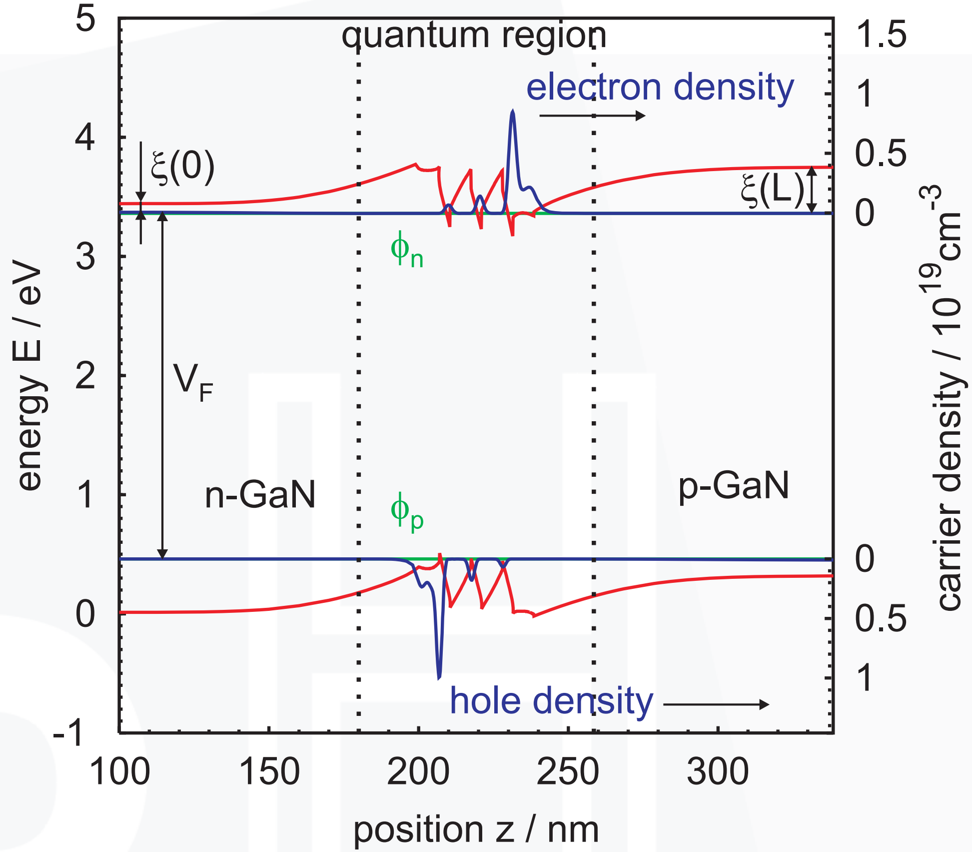
$$\Psi_n = 0$$

at boundaries of quantum region

- Hartree potential

$$\phi_{\mathrm{H}}(0) = 0$$
$$\phi_{\mathrm{H}}(L) = \xi(L) - \xi(0)$$

$V_{\mathrm{F}} = 2.9$ V



chemical potentials ξ solutions of bulk neutrality condition at $z = 0,\ L$

$$N_v \mathrm{F}_{1/2}\left(\frac{eV_{\mathrm{F}} - E_{\mathrm{g}} - e\xi}{k_{\mathrm{B}}T}\right) - N_c \mathrm{F}_{1/2}\left(\frac{e\xi}{k_{\mathrm{B}}T}\right) + N_{\mathrm{D}}^{+} - N_{\mathrm{A}}^{-} = 0$$

input parameter $V_{\mathrm{F}} = \phi_n - \phi_p$ Fermi voltage

Numerics

- Schrödinger equation: Galerkin method (sinus functions) $\Longrightarrow$ algebraic eigenvalue problem solved with LAPACK routine ZHEEV
- nonlinear Poisson equation: discretized with finite differences, solved with Newton's method
- iteration using implicit scheme where subband energies E_{n_c} are replaced by $E_{n_\mathrm{c}} - \left(\phi_\mathrm{H}^k(z) - \phi_\mathrm{H}^{k-1}(z)\right)$ in expression for n^{2D} (similarly for p^{2D}) $\Longrightarrow$ faster convergence
- luminescence and gain: free carrier theory with sech-type of broadening (FWHM 26 meV)
- $T = 300$ K in all simulations

