SPIE Photonics West: Light-Emitting Diodes: Materials, Devices, and Applications for Solid State Lighting XVI , San Francisco, USA, 21-26 January, 2012

Simulation of light-emitting diodes for new physics understanding and device design

Sergey Yu. Karpov

STR Group – Soft-Impact, Ltd (St.Petersburg, Russia)

Outline

- Lessons of ABC-model
  - interplay between recombination channels
  - figure of merit for LED structures
  - ways to improve LED structure performance
- Quantum corrections in LED modeling
  - quantum potential approach
  - LED structure with short-period superlattice active region
- Toward 'green gap' understanding

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ABC-model and processing of experimental data

$$j = j_{SR} + j_{rad} + j_{Auger} \quad , \quad \eta = j_{rad} / j$$

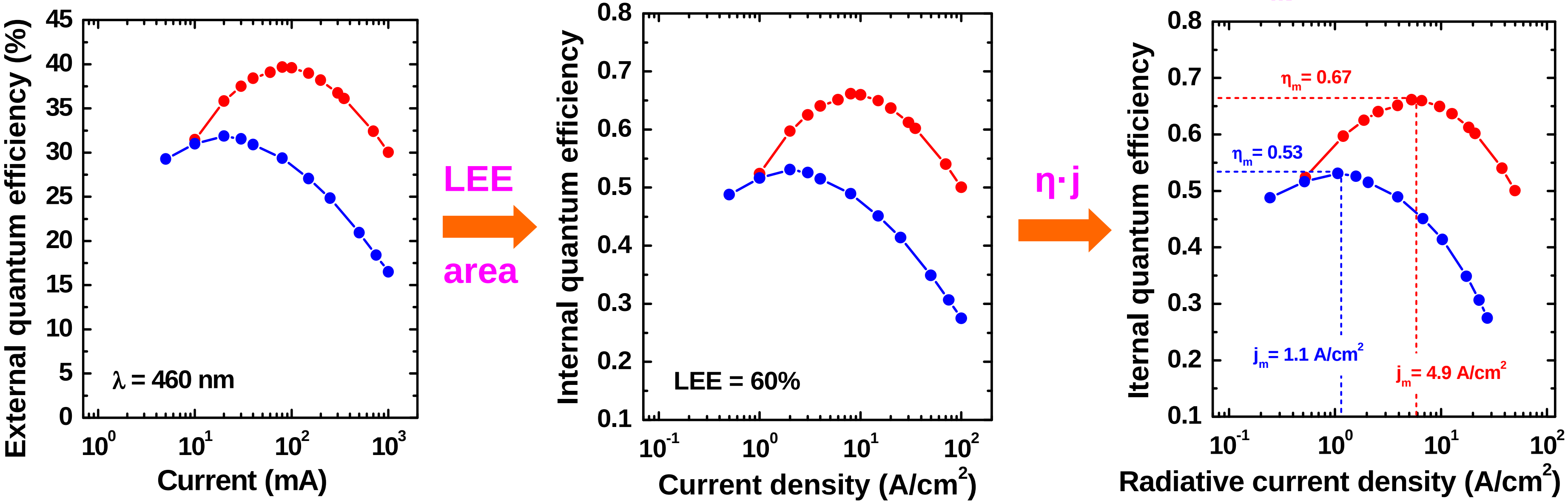
ABC-model:

$$\frac{j_{SR}}{qd} = An = n/\tau \quad , \quad \frac{j_{rad}}{qd} = Bn^2 \quad , \quad \frac{j_{Auger}}{qd} = Cn^3$$

here q is the electron charge, n is the electron/hole concentration in the active region, d is the width of recombination region, τ is the carrier life time, B and C are the radiative recombination and Auger recombination constant, respectively, weakly dependent on n

processing of experimental curve …

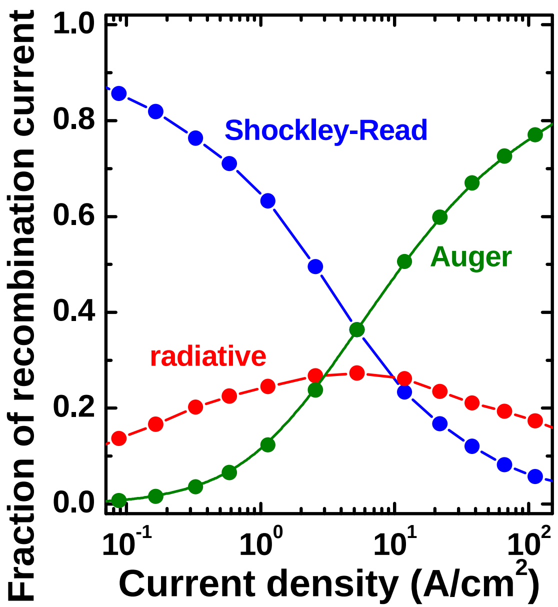
$$j_m = qdB/\tau C$$



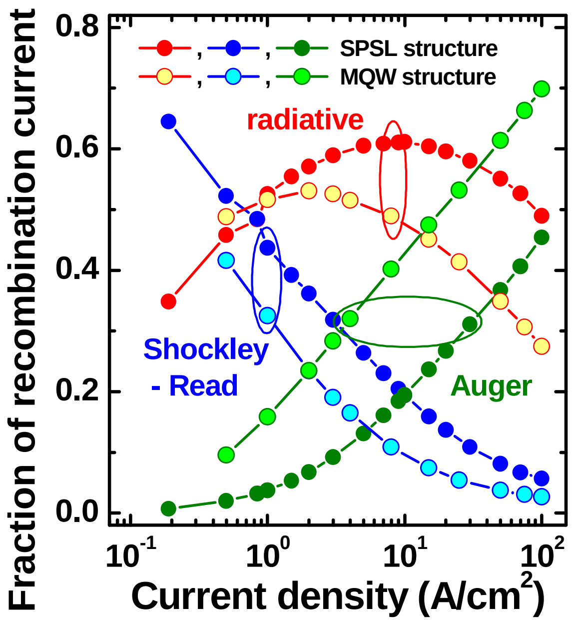
Interplay between recombination channels

contributions of various recombination channels to the total current density:

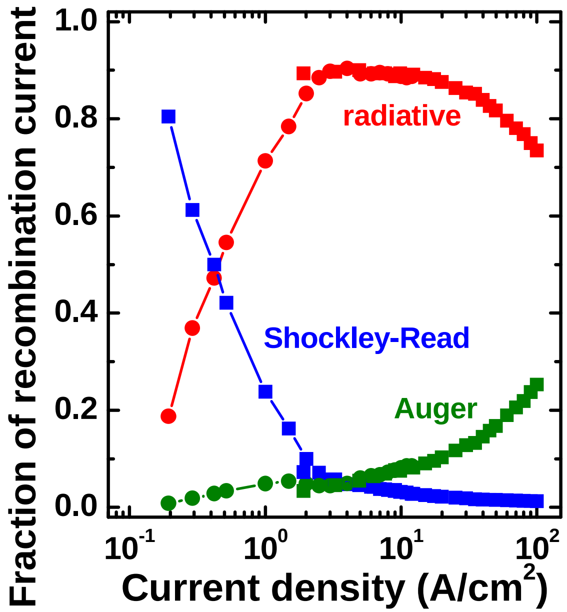
$$f_{SR} = \frac{j_{SR}}{j} = \frac{j_m}{j_m + j_{rad}}(1-\eta) \;, \quad f_{rad} = \frac{j_{rad}}{j} = \eta \;, \quad f_A = \frac{j_A}{j} = \frac{j_{rad}}{j_m + j_{rad}}(1-\eta)$$



A. Laubsch et al., Phys. Stat. Solidi (c) 6, S913 (2009)



D. Zakheim, et al., Phys. Stat. Solidi (c) 8, 2340 (2011)



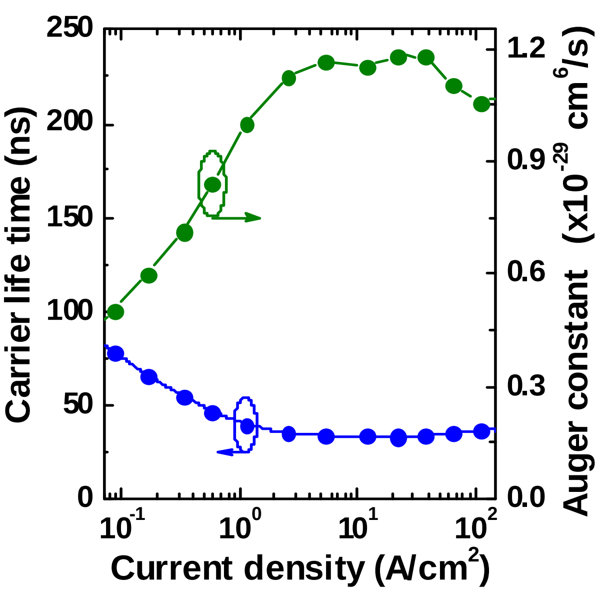
Y. Narukawa et al., J. Phys. D: Appl. Phys. 43, 354002 (2010)

