



Physics and Simulation of Nitride Light-Emitting Devices

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Outline

1. Introduction
2. Nitride Material Properties
3. Light-Emitting Diode (LED)
4. Laser Diode (LD)

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A Brief History

- 1970 Pankove demonstrates GaN LEDs
- 1986 Akasaki demonstrates Low Temp AlN buffer
- 1989 Akasaki p-type GaN by electron beam
- 1991 Nakamura two-flow MOCVD
- 1992 Nakamura p-type GaN by thermal annealing
- 1992 Nakamura demonstrates first InGaN growth
- 1993 Nakamura Blue LED
- 1995 Nakamura 1st Blue Laser Diode

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Application Examples (LED)

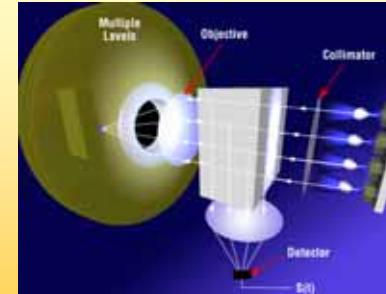


green traffic light



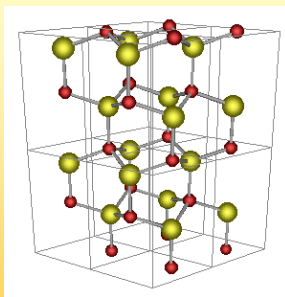
white LED headlight

Application Examples (LD)



blue lasers for optical data storage (HD-DVD)

Nitride Material Properties



wurtzite (hexagonal)
crystal structure

- large bandgap $\sim 1 - 6$ eV
- wide wavelength range
- high electron velocity
- high breakdown field
- high thermal conductivity
- chemically inert
- mechanically strong

Material Parameters

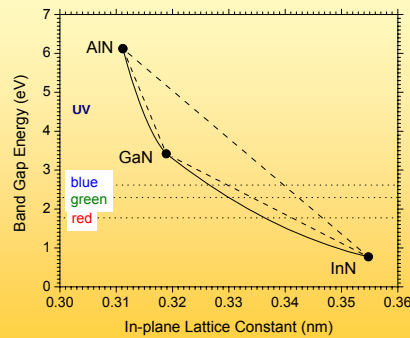
needed: more than 40 material parameters as function of layer composition

mobility (n,p)	$\mu(T,N,F)$	bandgap	$E_g(T)$
SRH lifetime (n,p)	τ	electron affinity	$\chi(T)$
spont. recomb. coeff.	B	electron effective mass	m
Auger coefficient (n,p)	C	hole effective mass par.	$A_1 - A_6$
optical dielectric constant	ϵ_∞	valence split energies	$\Delta_1 - \Delta_3$
dc dielectric constant	ϵ_0	deformation potentials	a, $D_1 - D_4$
refractive index	$n(\lambda)$	elastic constants	C_{13}, C_{33}
absorption coefficient	$\alpha(\lambda)$	lattice constant	a
thermal conductivity	κ	dopant activation energy	E_a
LO phonon energy	E_{LO}	etc.	

most of these parameters are not exactly known for nitride compounds

=> main source of uncertainty in nitride laser simulations

Direct Energy Gap



$$\text{Al}_x\text{Ga}_{1-x}\text{N}$$

$$E_g = 6.12x + 3.42(1-x) - 1.5x(1-x)$$

$$\text{In}_x\text{Ga}_{1-x}\text{N}$$

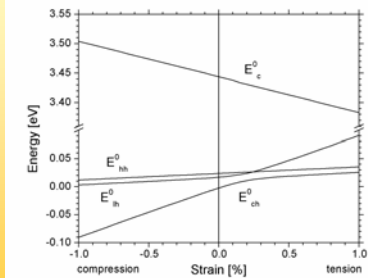
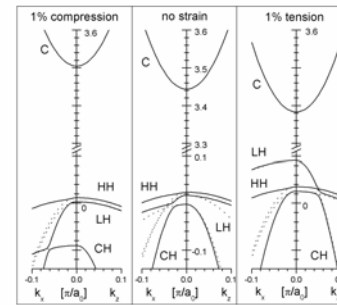
$$E_g = 0.77x + 3.42(1-x) - 1.43x(1-x)$$

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GaN Bandstructure: Strain Effects

