SPIE Photonics West: GaN materials and devices VI,
San Francisco, USA, 22-27 January, 2011

Modeling of III-nitride Light-Emitting Diodes: Progress, Problems, and Perspectives

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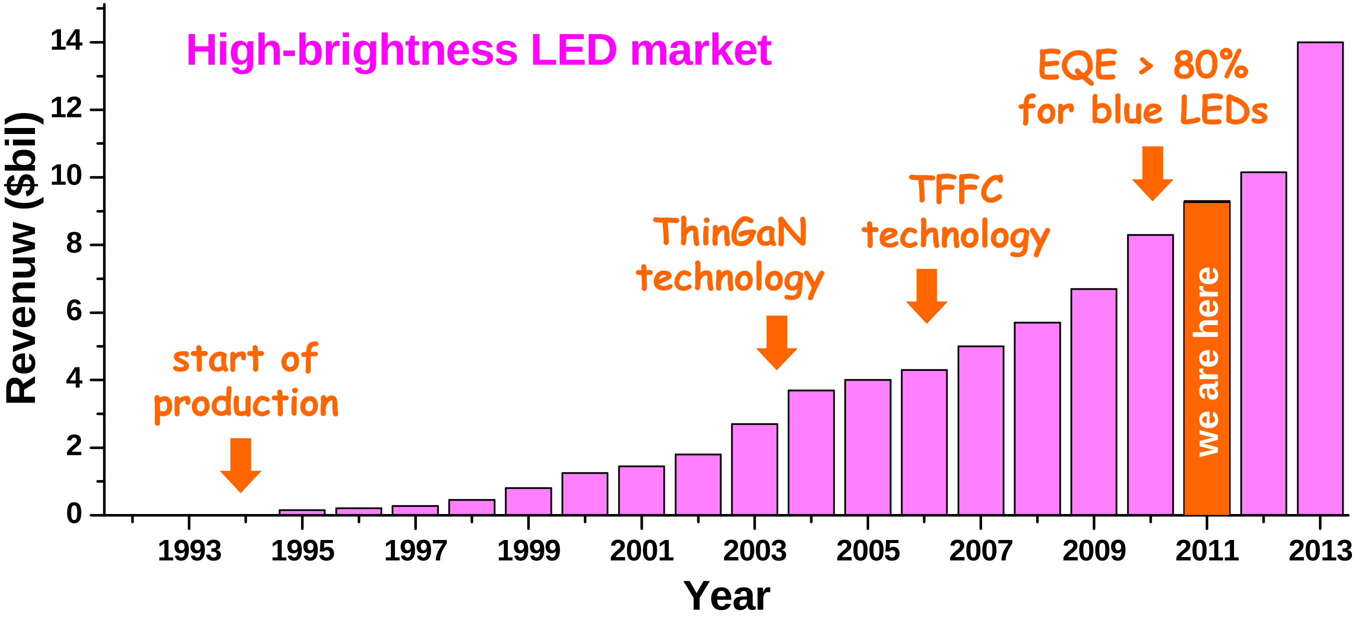
Development of III-nitride LED technology and basic research

Technological background:

- buffer layer in MOVPE for GaN
- p-doping of GaN
- InGaN growth, including QWs



Milestones of basic research:

spontaneous polarization in III-N materials

effect of InGaN composition fluctuations on IQE

correct bandgap of InN and InGaN alloys

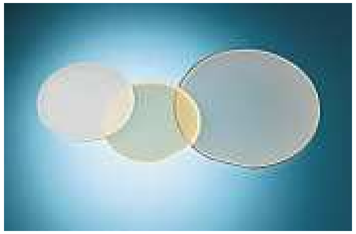
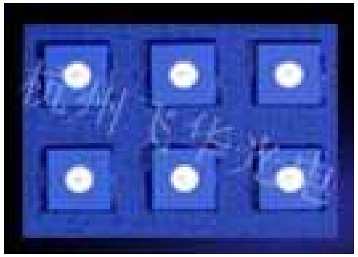
Auger recombination in InGaN

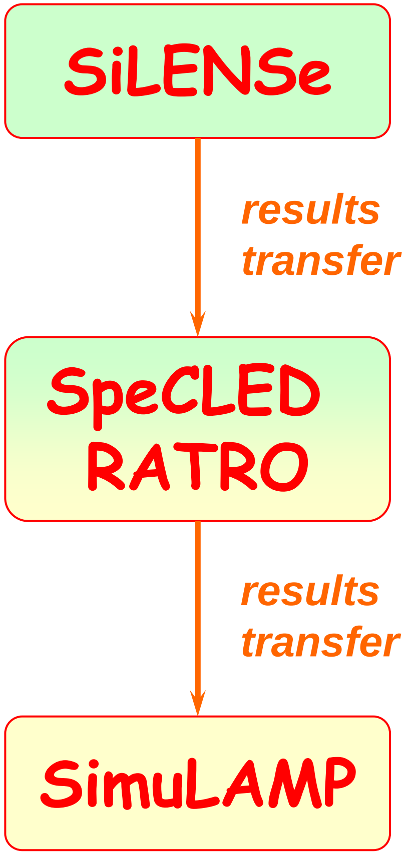
LED modeling

Outline

- Features of III-nitride LED modeling
- Critical physical mechanisms
  - carrier recombination in InGaN QW
  - polarization doping
  - current crowding in LED dice
  - light conversion
- Unsolved problems
- Future developments

Multi-scale problem and simulation approach

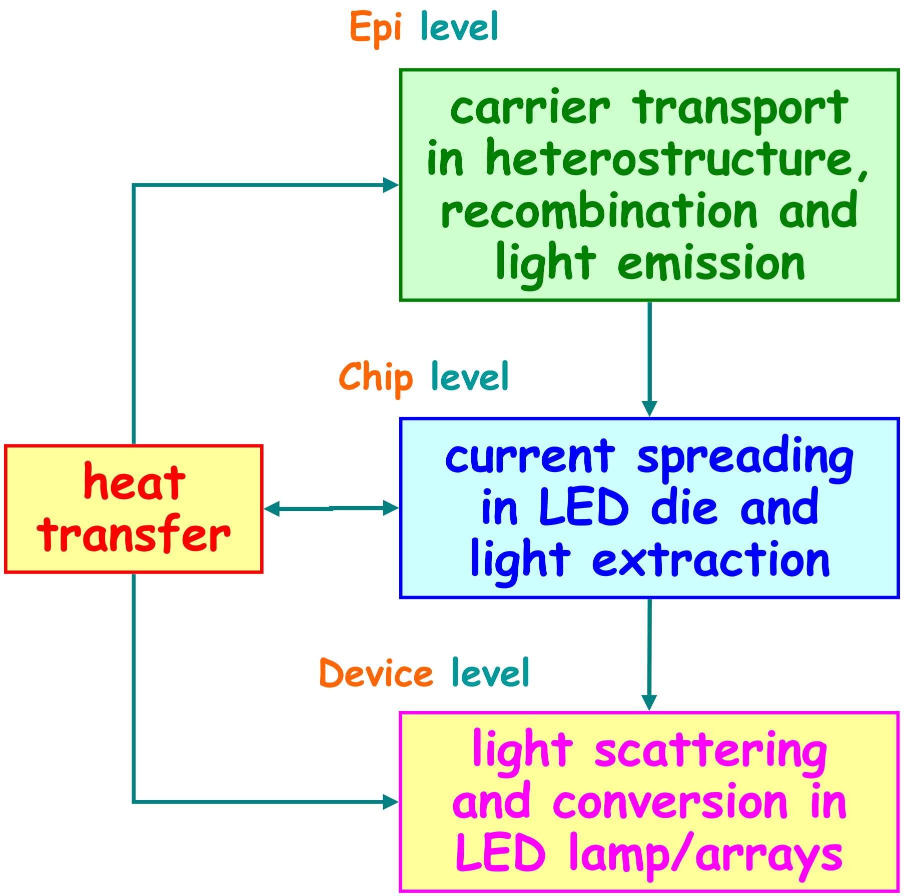
	Targets	Scales	Tools
Epi level 	Design and optimization of LED structures	~1-100 nm	**SiLENSe**
Chip level 	Design and optimization of LED chips	~1-1000 μm	**SpeCLED** **RATRO**
Device level 	Design and optimization of DC & AC LED lams, arrays, etc.	~0.01-1.0 cm	**SimuLAMP**



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

Interrelation of physical phenomena involved in LED operation

Mechanisms involved in LED operation



Epi level

carrier transport in heterostructure, recombination and light emission

Chip level

current spreading in LED die and light extraction

heat transfer

Device level

light scattering and conversion in LED lamp/arrays

Multi-disciplinary physics

- ✓ elasticity & electro-mechanical coupling
- ✓ dislocations & interaction with carriers
- ✓ electrostatics & spontaneous polarization
- ✓ band structure with strain effects
- ✓ carrier transport & recombination
- ✓ quantum mechanics

- ✓ current flow in a complex structure
- ✓ ray tracing and scattering by surface textures

- ✓ heat transfer

- ✓ electrodynamics & wave scattering
- ✓ light conversion, including multi-phosphor interaction
- ✓ spectral ray tracing
- ✓ colorimetry