Determination of recombination constants

$$\tau = \tau_B \frac{f_{rad}^{1/2}}{f_{SR}} \quad , \quad C = B^2 \tau_B \frac{f_A}{f_{rad}^{3/2}} \quad , \quad \text{where } \tau_B = \left(\frac{qd}{jB}\right)^{1/2}$$

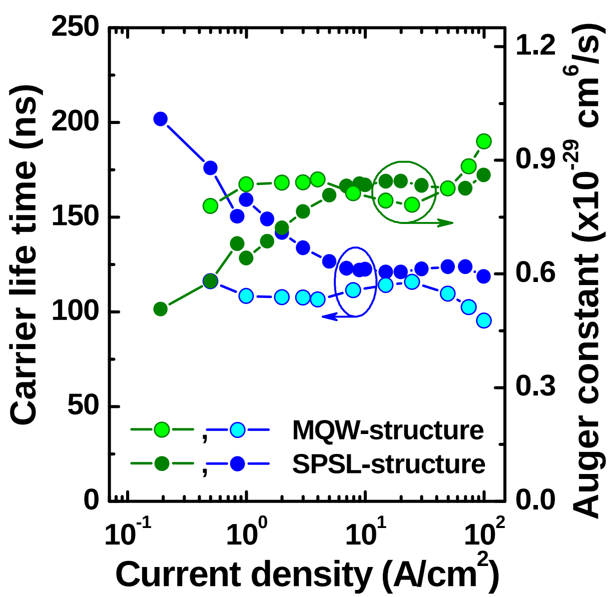
if one of the recombination constants, for instance B , is known, the other ones can be obtained from the contributions of various recombination channels in the total current density

$B = 1.4\times10^{-11}$ cm³/s



A. Laubsch et al., Phys. Stat. Solidi (c) 6, S913 (2009)

$B = 2.0\text{-}2.6\times10^{-11}$ cm³/s



D. Zakheim, et al., Phys. Stat. Solidi (c) 8, 2340 (2011)

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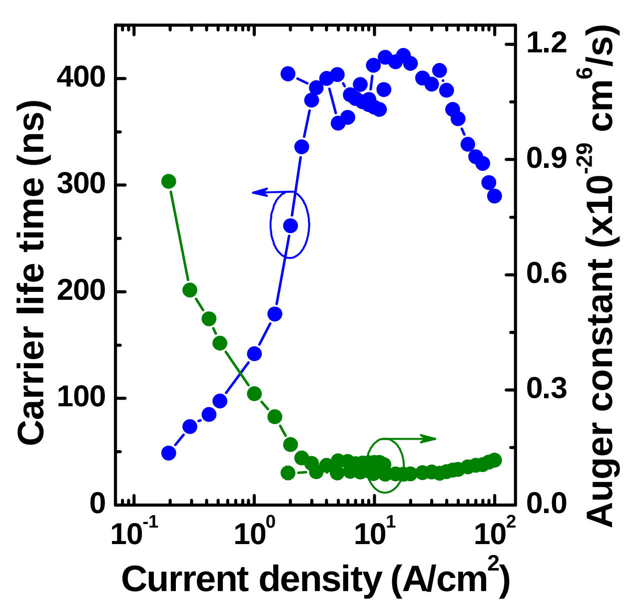


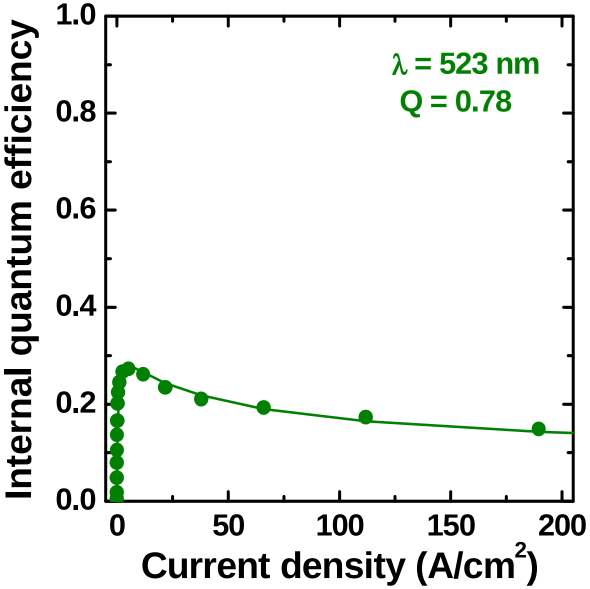
Y. Narukawa et al., J. Phys. D: Appl. Phys. 43, 354002 (2010)

Quality factor as a figure of merit for LED heterostructures

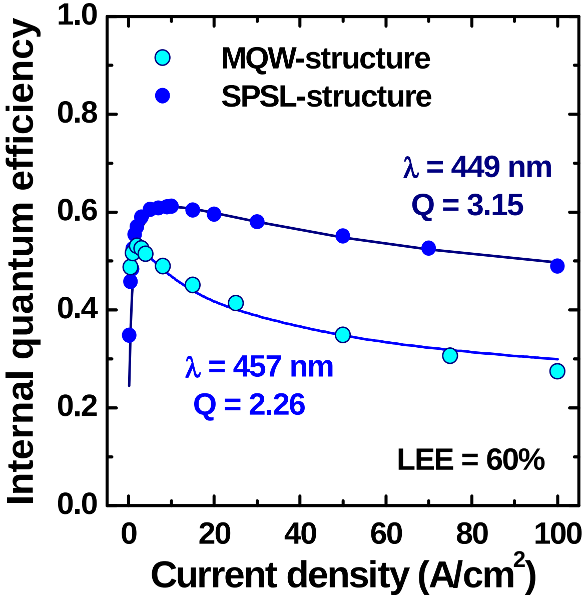
universal IQE dependence on the radiative current density:

$$\eta = \frac{Q}{Q + (j_{rad}/j_m)^{1/2} + (j_{rad}/j_m)^{-1/2}}$$

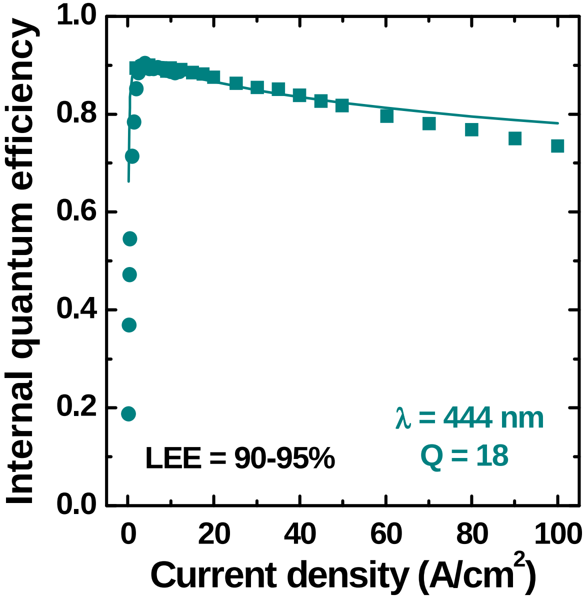
where $\eta_m = \frac{Q}{Q+2} \rightarrow Q = \frac{2\eta_m}{1-\eta_m}$



A. Laubsch et al., Phys. Stat. Solidi (c) 6, S913 (2009)



D. Zakheim, et al., Phys. Stat. Solidi (c) 8, 2340 (2011)

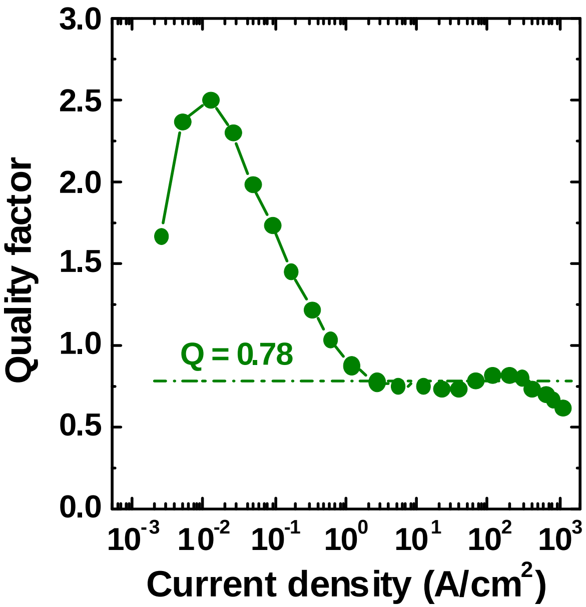


Y. Narukawa et al., J. Phys. D: Appl. Phys. 43, 354002 (2010)

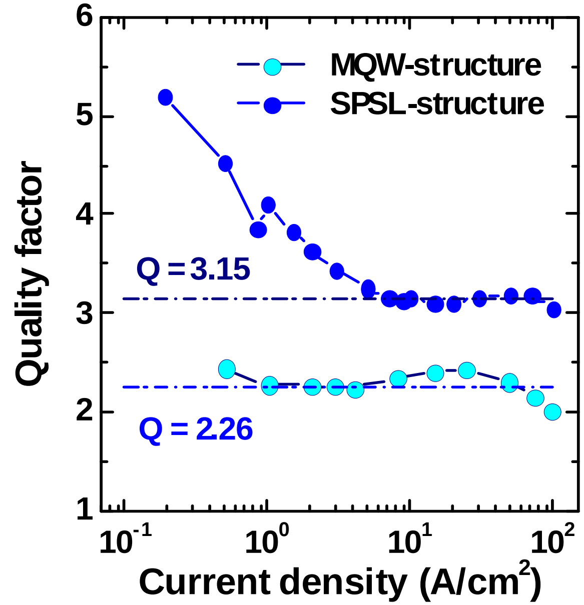
Applicability of the ABC-model to analysis of III-nitride LEDs

$$Q = \frac{j_{rad}}{(j_{SR}\, j_{Auger})^{1/2}} = B\left(\frac{\tau}{C}\right)^{1/2}$$