6 x 6 kp method for valence bands



HH - heavy hole bands
LH - light hole bands
CH - crystal-field split-hole band

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Band Structure Parameters

Parameter	Symbol	Unit	InN	GaN	AlN
electron eff. mass (c-axis)	m_c^*	m_0	0.11	0.20	0.33
electron eff. mass (transversal)	m_t^*	m_0	0.11	0.18	0.25
hole eff. mass parameter	A_1	-	-9.24	-7.24	-3.95
hole eff. mass parameter	A_2	-	-0.60	-0.51	-0.27
hole eff. mass parameter	A_3	-	8.68	6.73	3.68
hole eff. mass parameter	A_4	-	-4.34	-3.36	-1.84
hole eff. mass parameter	A_5	-	-4.32	-3.35	-1.92
hole eff. mass parameter	A_6	-	-6.08	-4.72	-2.91
direct bandgap	E_g	eV	1.89	3.42	6.28
spin-orbit energy	Δ_{so}	eV	0.001	0.013	0.019
crystal-field energy	Δ_{cr}	eV	0.041	0.042	-0.217
lattice constant	a_0	Å	3.548	3.189	3.112
elastic constant	C_{33}	GPa	200	392	382
elastic constant	C_{13}	GPa	94	100	127
hydrost. deform. potential (E_c)	a_c	eV	-	-4.08	-
shear deform. potential	D_1	eV	-	-0.89	-
shear deform. potential	D_2	eV	-	4.27	-
shear deform. potential	D_3	eV	-	5.18	-
shear deform. potential	D_4	eV	-	-2.59	-

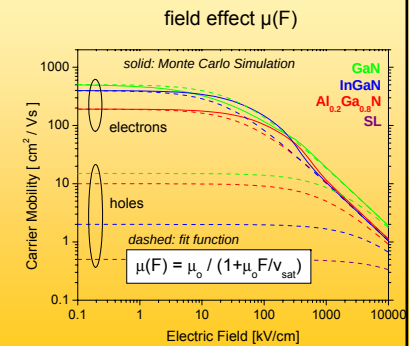
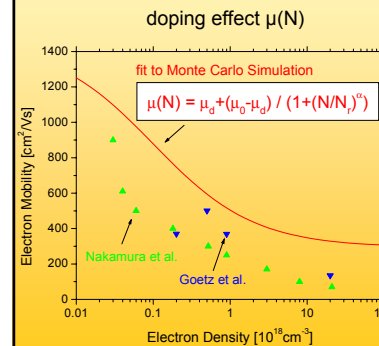
[Vurgaftman & Meyer, JAP 94, 3675, 2003]

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Carrier Mobility $\mu(N, F, T)$

PROBLEM: Mg acceptor $E_A > 0.17$ eV
hole mobility < 15 cm²/Vs
hole conductivity constant



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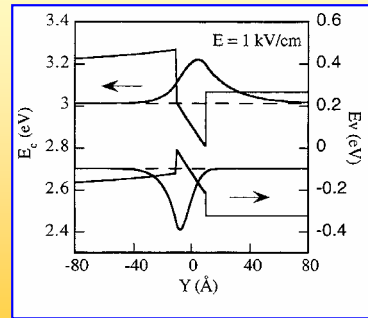
Built-in Polarization

fixed interface charges due to

- spontaneous polarization
- strain induced polarization

quantum well effects

- longer emission wavelength
- less transition strength

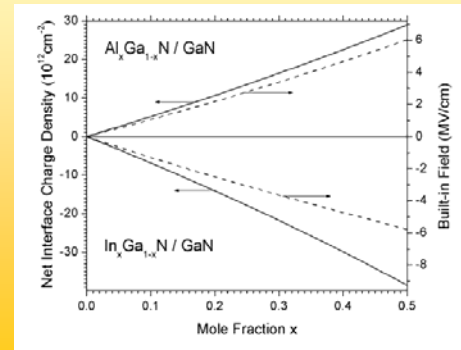


[Fiorentini et al., APL 80, 1204 (2002)]

Polarization Field

Parameter	Symbol	Unit	InN	GaN	AlN
Spontaneous polarization	P_{sp}	Cm^{-2}	-0.042	-0.034	-0.09
piezoelectric constant (z)	e_{33}	Cm^{-2}	0.810	0.670	1.50
piezoelectric constant (x,y)	e_{31}	Cm^{-2}	-0.410	-0.340	-0.53