Structure

layer	compound	d nm	D cm^{-3}	$P_{spont,z}$ 10^{-6} C cm^{-2}	$P_{piezo,z}$ 10^{-6} C cm^{-2}
confinement	n-GaN	200	$+10^{17}$	-3.40	0
barrier	$In_{0.015}Ga_{0.985}N$	7	$+10^{16}$	-3.36	$+0.22$
QW	$In_{0.09}Ga_{0.91}N$	3.5	$+10^{16}$	-3.17	$+1.42$
barrier	$In_{0.015}Ga_{0.985}N$	7	$+10^{16}$	-3.36	$+0.22$
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confinement	p-GaN	200	-10^{17}	-3.40	0

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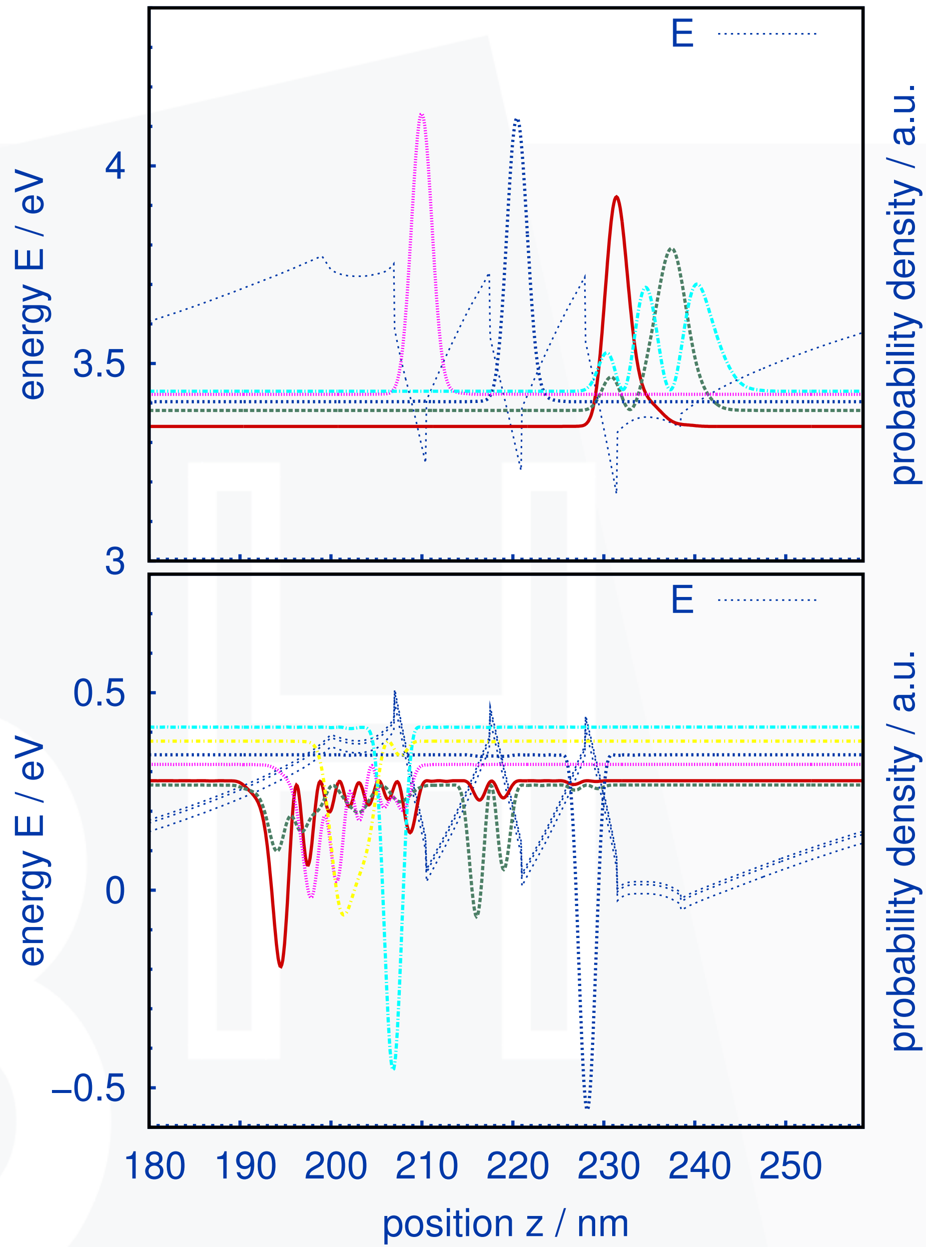
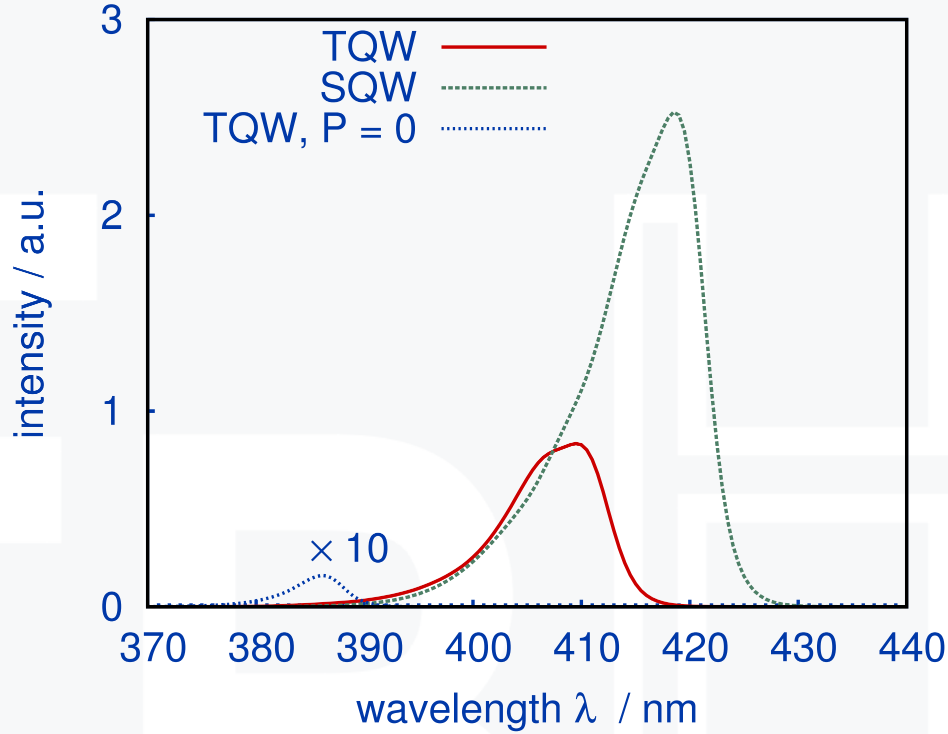
Quantum region