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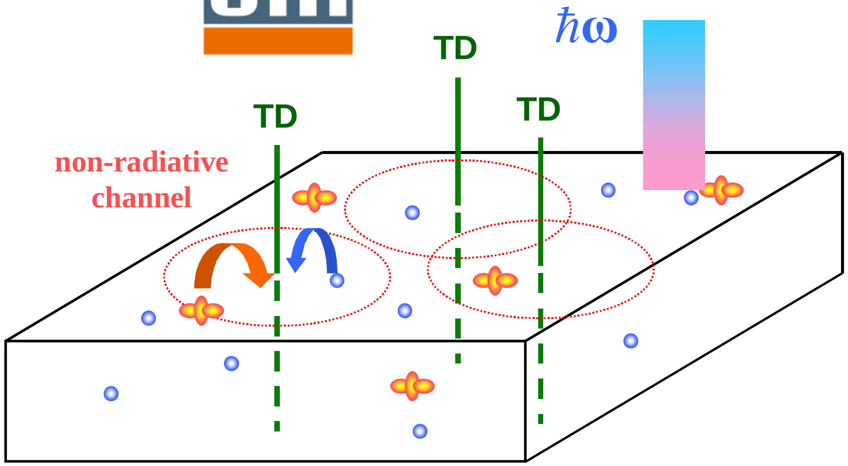
Carrier recombination in InGaN QW active region

Non-radiative recombination in III-nitride materials: effect of TDs

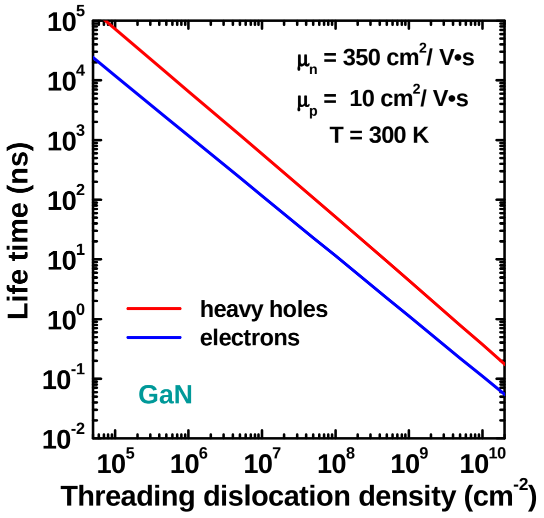


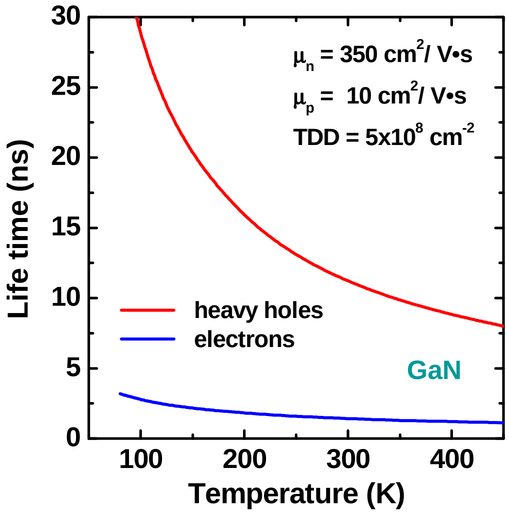
being non-radiative recombination centers, TDs affect appreciably the life times of electrons and holes :

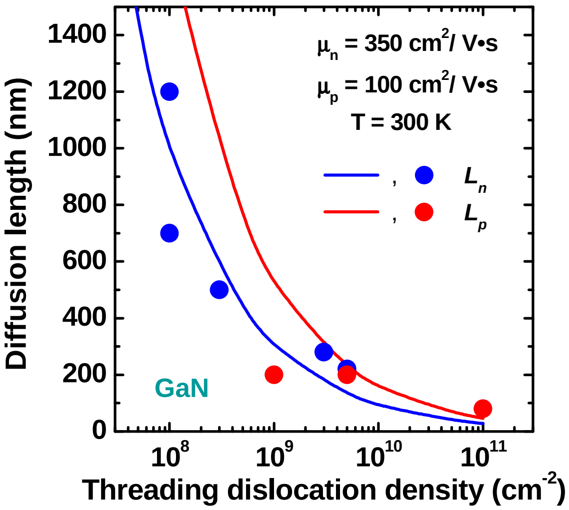
$$\tau_{dis} = \frac{q}{4\pi kT\mu N_d}\left\{\ln\left(\frac{1}{\pi a^2 N_d}\right) + \frac{2kT\mu}{qaV_{th}} - \frac{3}{2}\right\}$$

S. Yu. Karpov and Yu. N. Makarov, Appl. Phys. Lett. 81 (2002) 4721

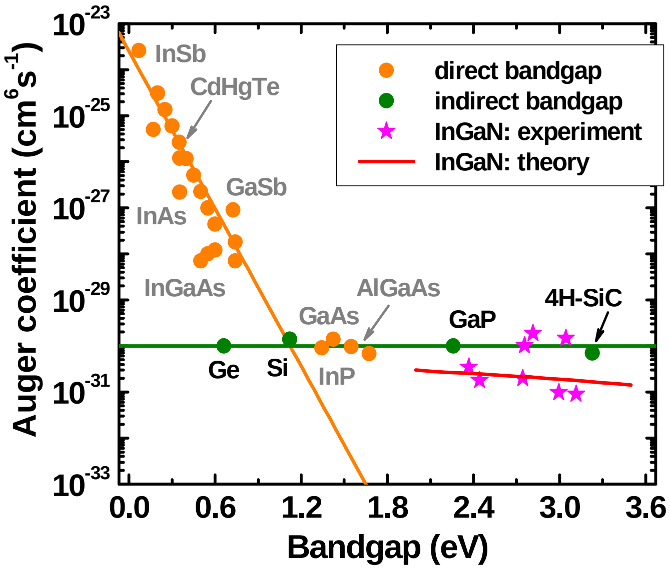
$$L_D = (kT\mu\tau_{dis}/q)^{1/2}$$







Auger recombination in III-nitride semiconductors



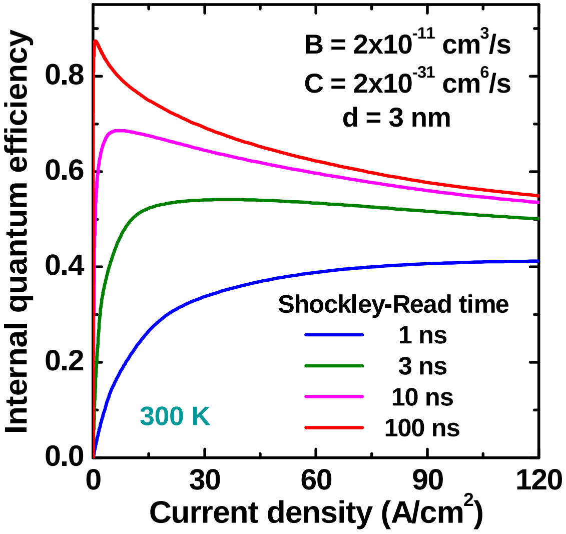
different trends in the Auger coefficient variation with the bandgap for direct- and indirect-bandgap materials; InGaN obeys the latter trend

ABC-model:

$$j = qd\,(An + Bn^2 + Cn^3)$$

$$\mathrm{IQE} = Bn/(A + Bn + Cn^2)$$

$$A = 1/\tau_{SR}$$

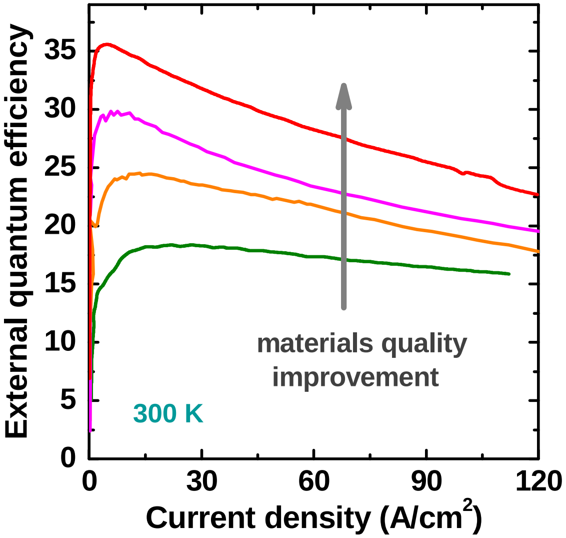


ab initio calculations for InGaN:

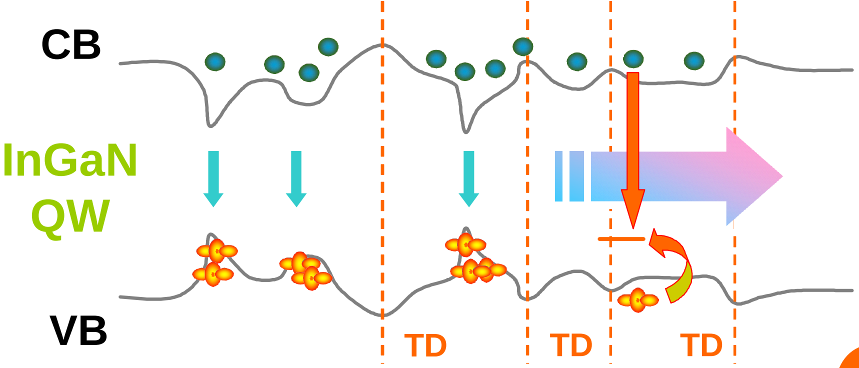
C. Van de Walle, private communication

experiment:

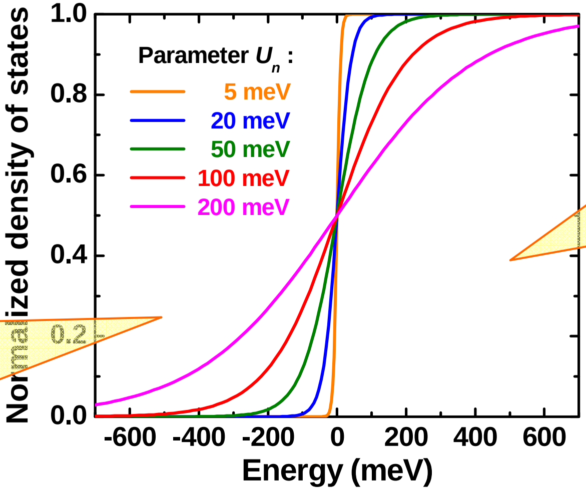
A. E.Chernyakov et al., Superlattices & Microstructures 45 (2009) 301



Localized and delocalized states in InGaN quantum wells

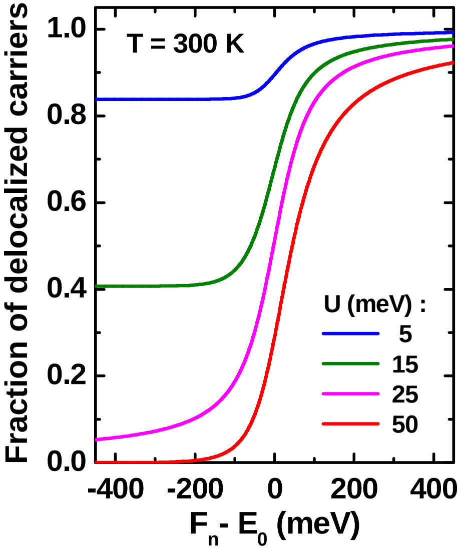


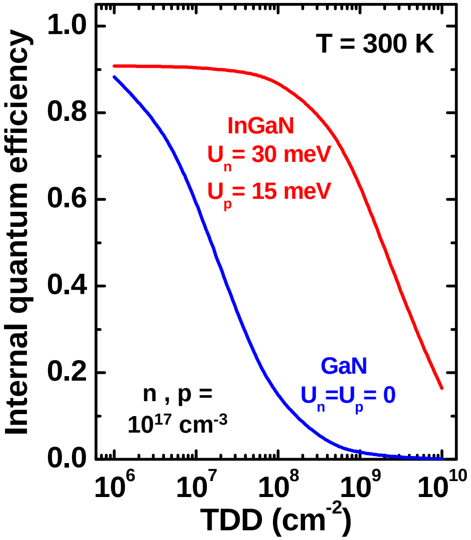
both QW thickness and composition fluctuations may produce DOS tails in the bandgap



localized carriers: do not take part in recombination at TDs

delocalized carriers: participate in recombination at TDs

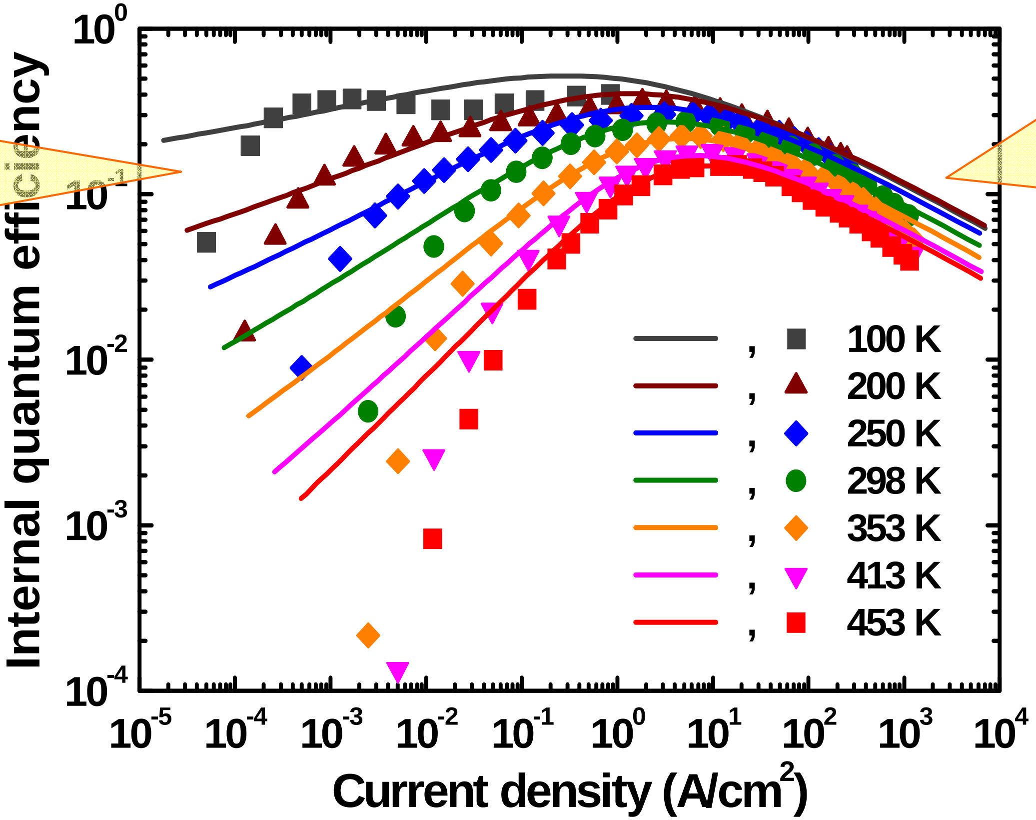




localized states due to composition/QW thickness fluctuation in InGaN increase the material IQE

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

$$B \propto T^{-1}$$

$$C = const(T)$$

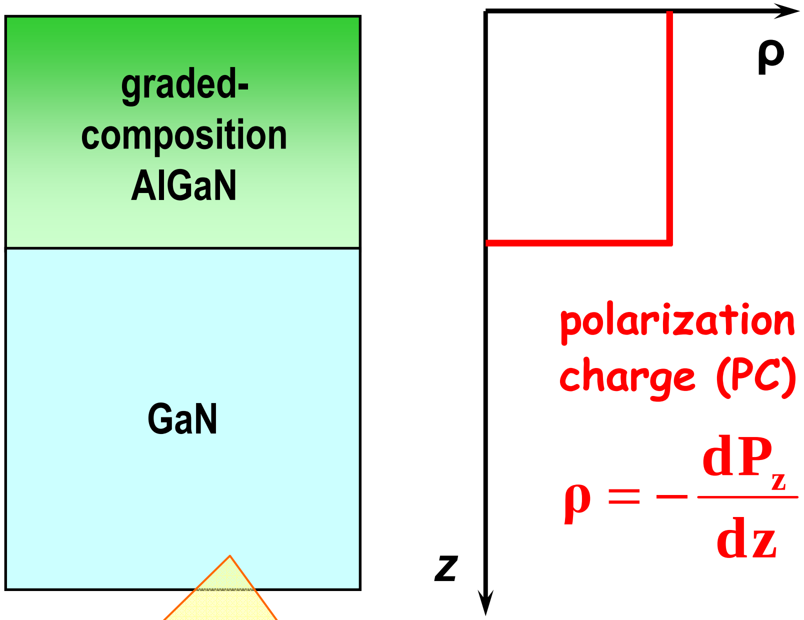
ABC model predicts well the IQE variation with the current density and temperature in the range of ~200-450 K

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)

Distributed polarization doping in LED structures

Distributed polarization doping (DPD) in graded-composition materials



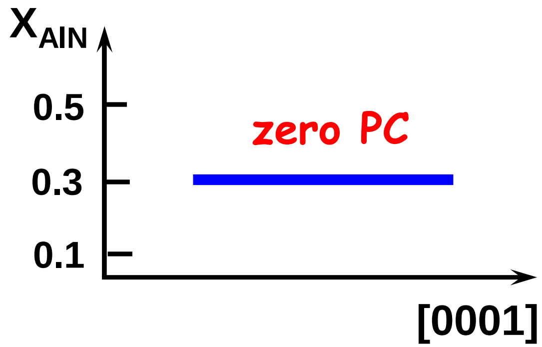
polarization charge (PC)

$$\rho = -\frac{dP_z}{dz}$$

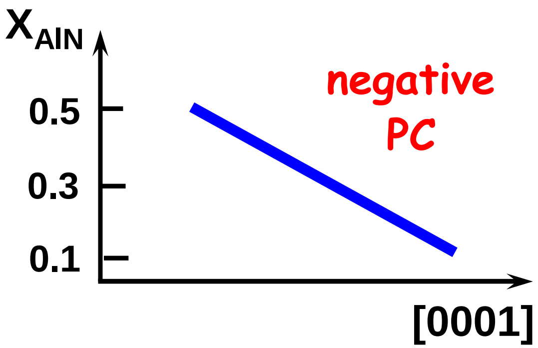
Distributed polarization doping has been proposed, for the first time, for HEMTs