$$P_{sp} + 2 \frac{a_s - a_0}{a_0} (e_{31} - \frac{C_{13}}{C_{33}} e_{33})$$



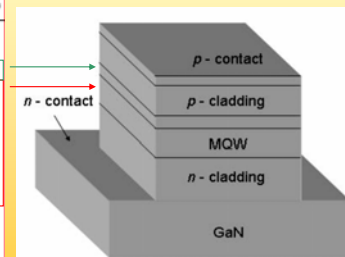
GaN-based Light Emitting Diodes



Ultraviolet LED Design

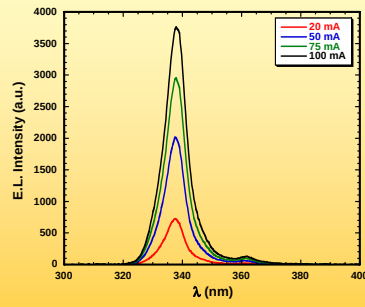
AlGaIn Multi-Quantum Well (MQW) Structure

Parameter	d Unit (nm)	N_{dop} ($1/\text{cm}^3$)	μ (cm^2/Vs)	n_r	κ_L (W/cmK)
p-GaN	5	1×10^{18}	10	2.77	1.3
p-AlGaIn SL cladding	126	4×10^{17}	0.5	2.48	0.2
p-Al _{0.3} Ga _{0.7} N blocker	15	1×10^{17}	5	2.02	0.1
i-Al _{0.16} Ga _{0.84} N well	5	—	300	2.79	0.2
n-Al _{0.16} Ga _{0.84} N barrier	13	2×10^{18}	185	2.48	0.2
i-Al _{0.16} Ga _{0.84} N well	5	—	300	2.79	0.2
n-Al _{0.16} Ga _{0.84} N barrier	13	2×10^{18}	185	2.48	0.2
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n-AlGaIn SL cladding	126	2×10^{18}	10	2.48	0.2
n-GaN contact layer	500	2×10^{18}	200	2.77	1.3

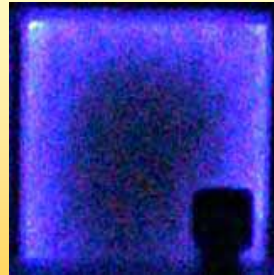


[Thomas Katona, PhD Thesis, UCSB 2003]

UV Emission Measurement



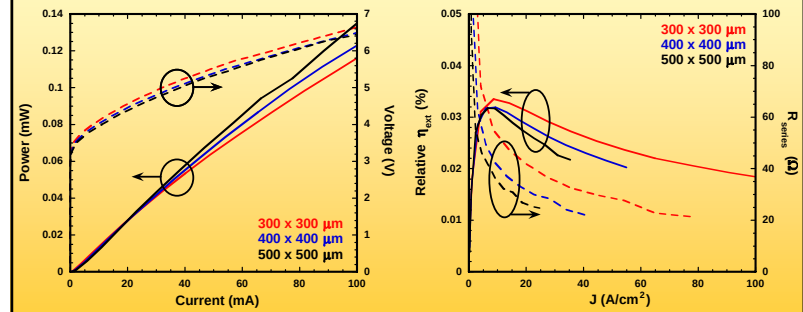
$\lambda_{\text{peak}} = 338 \text{ nm}$ FWHM = 8 nm



Power Measurements

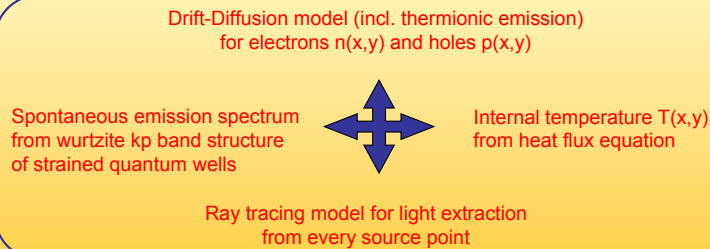
Max Power = 0.135 mW at 100mA DC

Max Quantum Efficiency = 0.033%



LED Simulation

three-dimensional physics-based model



APSYS by Crosslight Software

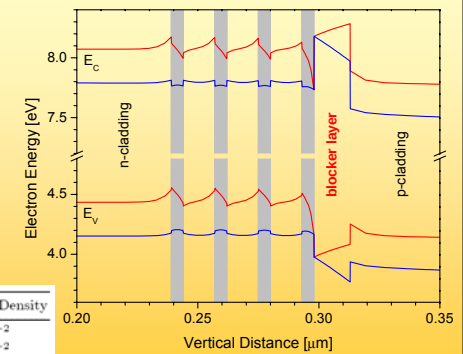
MQW Band Diagram

$\text{Al}_{0.3}\text{Ga}_{0.7}\text{N}$ blocker layer:

bandgap adjusted from 4.1 eV to 4.5 eV

Polarization charges

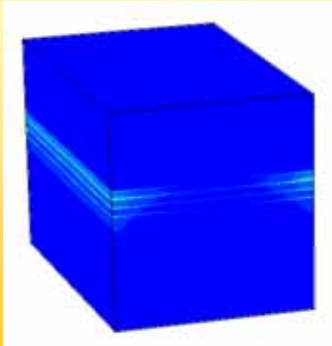
Interface	Built-in Charge Density
GaN/ $\text{Al}_{0.16}\text{Ga}_{0.84}\text{N}$	$+6.88 \times 10^{12} \text{ cm}^{-2}$
$\text{Al}_{0.16}\text{Ga}_{0.84}\text{N}/\text{Al}_{0.10}\text{Ga}_{0.90}\text{N}$	$-2.73 \times 10^{12} \text{ cm}^{-2}$
$\text{Al}_{0.10}\text{Ga}_{0.90}\text{N}/\text{Al}_{0.16}\text{Ga}_{0.84}\text{N}$	$+2.73 \times 10^{12} \text{ cm}^{-2}$
$\text{Al}_{0.10}\text{Ga}_{0.90}\text{N}/\text{Al}_{0.30}\text{Ga}_{0.70}\text{N}$	$+9.89 \times 10^{12} \text{ cm}^{-2}$
$\text{Al}_{0.30}\text{Ga}_{0.70}\text{N}/\text{Al}_{0.16}\text{Ga}_{0.84}\text{N}$	$-7.16 \times 10^{12} \text{ cm}^{-2}$
$\text{Al}_{0.16}\text{Ga}_{0.84}\text{N}/\text{GaN}$	$-6.88 \times 10^{12} \text{ cm}^{-2}$



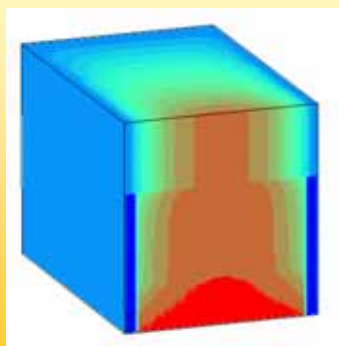
grey — quantum wells
blue — no polarization charges

3D Simulation Results

Internal Emission Rate



Vertical Current Density



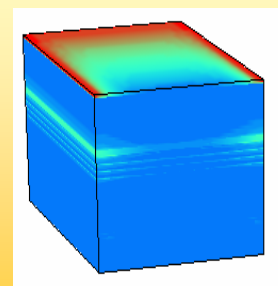
current = 100 mA, bias = 6.5 V

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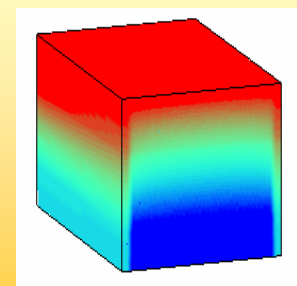
Self-Heating

Heat Source



75% Joule heat
24% recombination heat

Temperature

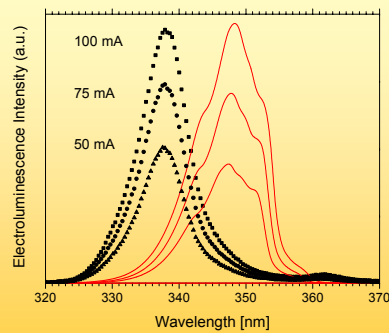


$T_{\max} = 360.6 \text{ K}$
 $T_{\min} = 360.4 \text{ K}$
 $R_{\text{th}} = 100 \text{ K/W}$

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Emission Spectrum



dots: measurement
lines: simulation

10 nm disagreement
• non-ideal QW growth
• band gap too small
• polarization too strong

thermal red-shift
• no peak shift measured
• 1 nm red-shift simulated

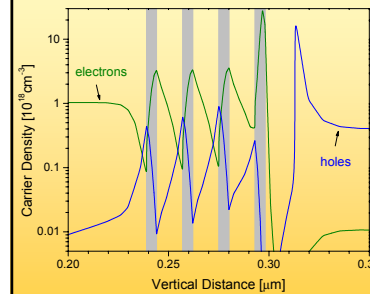
=> self-heating overestimated

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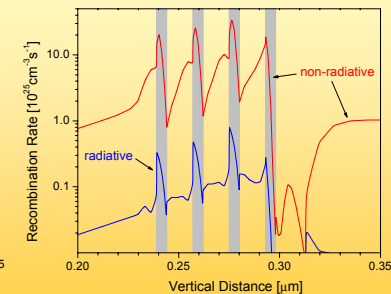
Carrier Recombination