conduction and valence band edges, probability densities

- first electron (hole) states are located in first (last) QW and left (right) barrier
- poor spatial overlap of highly occupied states
- states with better overlap less occupied



Luminescence spectra $V_F = 2.9$ V



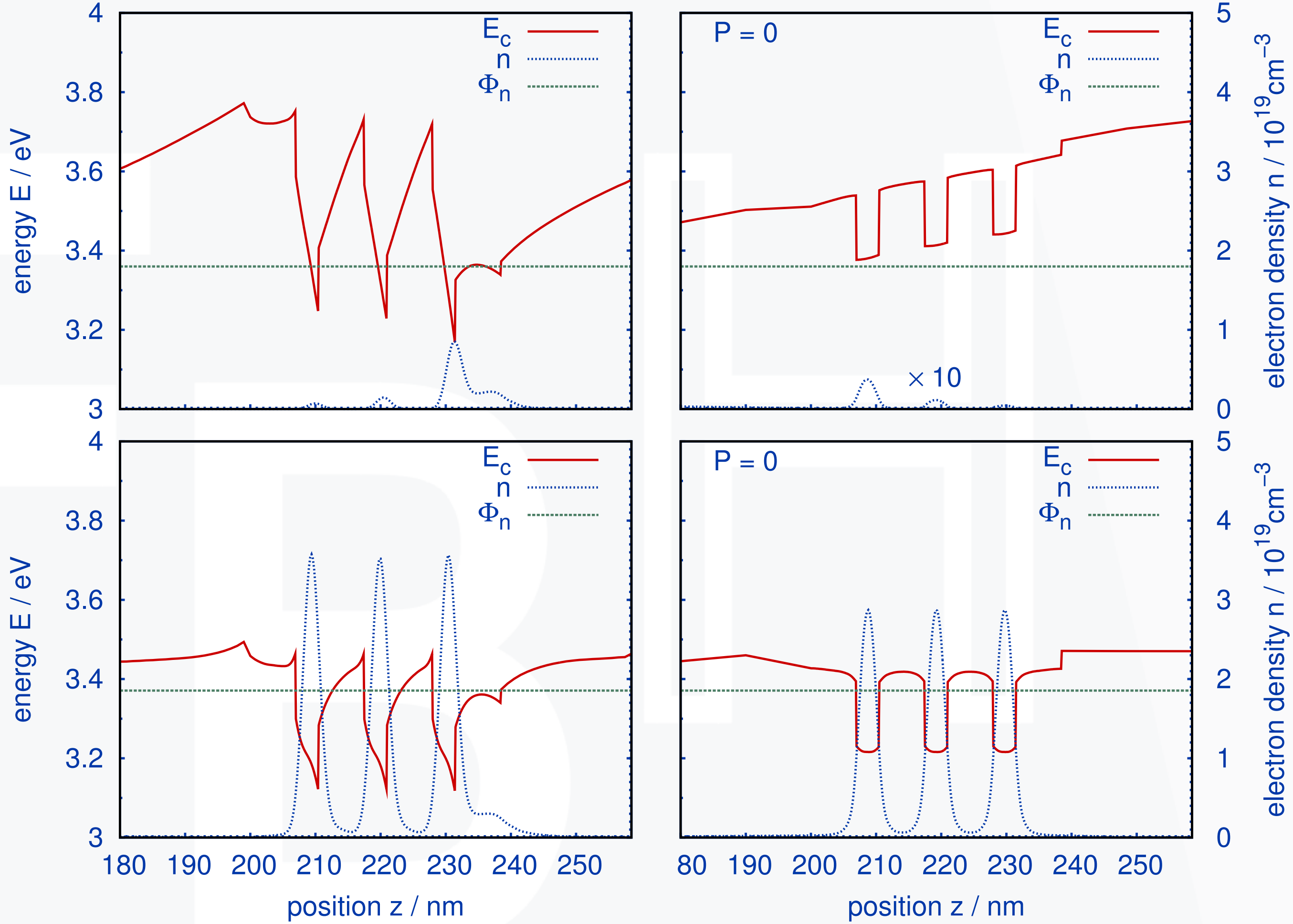
- luminescence peak of SQW red–shifted and larger due to larger spatial overlap of highly occupied states
- luminescence of TQW for vanishing polarization 2 orders of magnitude smaller