D. Jena et al., Phys.Stat.Solidi (c) 0 (2003) 2339

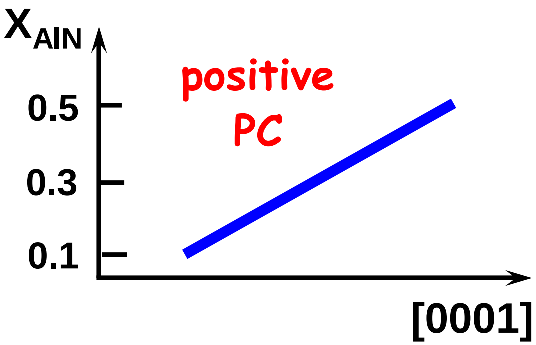
constant composition



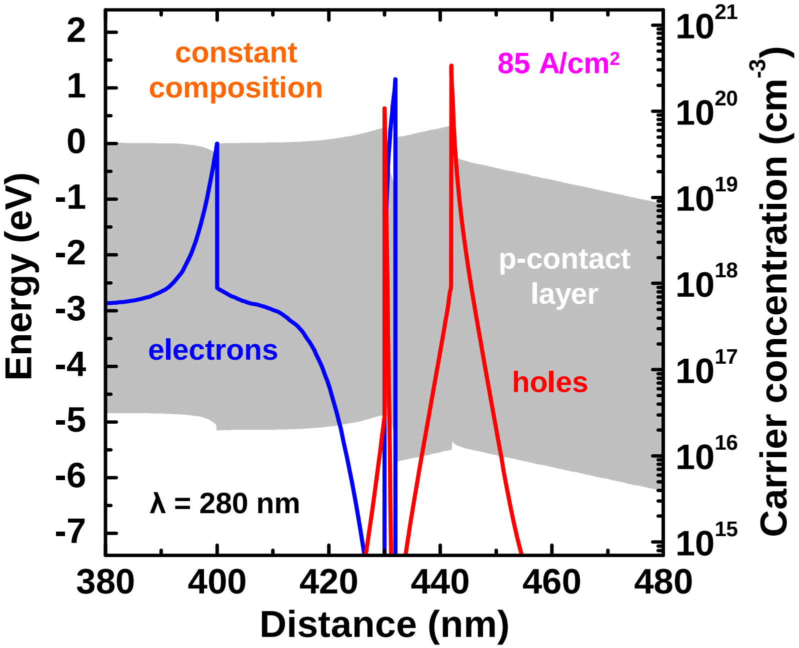
descending composition



ascending composition

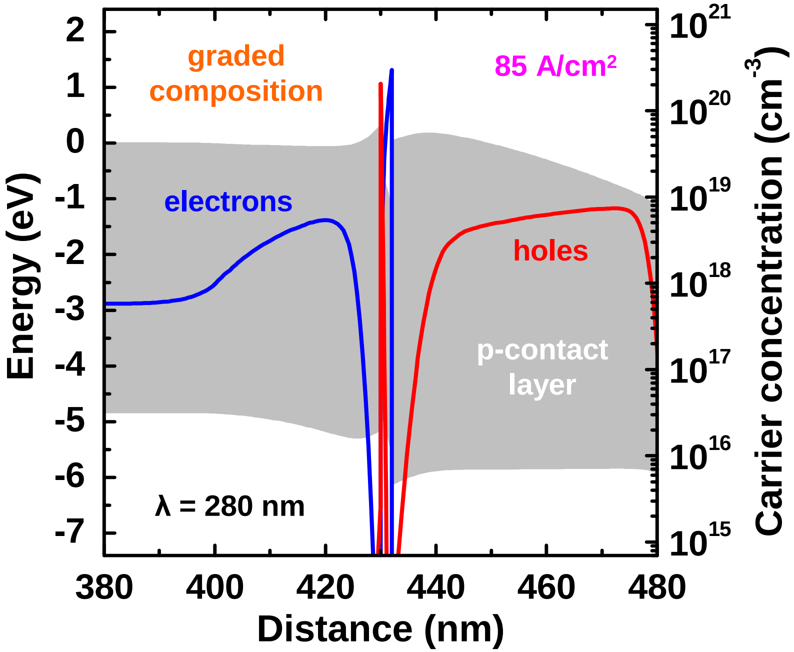


Using DPD for performance improvement in deep-UV LEDs



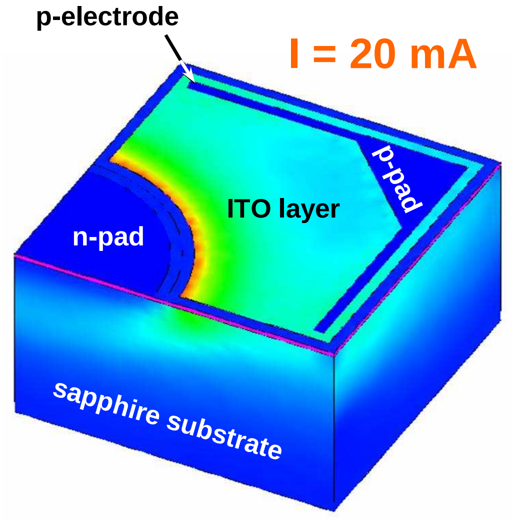
Ga-polar structure with constant-composition layers suffers from vanishing hole concentration in the contact layer

LED with parabolic composition profiles in EBL and HBL produces high electron and hole concentrations throughout the layers



Current crowding in LED dice

Current localization in LED die with ITO spreading layer



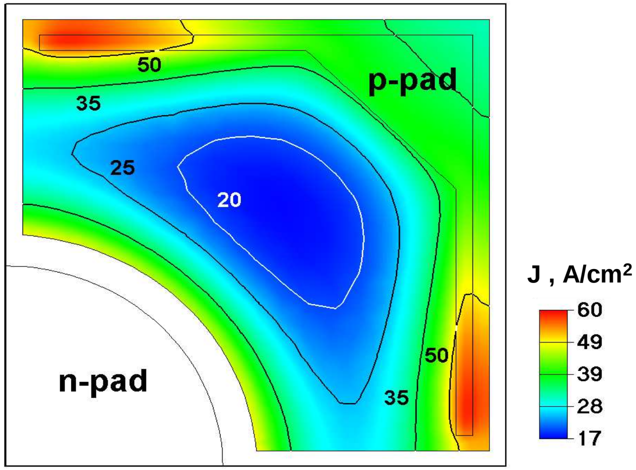
- the principal origin of current crowding is nonlinear resistance of the p-n junction, depending on temperature
- a more pronounced current crowding results in a lower LED series resistance:

$$R_s \approx \rho_n L_{sp} / P_n d_n$$

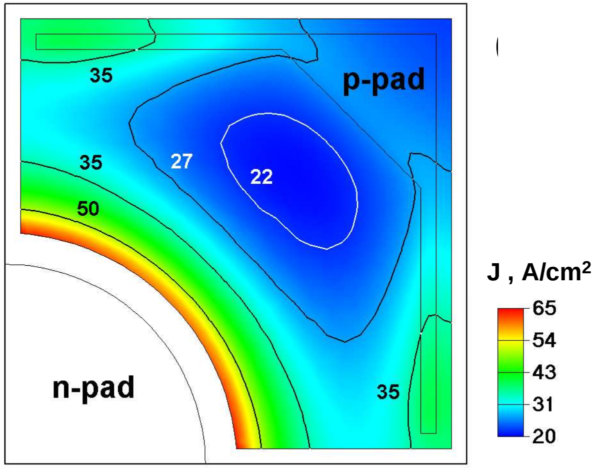
P_n and d_n are the specific resistance and thickness of the n-contact layer, L_{sp} is the current spreading length and P_n is the outer perimeter of the n-electrode