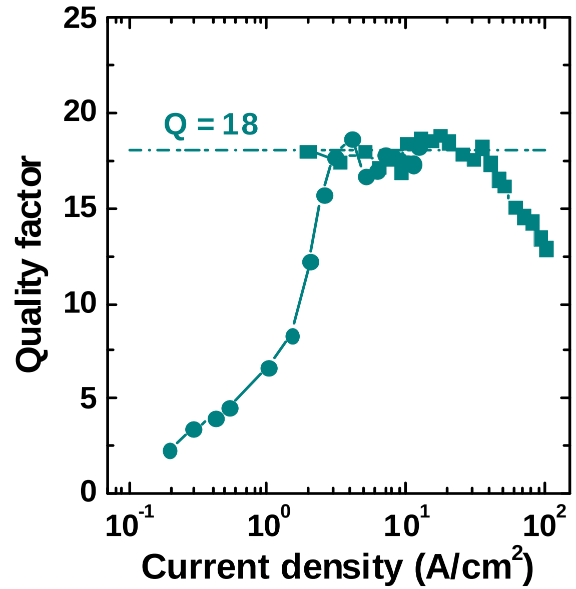
there is a wide practically important range of the current densities where Q-factor is nearly constant, in line with the ABC-model; beyond this range, the model is no longer applicable to LED structure analysis



A. Laubsch et al., Phys. Stat. Solidi (c) 6, S913 (2009)

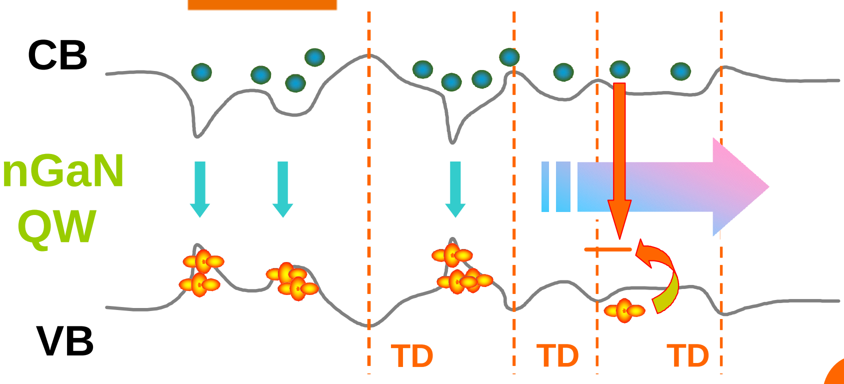


D. Zakheim, et al., Phys. Stat. Solidi (c) 8, 2340 (2011)

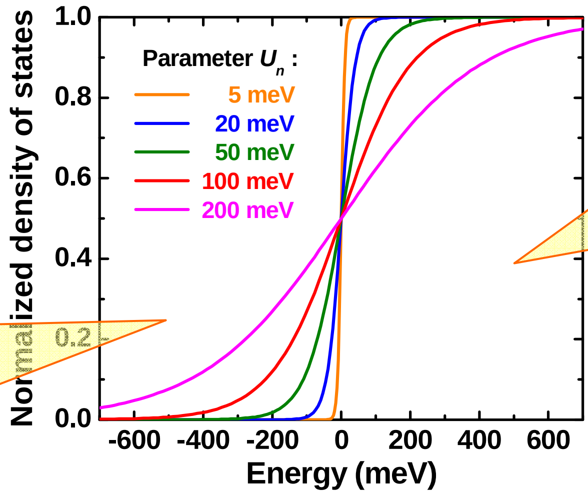


Y. Narukawa et al., J. Phys. D: Appl. Phys. 43, 354002 (2010)

Localized and delocalized states in InGaN quantum wells

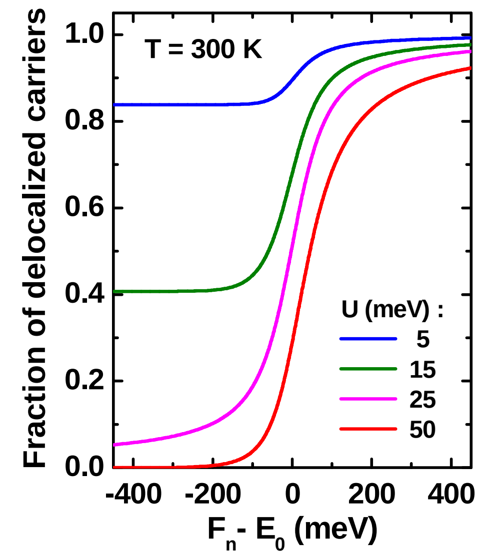


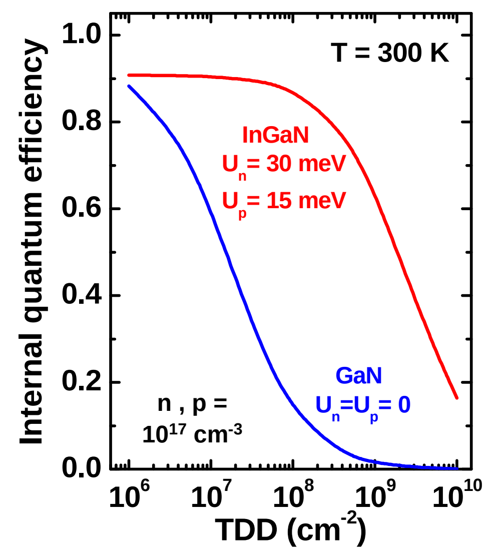
both QW thickness and composition fluctuations may produce DOS tails in the bandgap



localized carriers: do not take part in recombination at TDs

delocalized carriers: participate in recombination at TDs

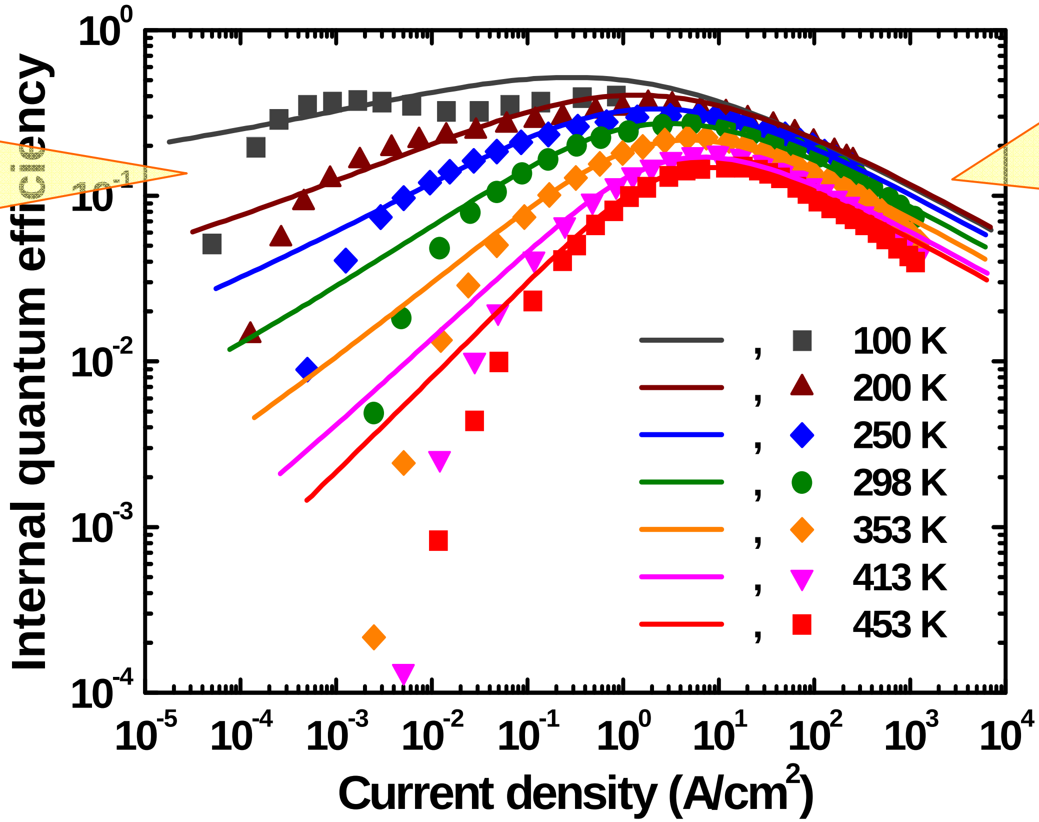




localized states due to composition/QW thickness fluctuation in InGaN increase the material IQE