Carrier Density



electron – hole separation in QW

Recombination Rate

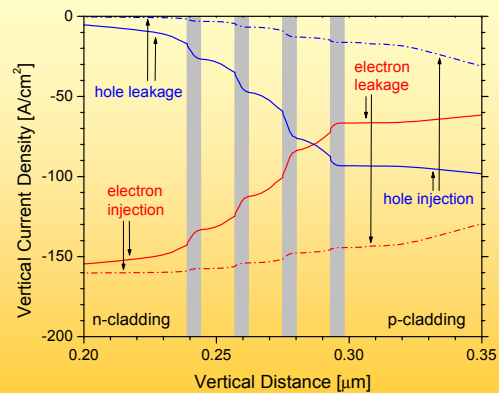


strong non-radiative recombination
non-radiative lifetime = 1 ns

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Carrier Leakage from MQW



solid lines: $E_{\text{block}} = 4.5 \text{ eV}$, dashed lines: $E_{\text{block}} = 4.1 \text{ eV}$

LED Efficiency

Quantum efficiency

$$\eta_{\text{det}} = \eta_{\text{int}} \eta_{\text{opt}} \eta_{\text{cap}}$$

detected eff. $\eta_{\text{det}} = 0.035 \%$

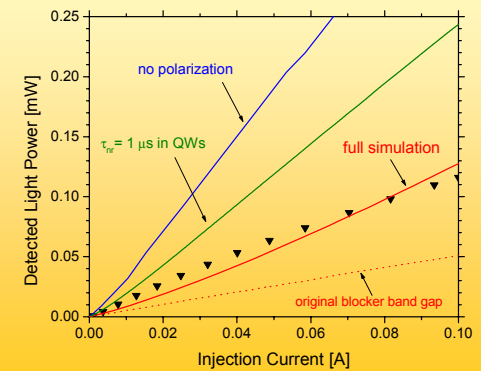
internal eff. $\eta_{\text{int}} = 1.0 \%$

optical eff. $\eta_{\text{opt}} = 4.5 \%$

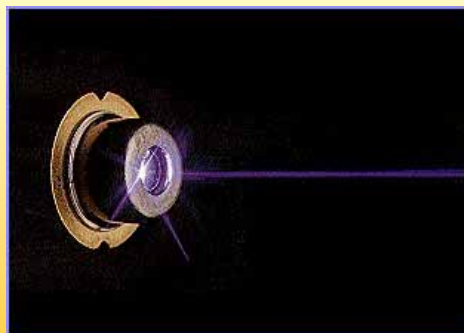
capture eff. $\eta_{\text{ext}} = 82 \%$

triangles: measurement

Light vs. Current

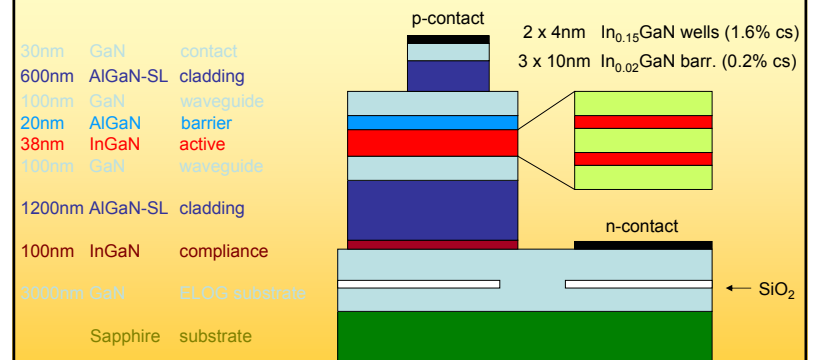


GaN-based Laser Diode



Ridge-Waveguide Laser Diode

[Nakamura et al., Jap. J. Appl. Phys, 37 (1998) L1020]