increasing series resistance

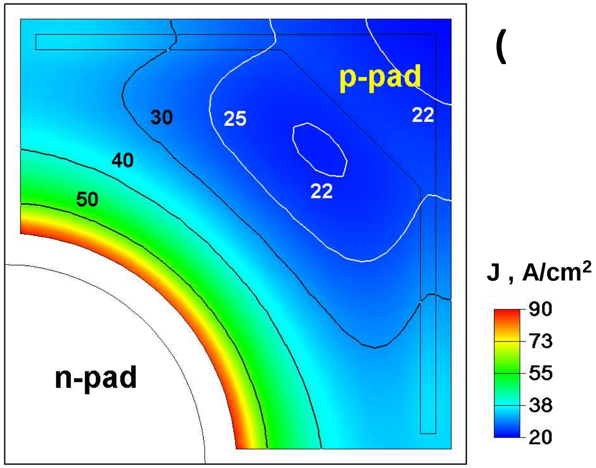
d_{ITO}= 20 nm



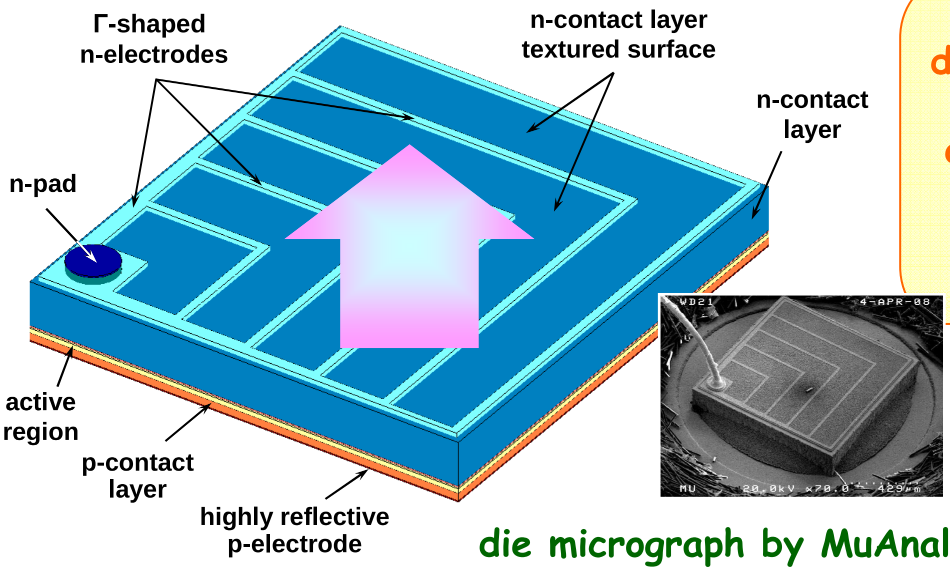
d_{ITO}= 50 nm



d_{ITO}= 100 nm

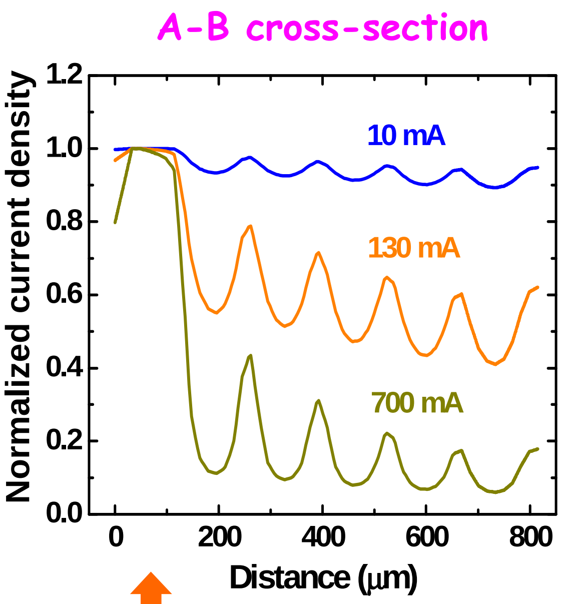


Current crowding effect on light extraction efficiency in a vertical LED die

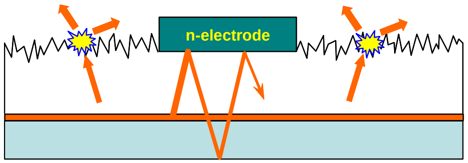


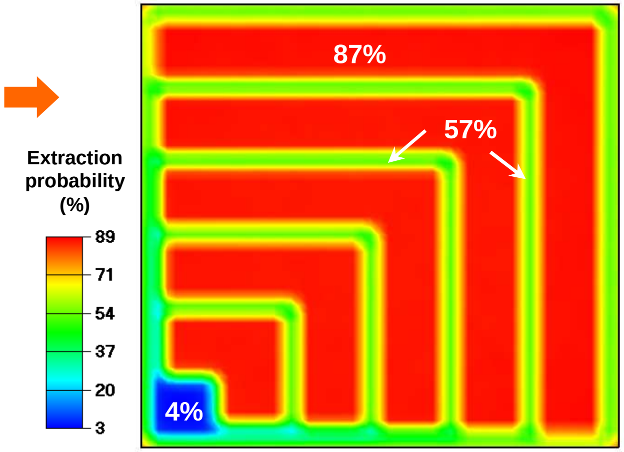
die micrograph by MuAnalysis, Inc., 2008

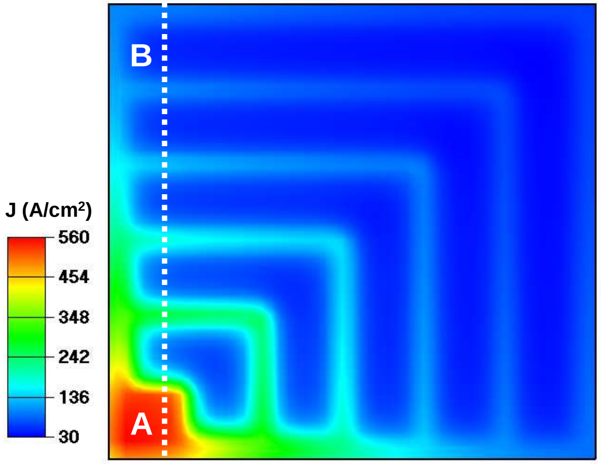
current density non-uniformity depends on the total operating current



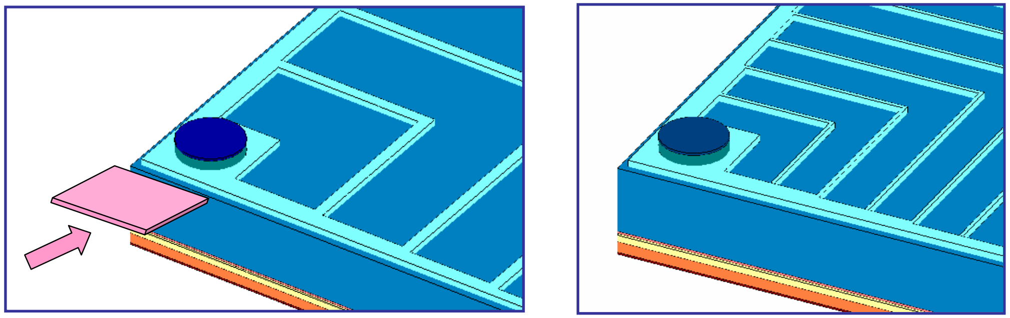
probability of light extraction falls down under and next to the n-electrodes



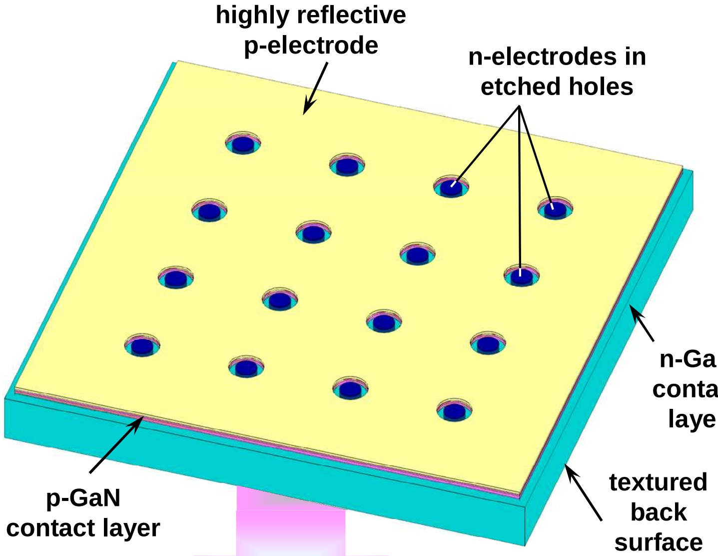




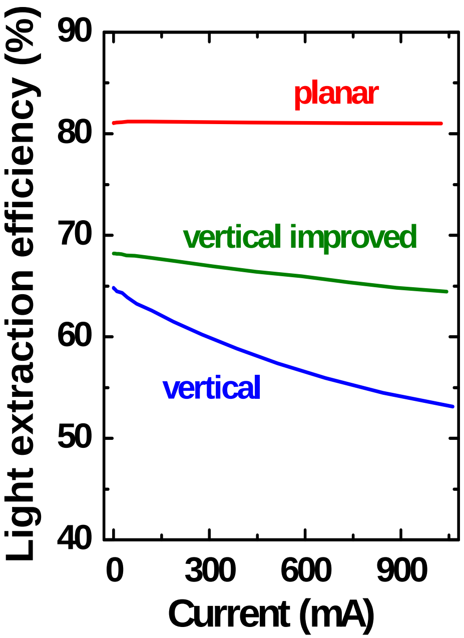
Reduction of the crowding effect on LEE via LED chip design



improvements in vertical die design

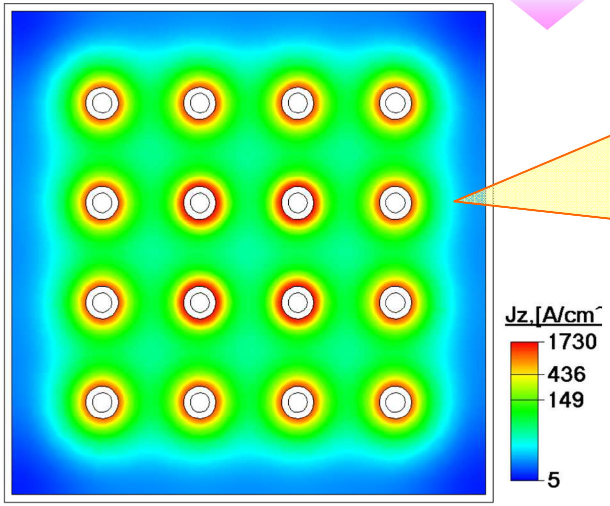


TFFC planar die



comparison of the die designs

M. V. Bogdanov et al., Phys.Stat.Solidi (c) 7 (2010) 2124

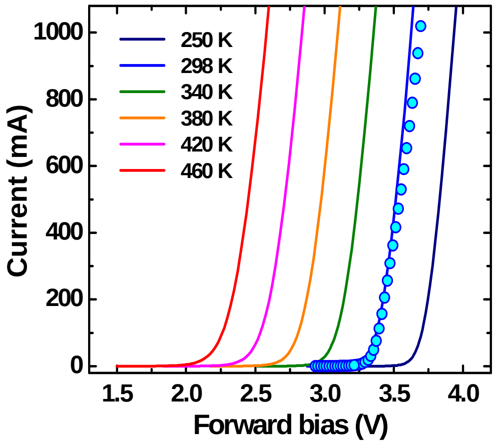


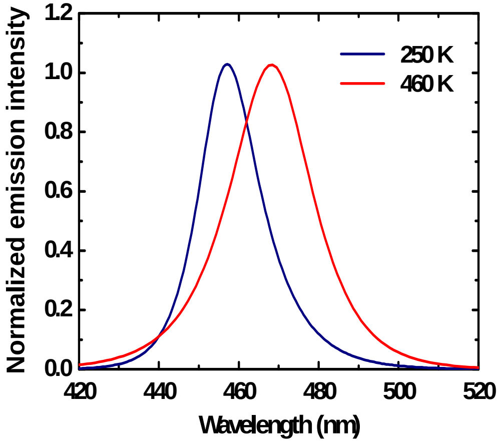
because of smaller total n-electrode perimeter, the current crowding is more pronounced