IQE of InGaN SQW LED structure *vs* current density and temperature

IQE increase at low temperatures and current densities due to carrier localization



non-thermal efficiency droop caused by Auger recombination practically independent of temperature

$B \propto T^{-1}$

$C = const\,(T)$

ABC model predicts well the IQE variation with the current density and temperature in the range of ~200-450 K

Experiment: A. Laubsch et al., Phys, Stat. Solidi (c) 6 (2009) S913 (symbols)

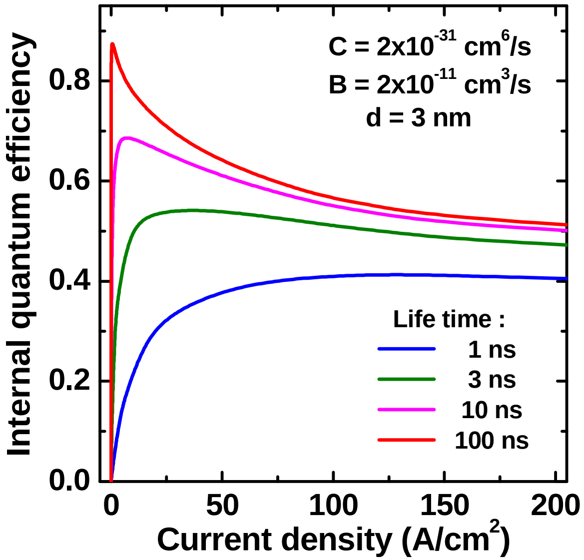
Theory: S. Yu. Karpov, Phys. Stat. Solidi RRL 4 (2010) 320 (lines)

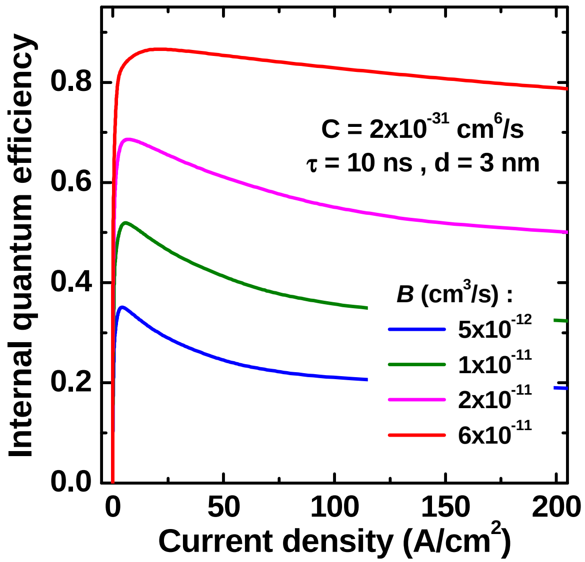
Ways to improve the LED structure performance

- increasing quality factor
- shift of j_m to the practically important region

$$Q = B(\tau/C)^{1/2}$$

$$j_m = qdB/\tau C$$

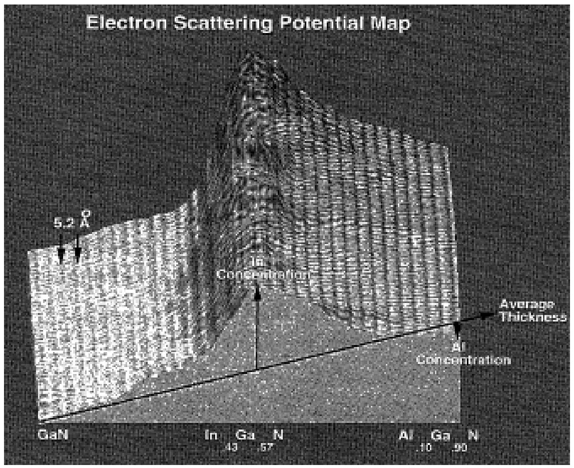


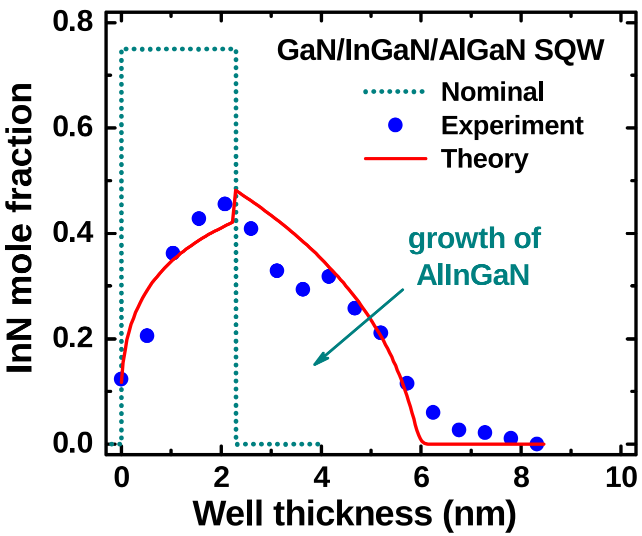


materials quality improvement, leading to longer carrier life times: no reason for violet and blue LEDs

increasing *B* constant:, cavity effects, bandgap engineering (indium surface segregation during MOVPE should be accounted for)

Effect of indium surface segregation on InGaN QW profile





Indium surface segregation results in:

- ✓ delayed indium incorporation at the bottom QW interface
- ✓ indium tail in the AlGaN or GaN cap layer

Experiment:

C. Kisielowski et al., Jpn. J. Appl. Phys. 36 (1997) 6932

Theory:

R. A. Talalaev et al., Phys. Stat. Solidi (c) 0 (2002) 311

Ways to control segregation:

- ✓ indium deposition prior InGaN QW growth
- ✓ growth interruption
- ✓ temperature ramping, etc.

improvement of the overlap between electron and hole wave functions requires understanding of indium surface segregation effect on the QW profile

Ways to improve the LED structure performance

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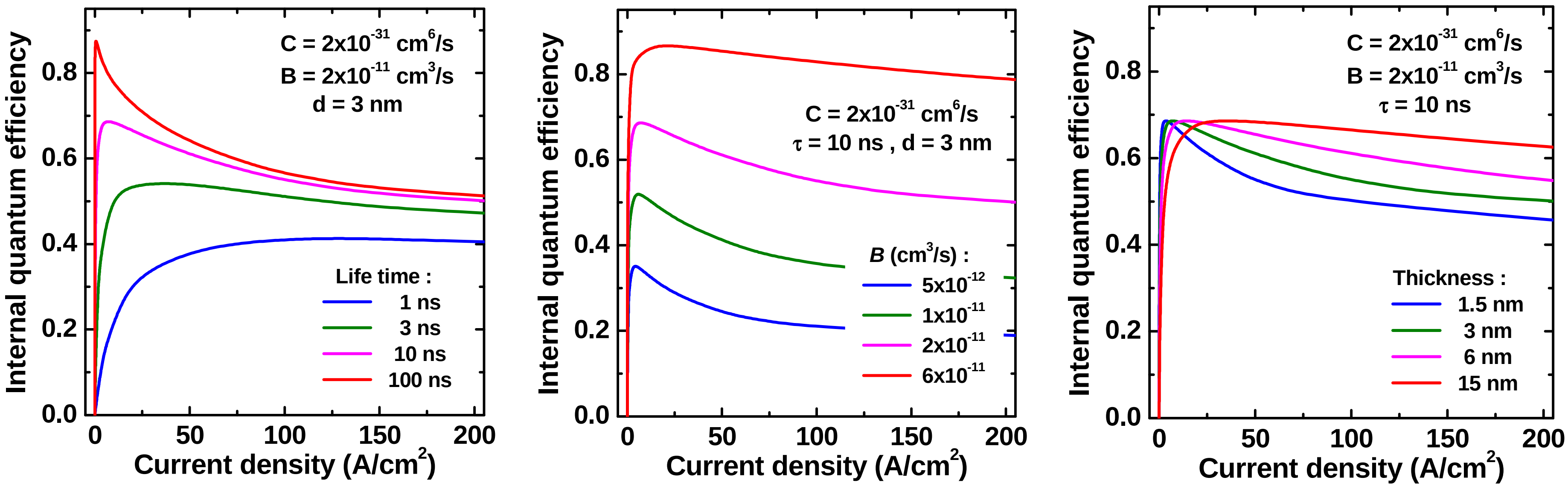
$$Q = B(\tau/C)^{1/2}$$

$$j_m = qdB/\tau C$$



materials quality improvement, leading to longer carrier life times: no reason for violet and blue LEDs

increasing *B* constant: cavity effects, bandgap engineering (indium surface segregation during MOVPE should be accounted for)

increasing recombination volume: the approach quite feasible for practical utilization

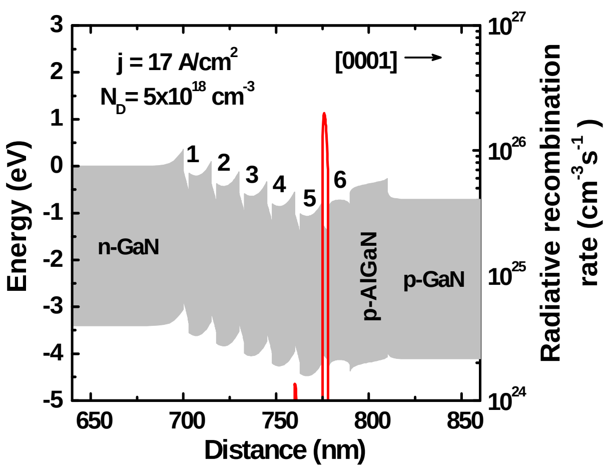
How to increase the recombination volume ?