ridge width = 3 μm, cavity length = 450 μm, facet reflectivity = 0.18 / 0.95

Layer Parameters

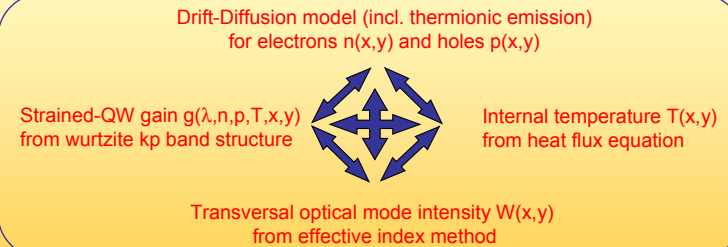
Parameter	l	N_{dop}	μ	n	κ
Unit	nm	$1/\text{cm}^3$	cm^2/Vs	-	W/cmK
p-GaN (contact)	30	2×10^{20}	15	2.54	1.3
p-Al _{0.14} Ga _{0.86} N/GaN SL (cladding)	600	1×10^{20}	0.5	2.48	0.2
p-GaN (waveguide)	100	5×10^{18}	15	2.54	1.3
p-Al _{0.2} Ga _{0.8} N (stopper)	20	1×10^{19}	10	2.23	0.8
n-In _{0.02} Ga _{0.98} N (barrier)	10	7×10^{16}	100	2.61	0.2
n-In _{0.15} Ga _{0.85} N (quantum well)	4	7×10^{16}	100	3.0	0.2
n-In _{0.02} Ga _{0.98} N (barrier)	10	7×10^{16}	100	2.61	0.2
n-In _{0.15} Ga _{0.85} N (quantum well)	4	7×10^{16}	100	3.0	0.2
n-In _{0.02} Ga _{0.98} N (barrier)	10	7×10^{16}	100	2.61	0.2
n-GaN (waveguide)	100	7×10^{17}	550	2.54	1.3
n-Al _{0.14} Ga _{0.86} N/GaN SL (cladding)	1200	3×10^{18}	10	2.48	0.2
n-In _{0.1} Ga _{0.9} N (compliance)	100	3×10^{18}	390	3.0	1.0
n-GaN (substrate)	3000	3×10^{18}	410	2.54	1.3

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Laser Simulation

two-dimensional physics-based model



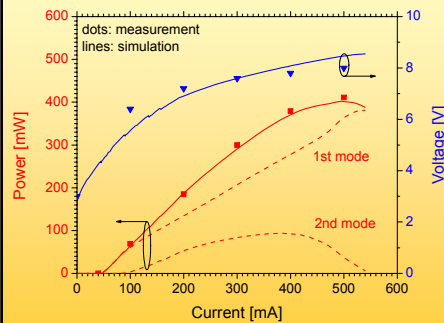
LASTIP by Crosslight Software

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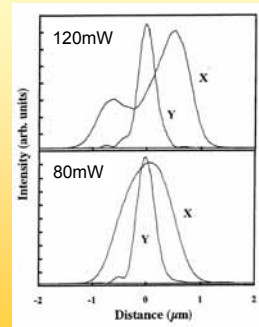
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Comparison to Measurements

CW simulation vs. measurement



measured near-field



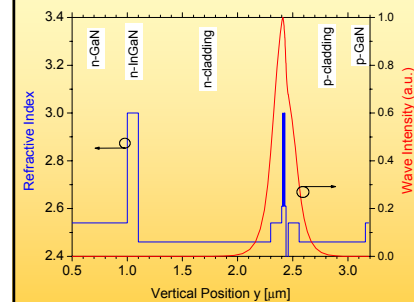
fit parameters $\alpha_i = 12 \text{ cm}^{-1}$ $\tau_{\text{SRH}} = 0.5 \text{ ns}$ (QW) $R_{\text{th}} = 75 \text{ K/W}$

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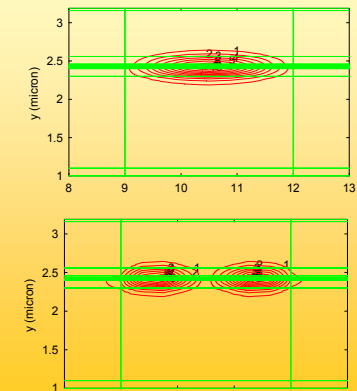
Optical Modes

vertical profile of index and mode



optical confinement factor
= 0.015 per quantum well

near field profile

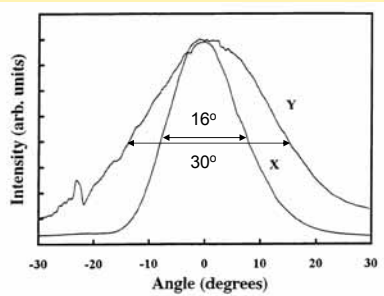


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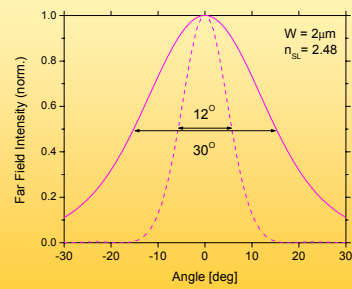
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Far-Field Pattern (2μm ridge width)