Light conversion in LED lamps

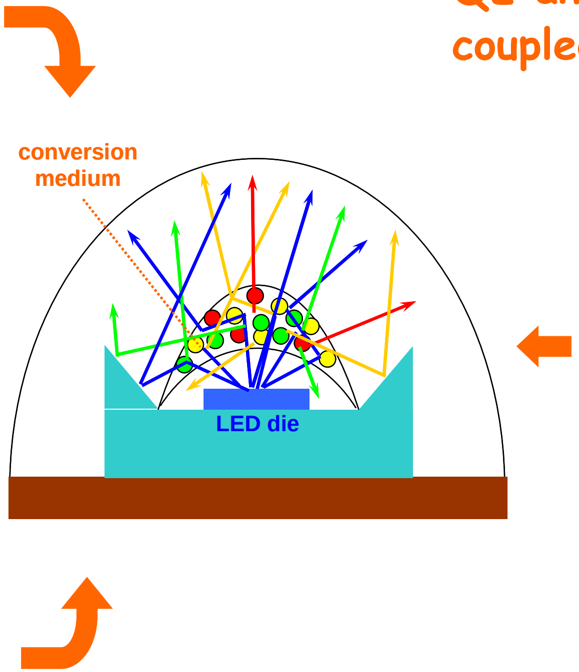
Modeling of light conversion in white-LED lamps

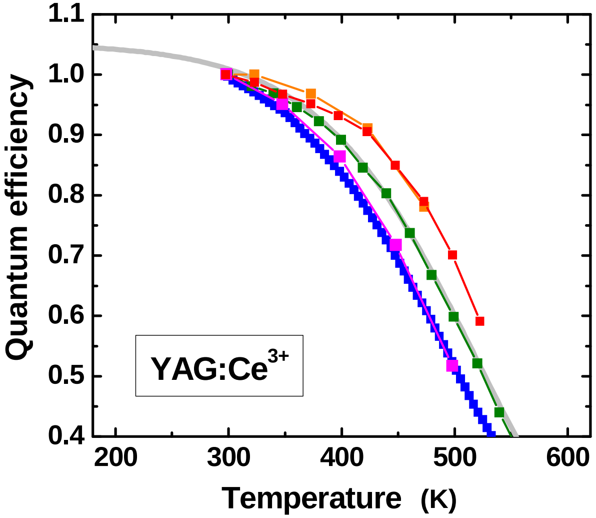
- many phosphors and/or conversion media → spectral ray-tracing
- temperature-dependent phosphor QE and LED characteristics → coupled optical/thermal analysis





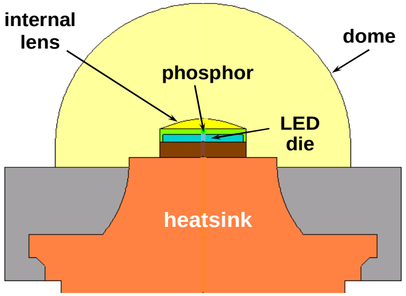
temperature-dependent LED characteristics

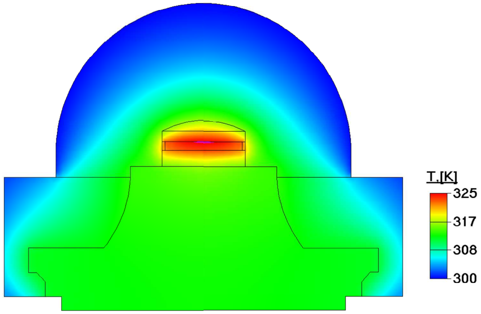




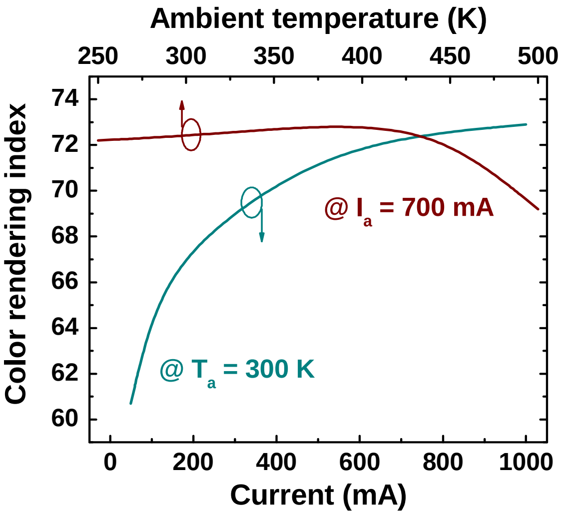
- Mie theory is now widely used for modeling light scattering and absorption by phosphor particles

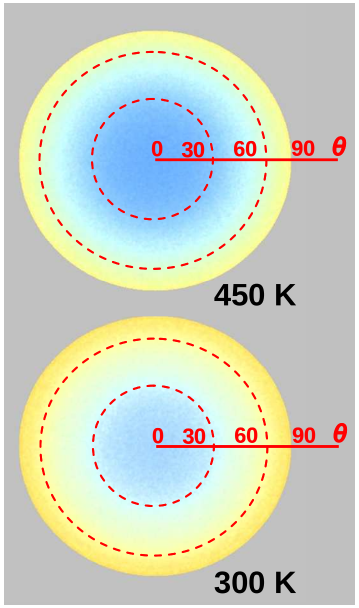
Effect of white LED operation conditions on the white light quality





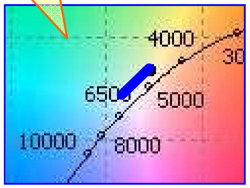
conversion medium is primarily heated by LED

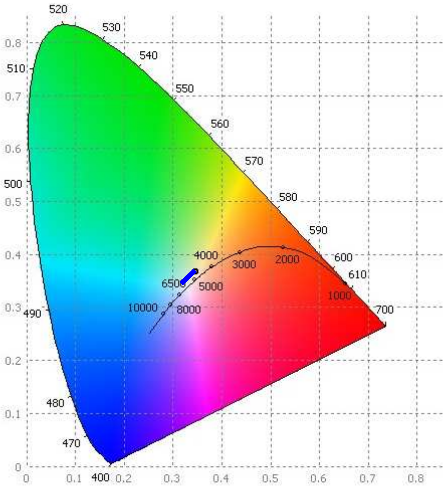


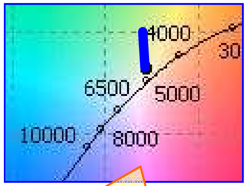


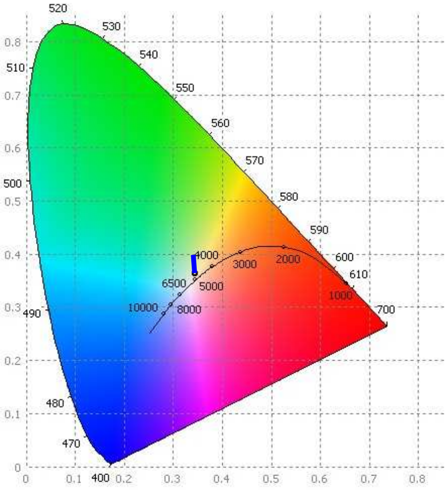
color angular non-uniformity in the far-field zone

chromatic coordinates variation with temperature









current dimming moves the chromatic coordinates away from the black-body radiation locus