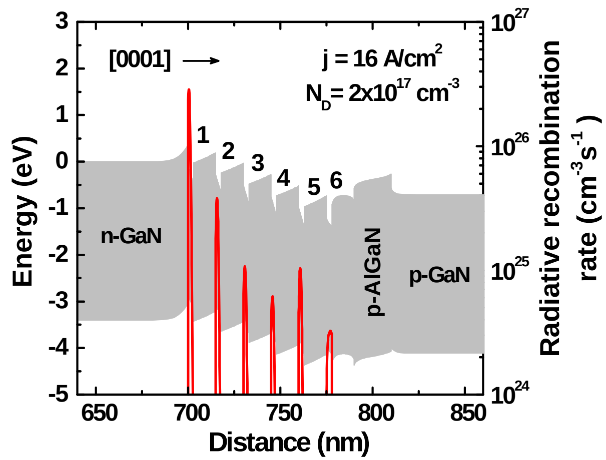
- using a wide single active layer – problematic growth of high-quality InGaN
- using of MQW LED structures – does not work because of non-uniform carrier injection

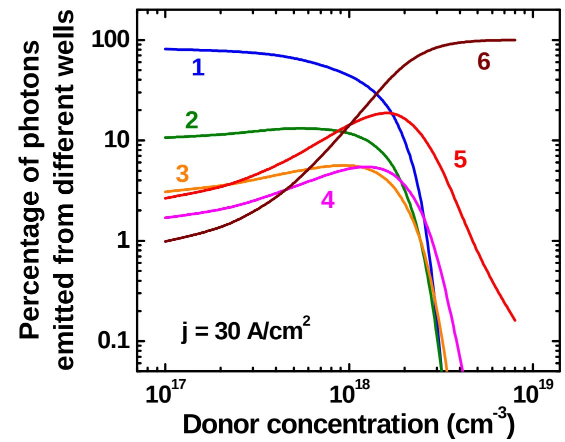
N. Gardner et al., Appl. Phys. Lett. 91 (2007) 243506

A. David et al., Appl. Phys. Lett. 92 (2008) 053502;

K. A. Bulashevich et al., Phys. Stat. Solidi (c) 6 (2009) S804







- using of short-period superlattice (SPSL) active region

X. Ni et al., Proc. SPIE 7216 (2009) 716W-1;

D. A. Zakheim et al., Phys. Stat. Solidi (c) 6 (2011) 2340

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- Lessons of ABC-model
  - interplay between recombination channels
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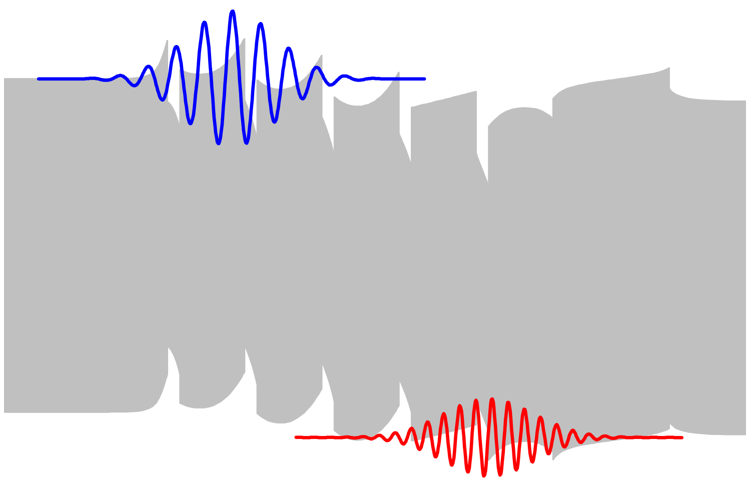
Quantum corrections in LED modeling

quantum potential accounts for delocalization of electrons and holes in the LED structure



actually, the carrier transport is affected not only by the potential in a particular point but also by its distribution in the surrounding region

- differential formulations

$$U_Q = -4\sigma^2 kT \frac{\nabla^2(\sqrt{n})}{\sqrt{n}}$$ – Bohm potential

$$U_Q = -\sigma^2 kT\, \nabla^2(\ln n)$$ – Wigner potential

$$U_Q = \sigma^2\, \nabla^2 U_C$$ – Wigner-Kirkwood expansion

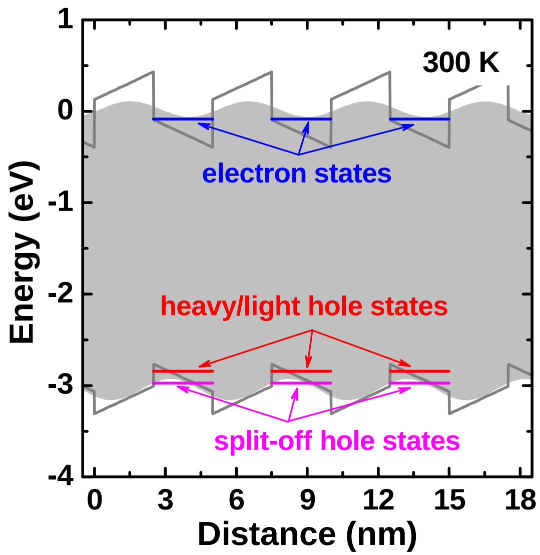
- integral formulation

$$U_{eff}(r) = U_C + U_Q = \int d^3 r' \cdot U_C(r - r') G(r', \sigma)$$

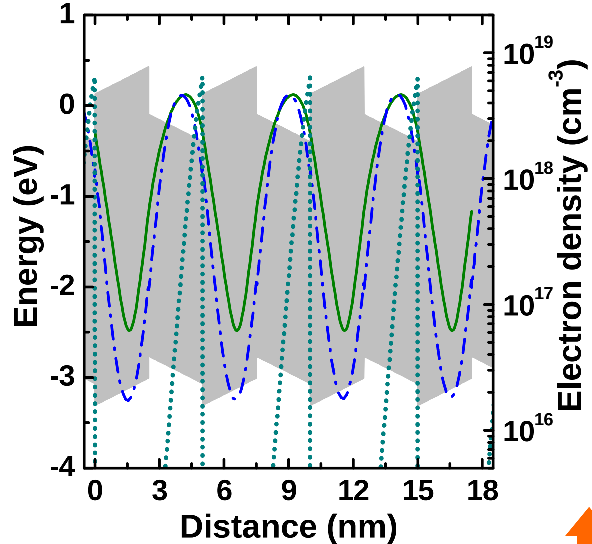
$$\sigma^2 = \gamma \frac{\hbar^2}{8 m_n kT} = \gamma \frac{\lambda_{DB}^2}{16\pi}$$

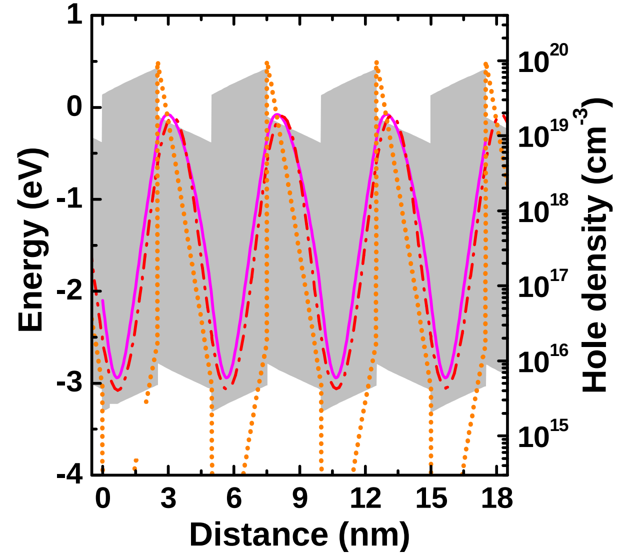
the values of γ from 2/3 to 3π are used in practical simulations

Testing and tuning of the quantum-potential model



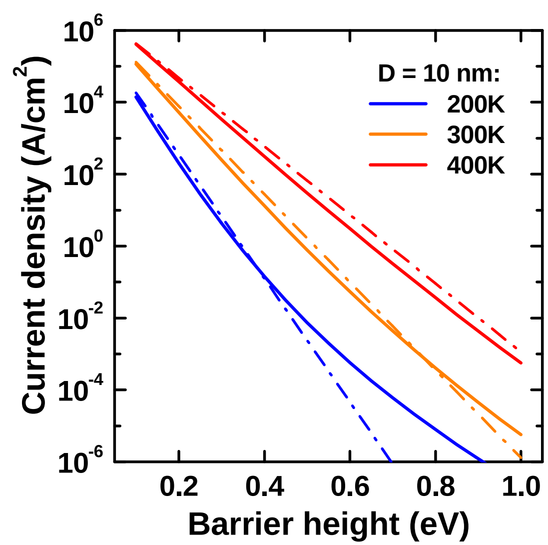
band edges of effective potential correspond well to the ground states of electrons/holes in the actual QWs