Conduction band edges and electron densities

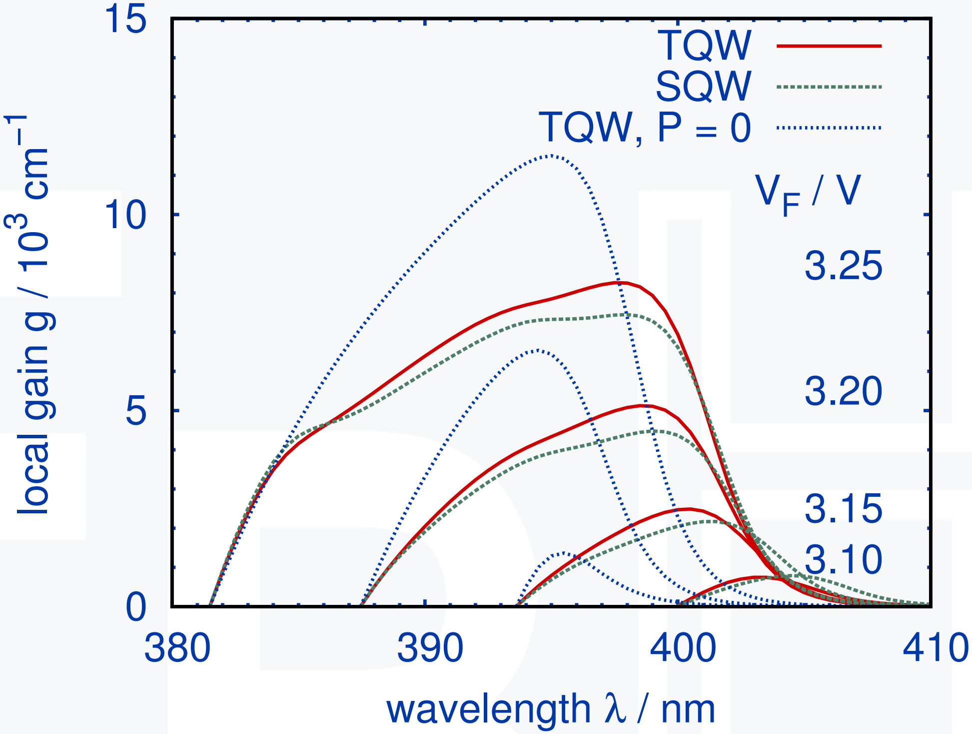
$P \neq 0$ $P = 0$

$V_F = 2.9$ V

$V_F = 3.2$ V



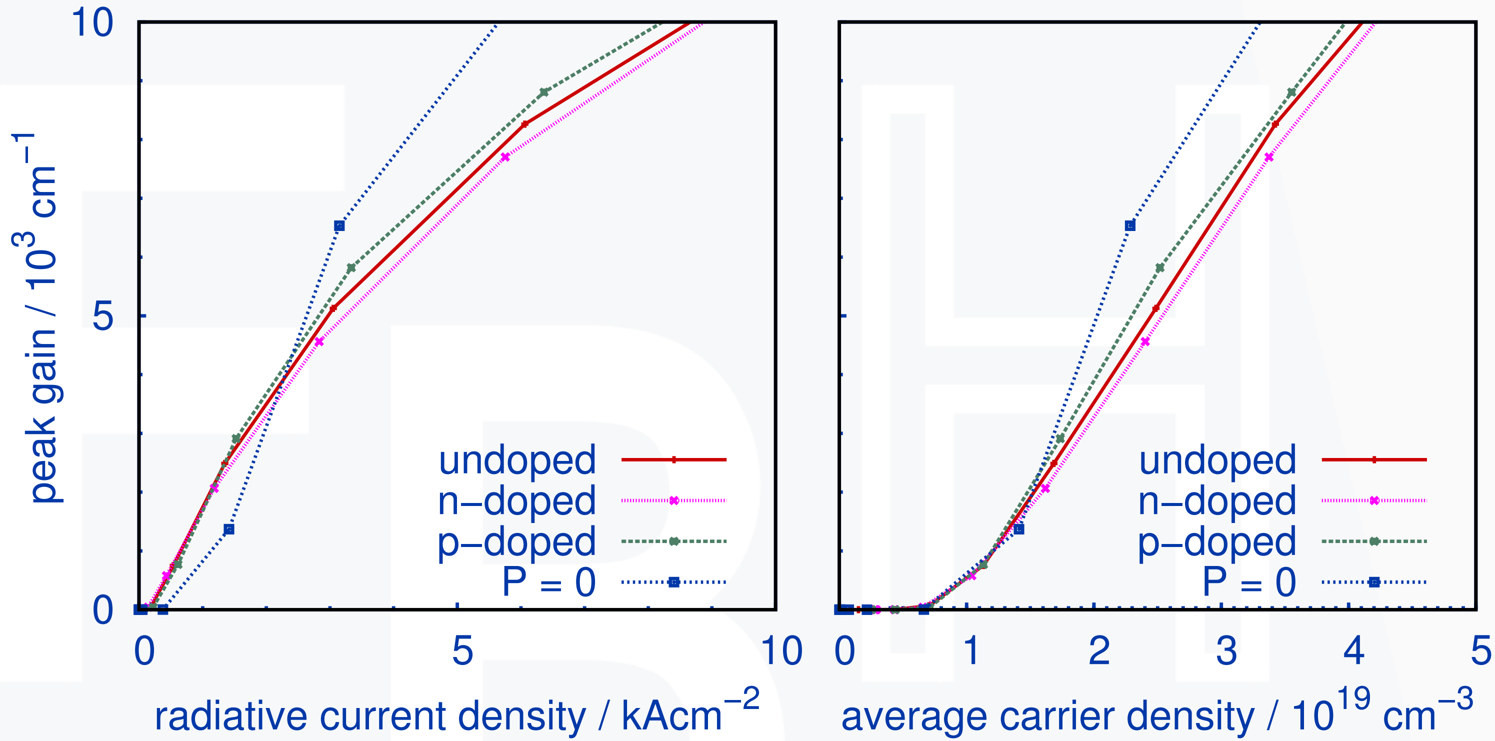
Gain spectra



- gain with full polarization fields enhanced at smaller bias, reduced at larger bias, blue–shifted compared to the case of $P = 0$
- almost no difference in gain spectra between SQW and TQW

Impact of doping of barriers on gain peak of TQW

n-doping: $N_{\mathrm{D}}^{+} = 5 \times 10^{18}$, p-doping: $N_{\mathrm{A}}^{-} = 5 \times 10^{18}$



almost no difference in gain peak dependence on radiative current density or on carrier density between undoped and doped barriers

Summary

- self–consistent solution of the Poisson equation and an eight–band $\boldsymbol{k}\cdot\boldsymbol{p}$ Schrödinger equation for wurtzite strained InGaN quantum wells taking into account proper boundary conditions for the Hartree and chemical potentials
- application to SQW and TQW structures embedded in a p-n junction
- stronger and red–shifted luminescence of SQW compared to TQW for the same Fermi voltage (bias)
- enhancement of luminescence and gain at lower bias due to polarisation fields
- almost identical gain spectra of SQW and TQW structures
- only minor impact of doping of barriers on gain