O. V. Khokhlev et al., Proc. 3rd Int. Conf. on White LEDs & Solid State Lighting (2010) 29

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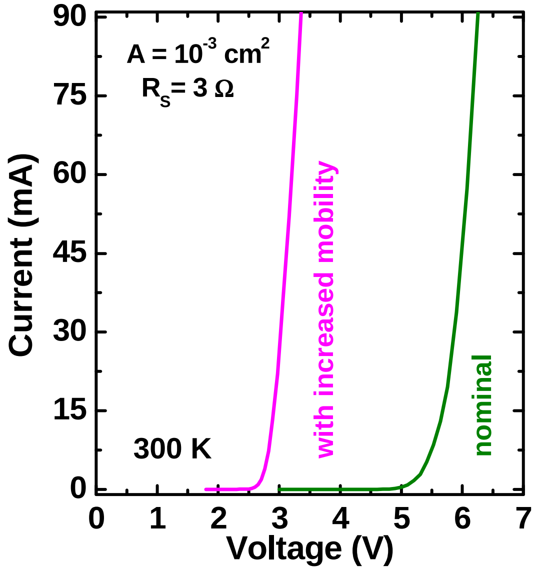
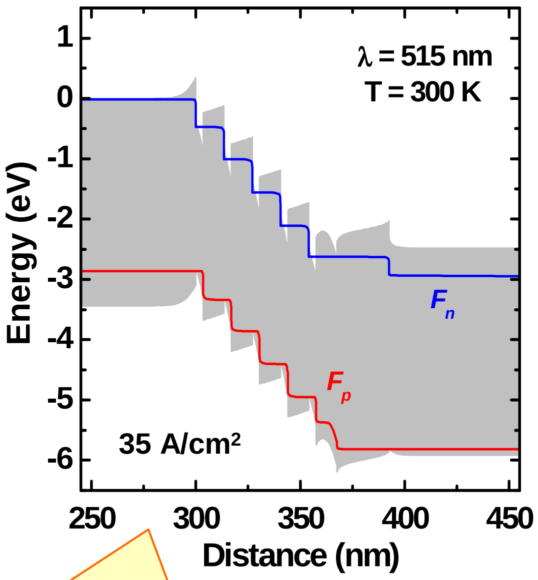
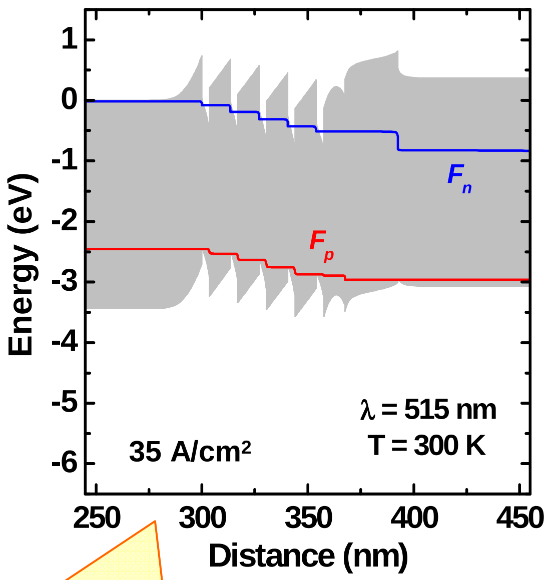
Overestimated operation voltage in III-nitride LEDs



with nominal mobilities in the structure



with artificially increased mobilities



high ballistic electron leakage is expected

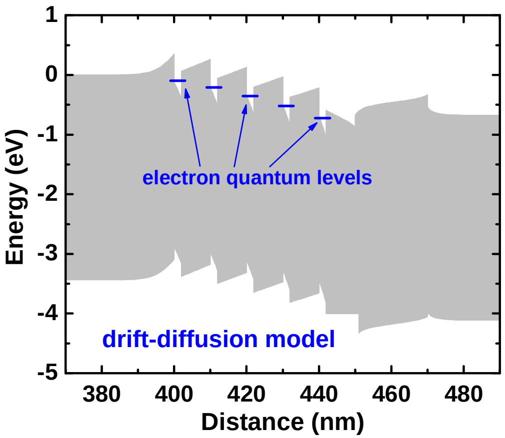
no electron leakage at flat band diagram

Possible channels of additional conductivity:

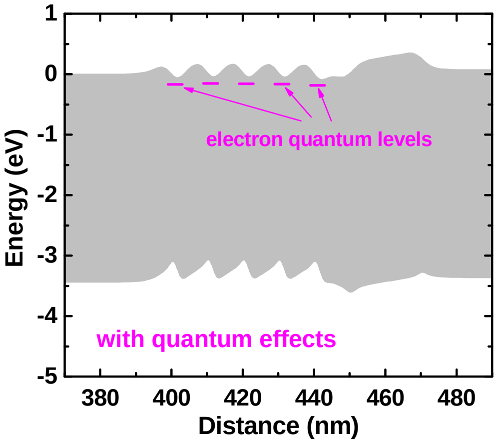
- direct or defect-assisted tunneling in MQW barriers
- dislocation-mediated conductivity
- ballistic transport in the barriers & incomplete carrier capture in the QWs
- reduction of the barrier heights due to composition fluctuations in InGaN

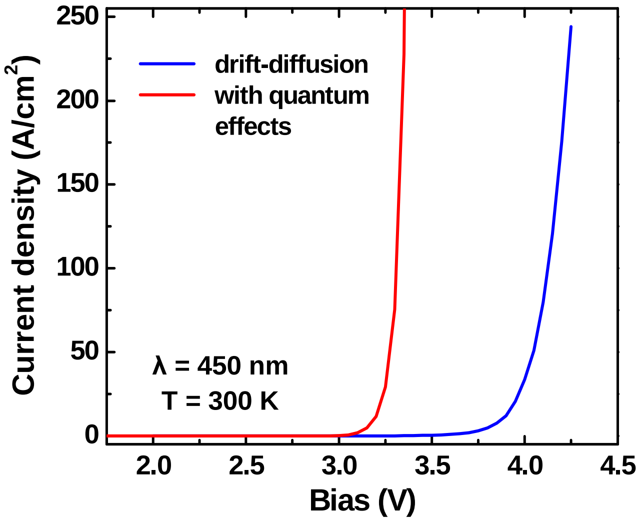
Using of quantum potential for solution of transport equations

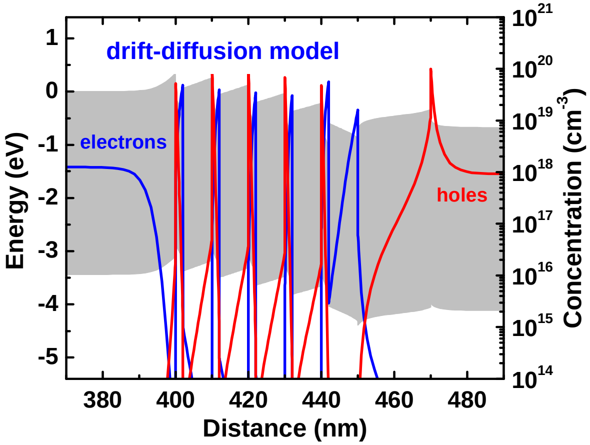
actual band diagram

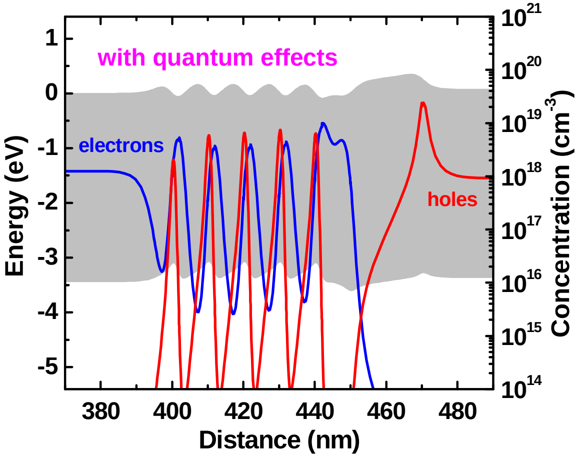


effective band diagram









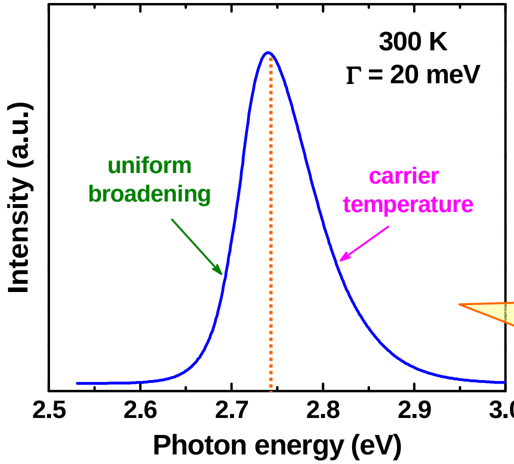
use of quantum potential improves operation voltage predictability and modifies properly the electron and hole density distributions

quantum potential accounts approximately tunneling and confinement effects

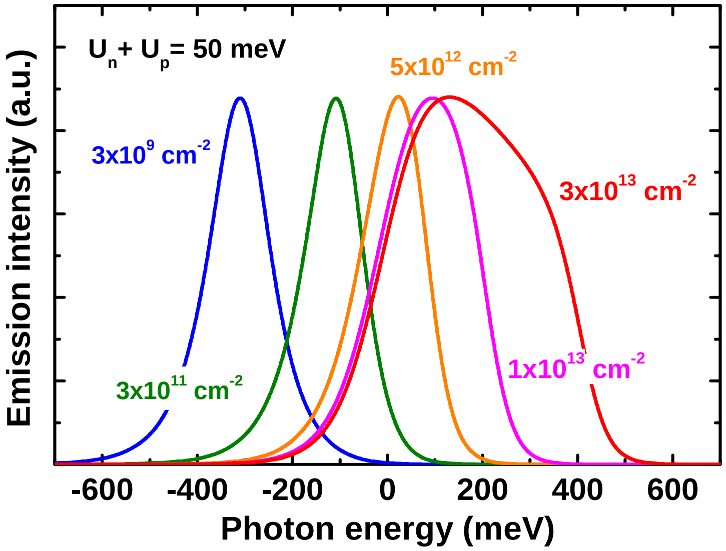
Prediction of emission spectra and their blue shift with current

Model: M. A. Jacobson et al., Semiconductors 39 (2005) 1410

with account of localized states formed by composition/thickness fluctuations in InGaN QW