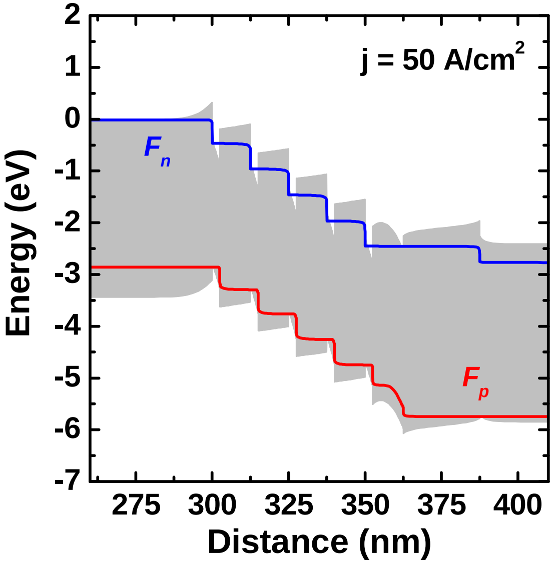
quantum potential provides much more realistic carrier density distributions than conventional drift-diffusion

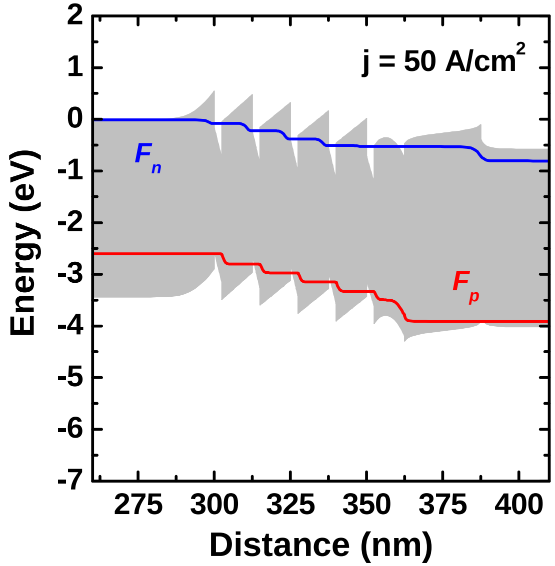
γ = 0.7 has been found from the fitting of tunneling current through a triangular barrier with the base D

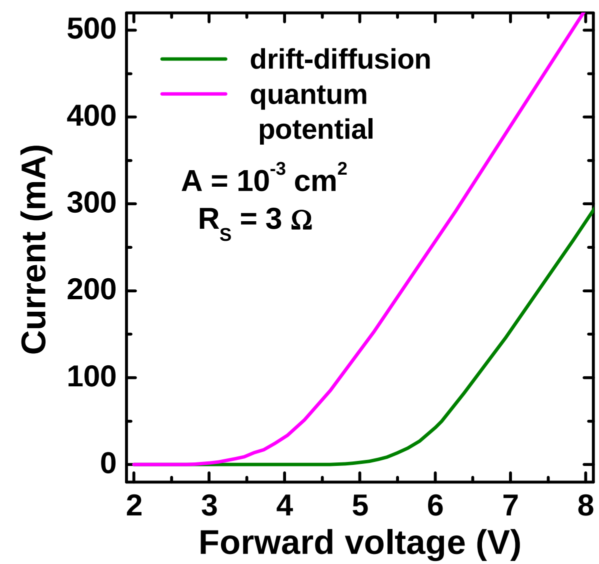


Band alignment in quantum-potential and drift-diffusion models

http://www.str-soft.com/SimuLED/SiLENSe







drift-diffusion model

quantum-potential model

much more realistic I-V characteristic is provided by quantum-potential approach for green (λ = 500 nm) MQW LED structure

quantum-potential model predicts more flat conduction and valence band alignment without ballistic leakage of electrons to p-region of an LED structure

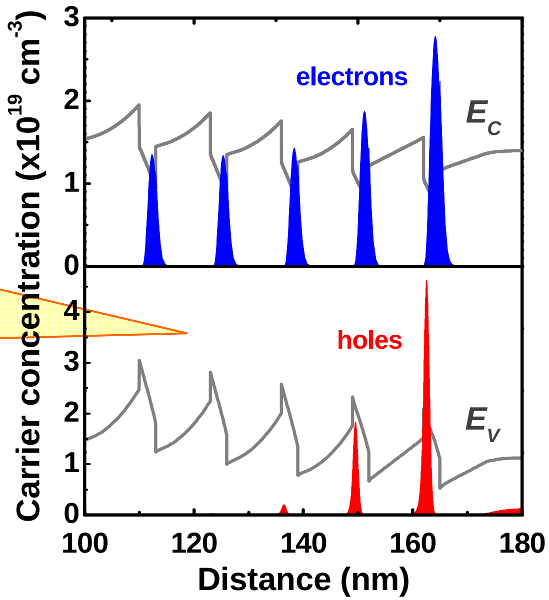
Comparative analysis of MQW and SPSL structure operation

D. A. Zakheim, et al., Phys. Stat. Solidi (a) accepted for publication

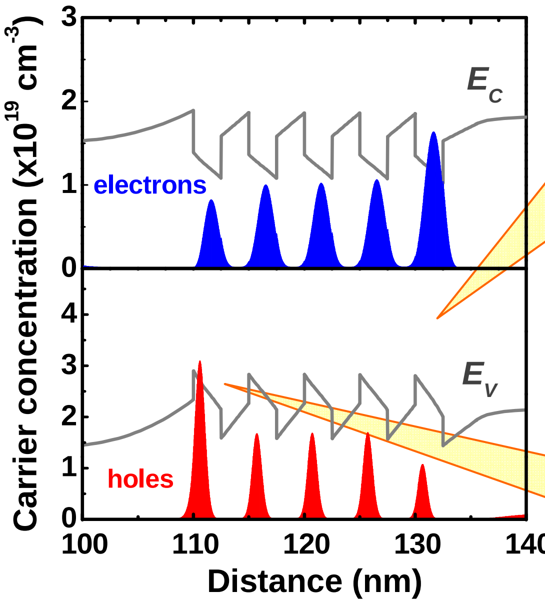
MQW structure: n-GaN contact layer, 5×(3 nm InGaN QW/10 nm GaN barrier), 20 nm p-$Al_{0.15}Ga_{0.85}N$ electron blocking layer, 110 nm p-GaN contact layer

SPSL structure: n-GaN contact layer, 5×(2.5 nm InGaN QW/2.5 nm GaN barrier), 120 nm p-GaN contact layer

non-uniform hole injection in the active region



MQW structure



SPSL structure

reduced peak electron and hole density suppressing the rate of Auger recombination