measured



calculated

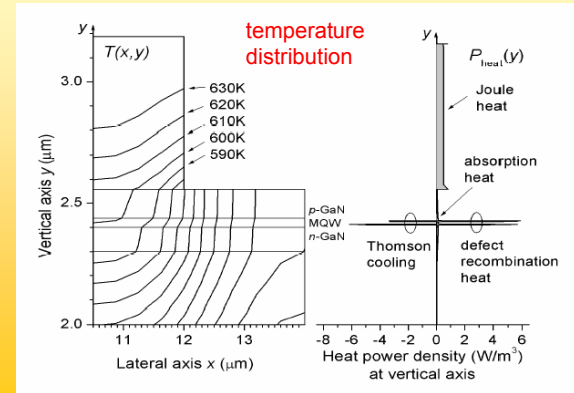


Self-Heating

thermal resistance:

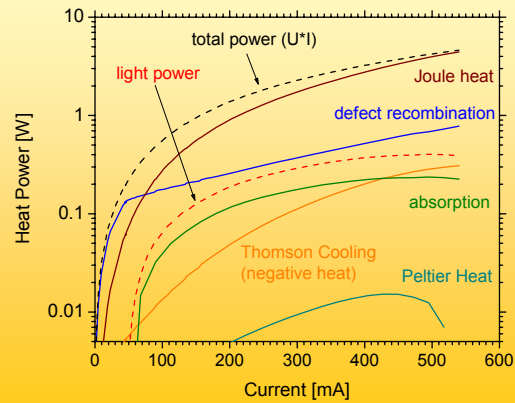
$$R_{th} = \frac{\Delta T_{MQW}}{P_{heat}} = \frac{300K}{4W} = 75 \frac{K}{W}$$

external
 $R_{th} = 30 K/W$

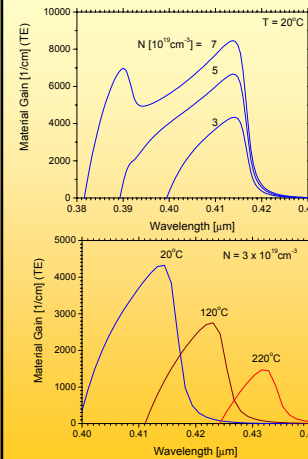


Heat Sources

heat power contributions vs. current



Optical Gain



considered:

- wurtzite band structure incl. strain
- independent quantum wells
- self-consistent carrier density
- band gap renormalization:

$$\Delta E_g = (-4.5 \times 10^{-8} \text{ eVcm}) N^{1/3}$$

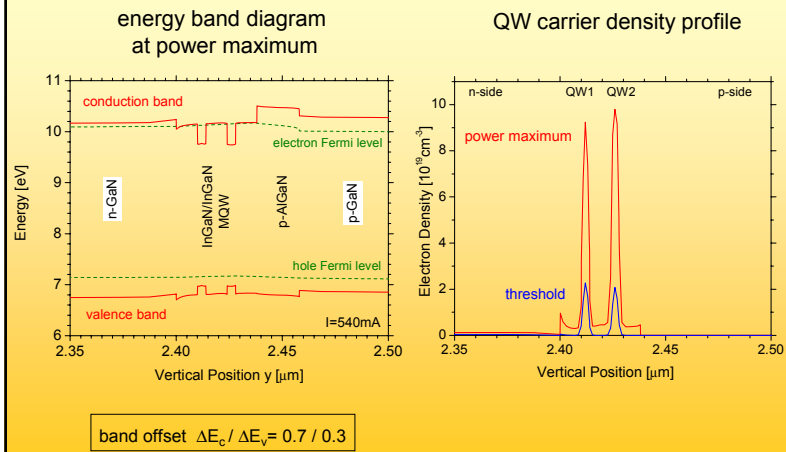
- thermal band gap shrinkage:

$$dE_g/dT = -0.6 \text{ meV/K}$$

$$d\lambda_g/dT = 0.09 \text{ nm/K}$$

- (QW polarization and screening)