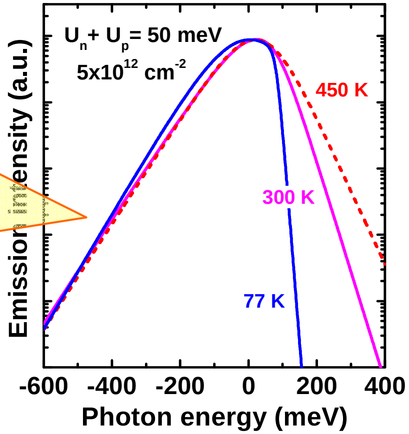


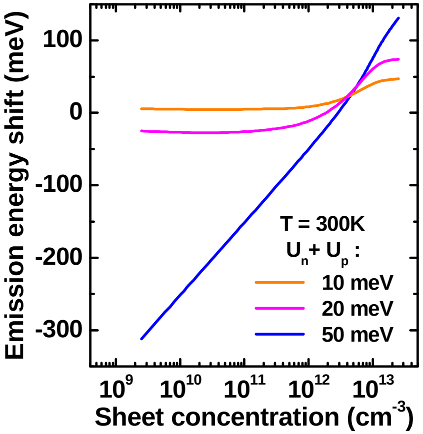
theoretical spectra shapes do not fit the experimental ones



the model of localized states predicts enhanced emission spectrum blue shift caused by filling the DOS tails

low-energy spectrum wing is determined by DOS tail due to fluctuations of thickness or composition of InGaN QW

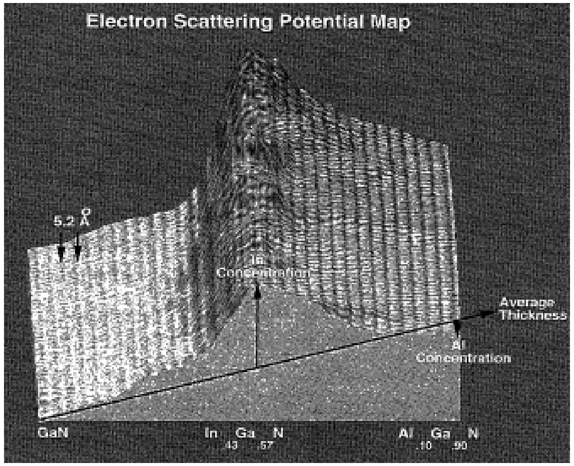




Outline

- Features of III-nitride LED modeling
- Critical physical mechanisms
  - carrier recombination in InGaN QW
  - polarization doping
  - current crowding in LED dice
  - light conversion
- Unsolved problems
- Future developments

Technological factor: effect of In surface segregation on InGaN QW profile



Experiment:

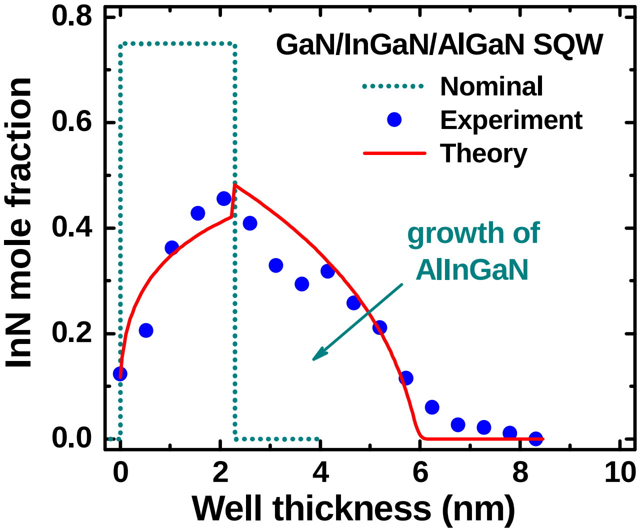
C. Kisielowski et al., Jpn. J. Appl. Phys. 36 (1997) 6932

Indium surface segregation results in:

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

Other transient effects:

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



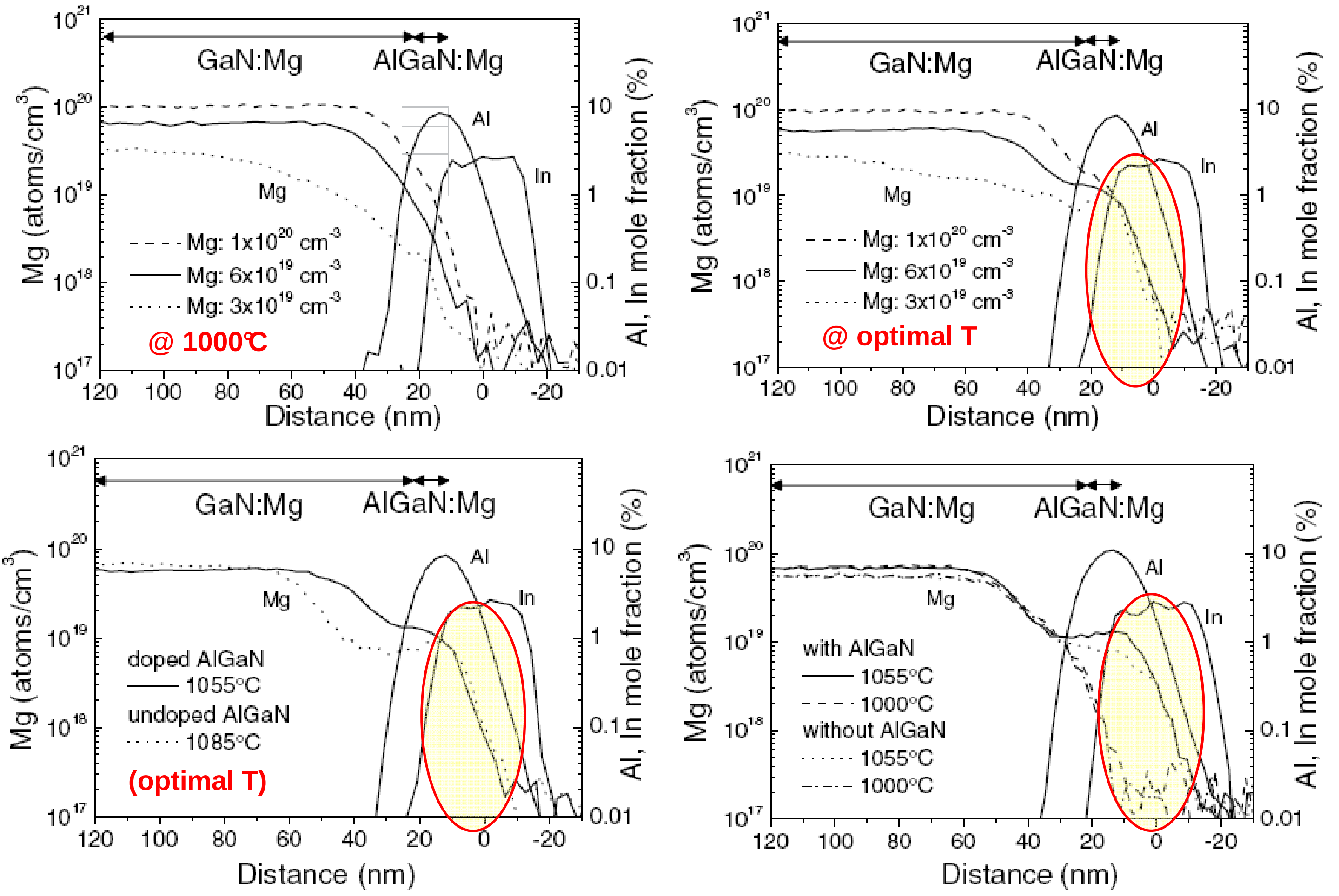
Theory:

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

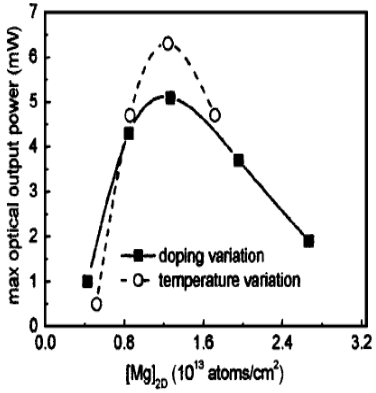
Now it has become possible to make coupled simulation of LED structure growth by MOVPE and operation of the grown device

Technological factor: redistribution of impurities during LED structure growth

**K. Köhler et al.,
J. Appl. Phys. 97
(2005) 104914 ;
Phys. Stat. Solidi (a)
203 (2006) 1802**



optimum doping for high LED efficiency



back diffusion of Mg removes the acceptors from the active region toward the AlGaN EBL and *p*-contact layer

Conclusions

- to account for and utilize in practice unique properties of III-nitride materials, a number of critical mechanisms should be considered: multi-channel recombination in LED active region, distributed polarization doping, 3D coupled current spreading & heat transfer in LED dice, multi-phosphor light conversion, etc.

- a number of issues, like enhanced electrical conductivity in LED structures, impact of carrier localization on the emission spectra, cavity effects, microscopic nature of Auger recombination, etc. should be studied experimentally and theoretically in future to generate respective physical models

- strong influence of technological factors on III-nitride LED properties requires a coupled simulations of the heterostructure epitaxial growth and device operation

Acknowledgment

I am grateful to my colleagues
K. A. Bulashevich
O. V. Khokhlev
I. Yu. Evstratov
V. F. Mymrin
M. S. Ramm
M. V. Bogdanov
A. I. Zhmakin
contributed much to development, numerical implementation, and validation of models for III-nitride LED simulation