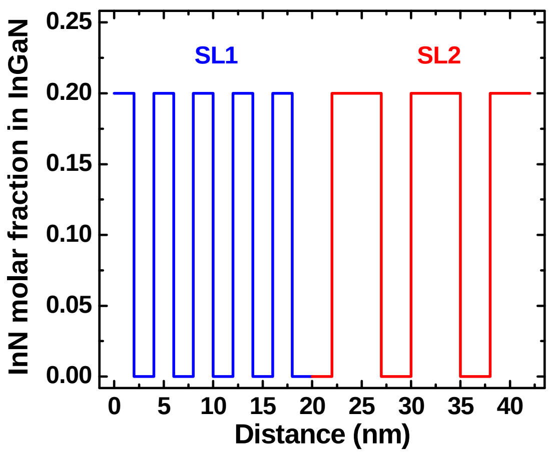
effect of built-in polarization field

j = 200 A/cm^2

Macroscopic polarization and built-in interface charges

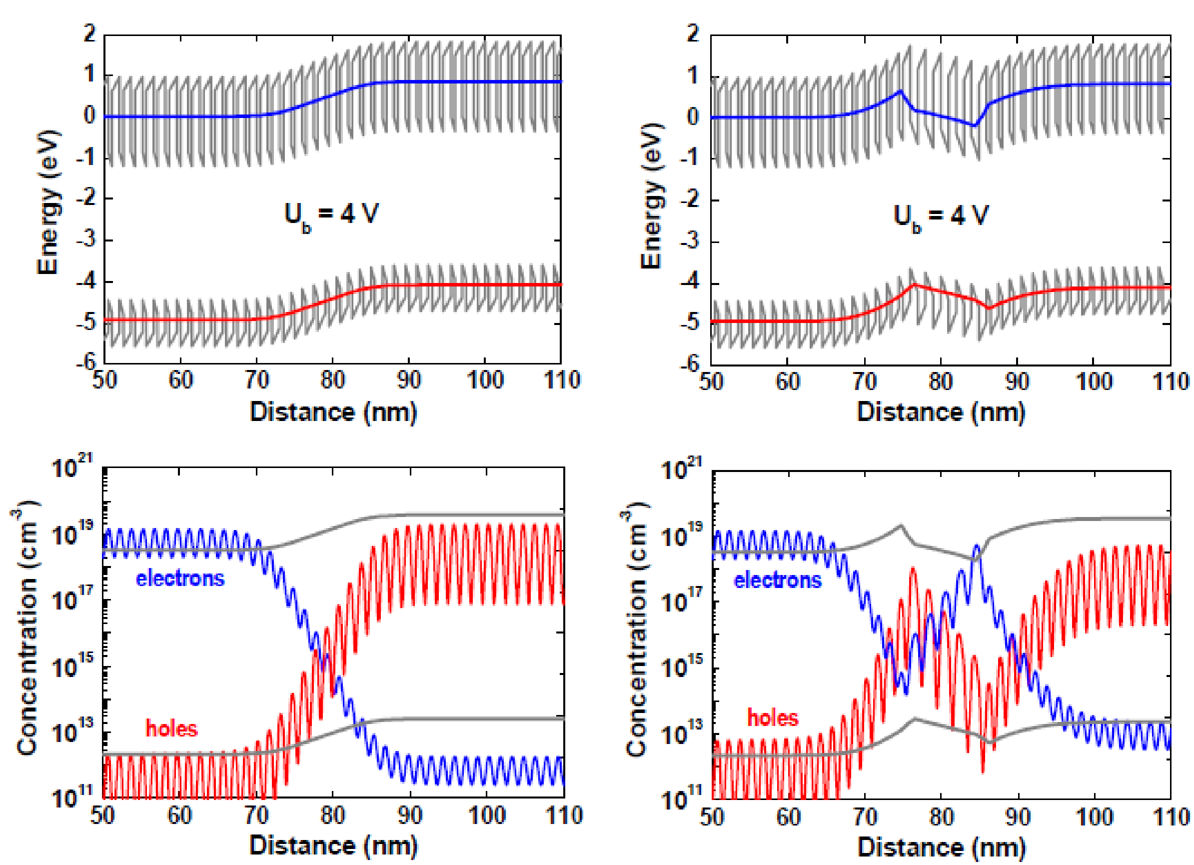
macroscopic charges are formed at a junction between two SLs with different macroscopic polarization vectors

K. A. Bulashevich, et al., Phys. Stat. Solidi (c) 2 (2005) 2394



$$P_{macr} = \frac{P_W d_W + P_B d_B}{d_W + d_B}$$

every superlattice can be characterized by a macroscopic electric polarization dependent on properties of the well and barrier layers



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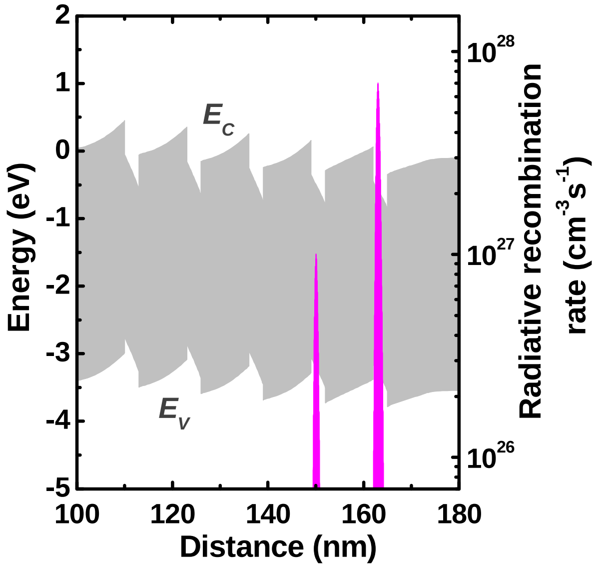
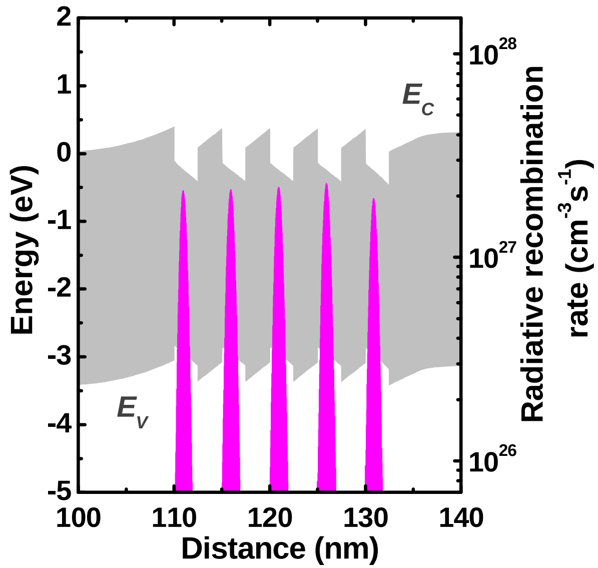
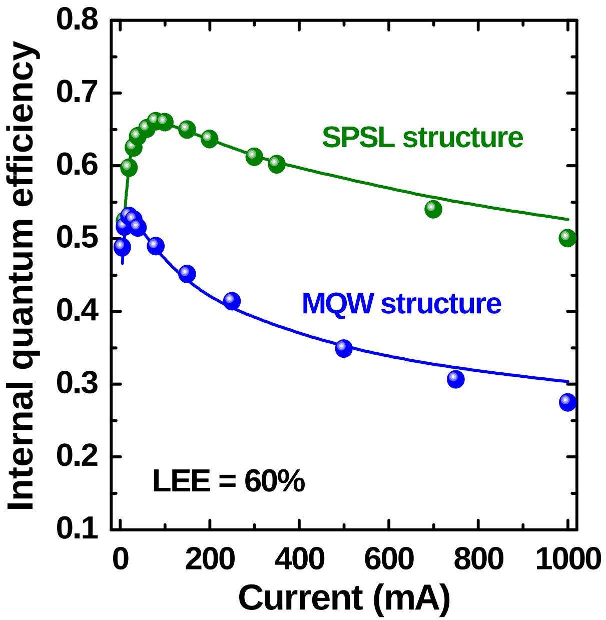


very non-uniform recombination rate distribution among individual QWs: only one QW operates

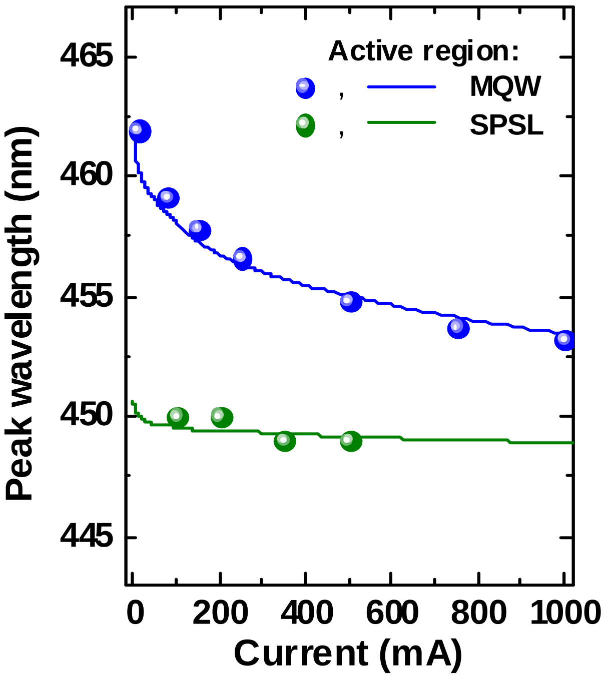


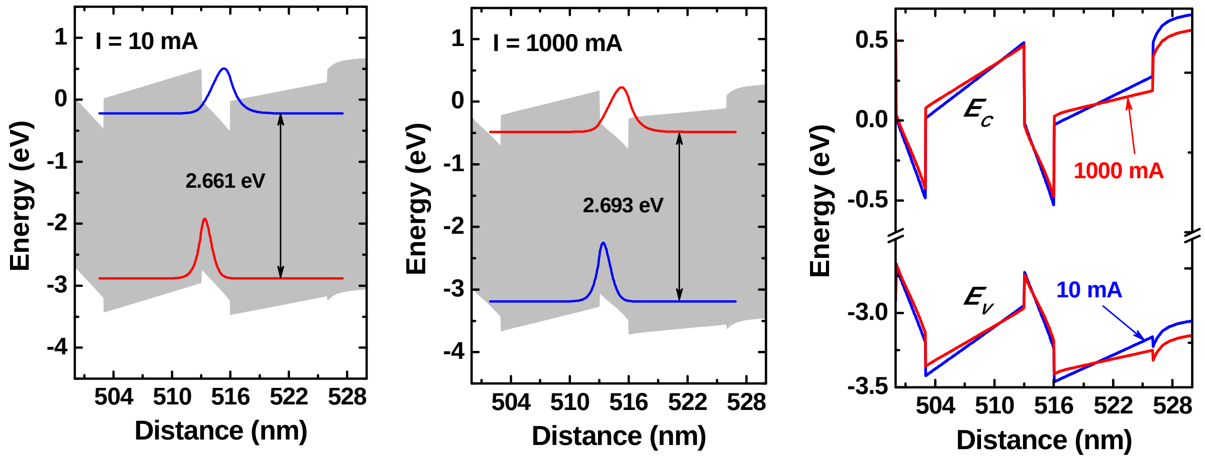
all the QWs give comparable rise to the recombination rate: this corresponds to an increased recombination volume

greater j_m for SPSL structure, which is the evidence for a larger recombination volume, and reduced efficiency droop due to suppression of Auger recombination