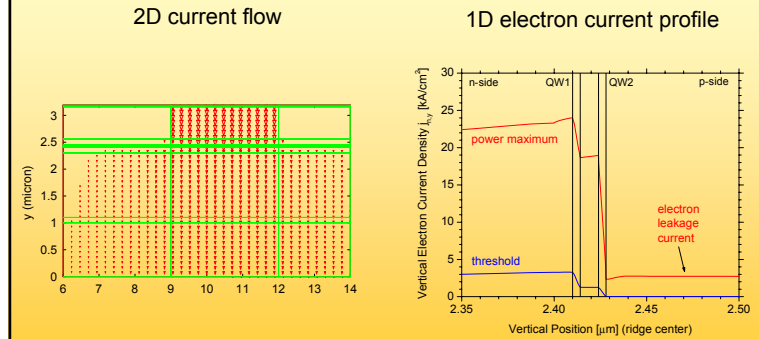
Quantum Well Active Region



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Leakage Current

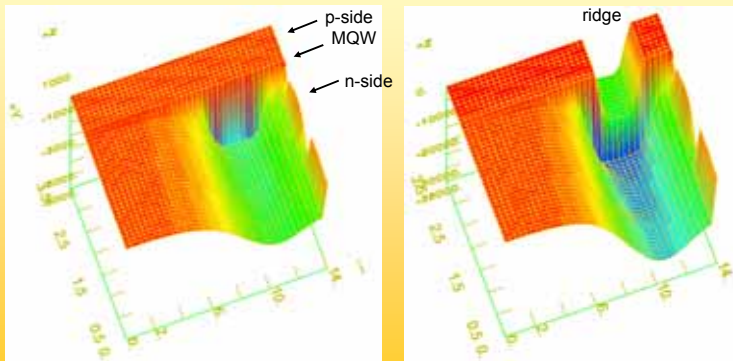


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Electron Leakage (2D)

2D surface plot of vertical electron current density $j_{n,y}(x,y)$ [A/cm²]



laser threshold

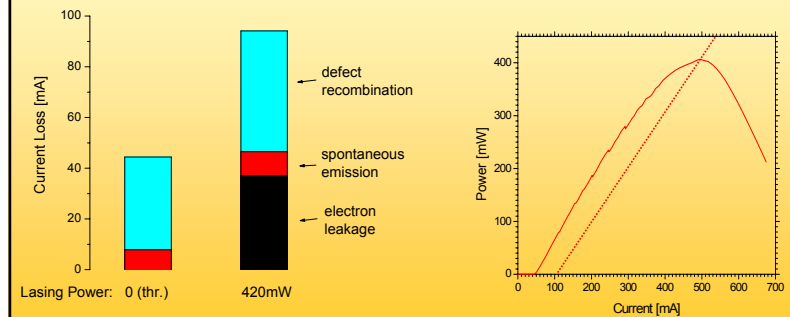
power roll-off

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Carrier Loss Comparison

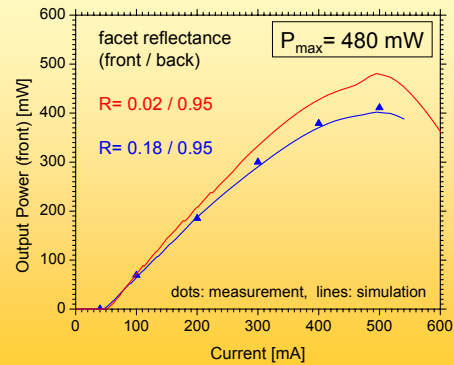
vertical electron leakage into p-region
limits maximum lasing power



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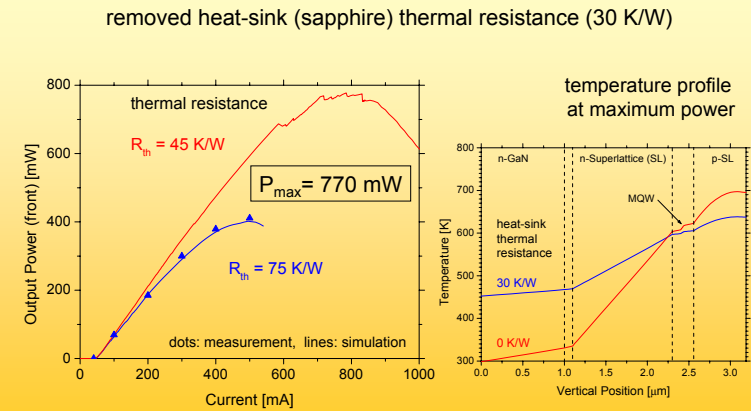
Optimization: Facet Coating



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Optimization: Heat Sinking



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Summary

1. GaN optoelectronics creates new opportunities and challenges for device simulation
2. Realistic results possible by careful investigation of material properties
3. New results on GaN-VCSELs: **TuC2**

further information: piprek@ieee.org

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