High stability of the emission wavelength in SPSL structure





since carrier recombination occurs primarily in one QW in the MQW structure, slight modification of the well profile with the bias applied is responsible for blue shift of the emission spectra

narrower barriers and uniform distribution of the recombination rate among all QWs results in a minor bias effect on the band alignment and, hence, on the emission spectra

Experiment: D. A. Zakheim et al., Phys. Stat. Solidi (c) 6 (2011) 2340

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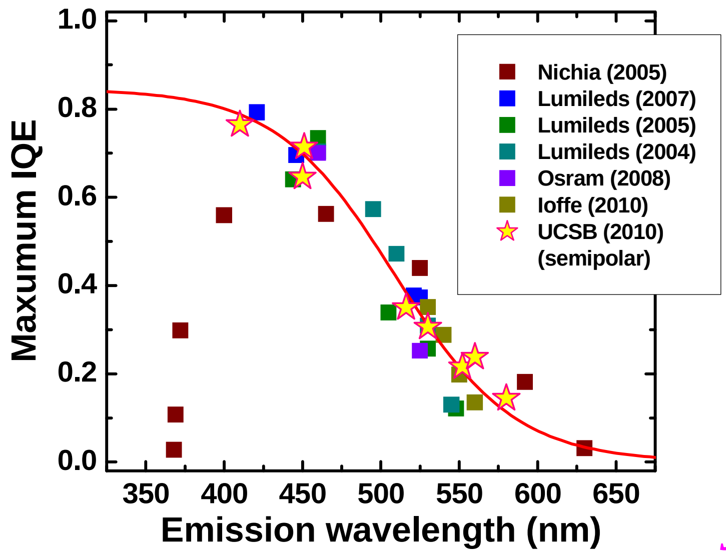
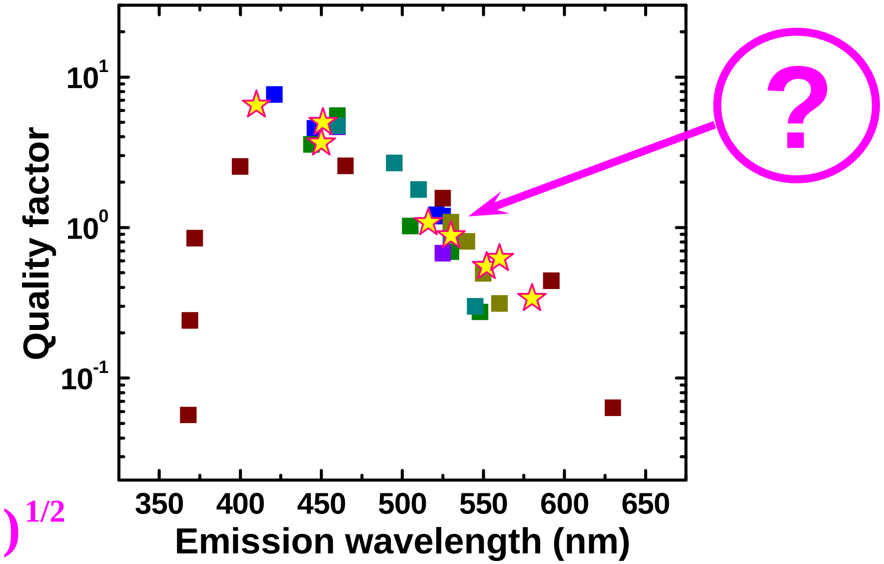
‘Green gap’ in the emission efficiency of III-nitride LEDs



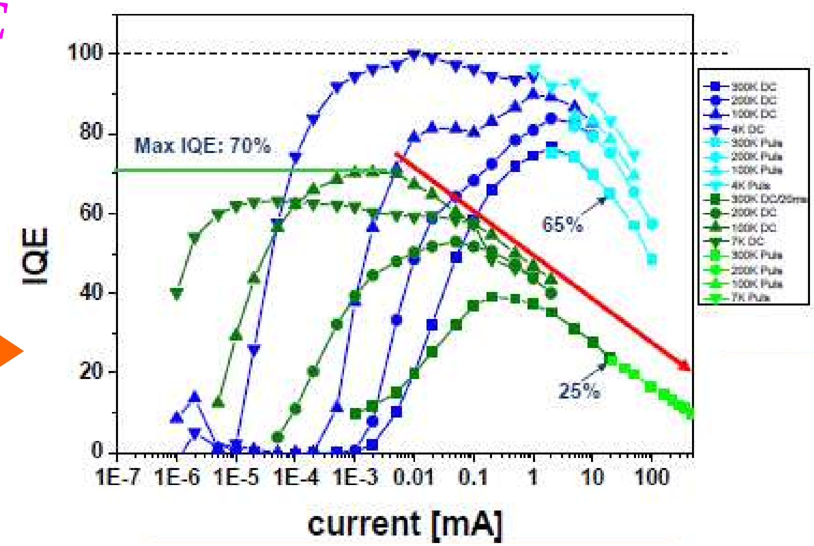


$$Q = B(\tau/C)^{1/2}$$

$$j_m = qdB/\tau C$$

data on EQE of LEDs emitting light with different wavelengths have been collected from various sources and recalculated to IQE dependence on the wavelength

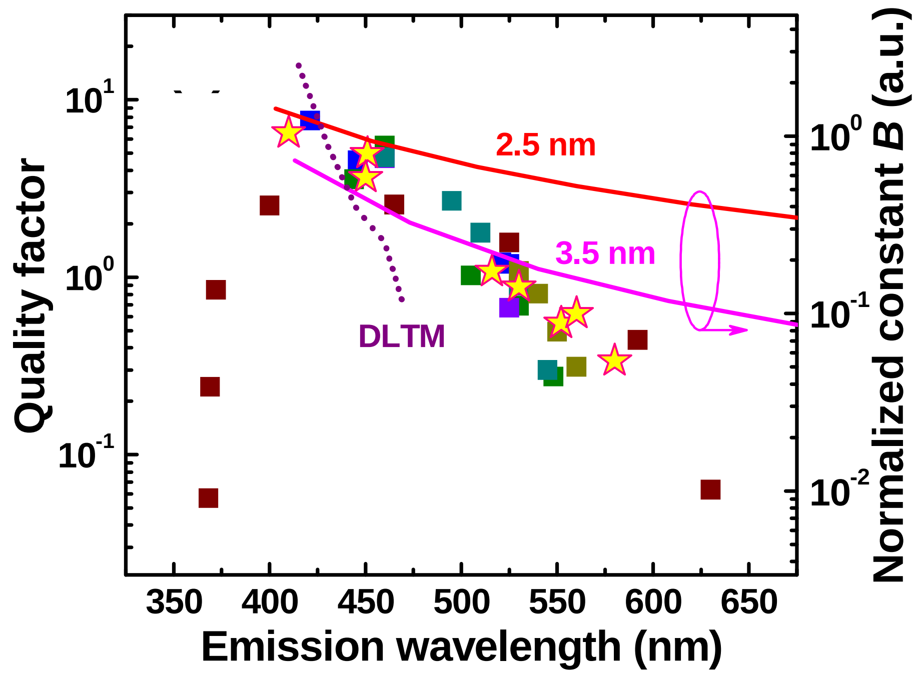
M. Sabathil et al., presentation at IWN, Montreaux (2008)



Degradation of the LED structure quality factor with the wavelength

$$B \propto \left| \int_{-\infty}^{\infty} dz \cdot \Psi_e(z)\, \Psi_{hh}(z) \right|^2$$

- decrease of the electron/hole wave function overlap with the wavelength may be attributed to the efficiency lowering in the range of ~430-520 nm
- at longer emission wavelengths, the efficiency decays faster then it is predicted theoretically – the evidence for additional mechanisms reducing efficiency ?



DLT measurements: A. David & M. Grundmann, Appl. Phys. Lett. 97 (2010) 033501

situation still remains ambiguous: theoretical estimates based on quantum-mechanical calculations disagree with available data of DLT measurements

Conclusions

- a figure of merit, the quality factor, is suggested to compare LED structures of various designs and emitting light at different wavelengths
- further improvement of the materials quality seems to be no longer effective for increasing the emission efficiency of violet and blue LEDs
- implementing the concept of large recombination volume, the LED structures with SPSL active regions are quite promising for reducing the efficiency droop and providing higher wavelength stability under current variation
- control of the value of radiative recombination constant by bandgap engineering, cavity effects, and other possible approaches seems to be beneficial for further improvements of the LED efficiency, especially in the green spectral range; a deeper understanding of indium surface segregation effects on the conduction/valence band profile is necessary for this purpose