GaN-based Devices: Physics and Simulation

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Collaborators

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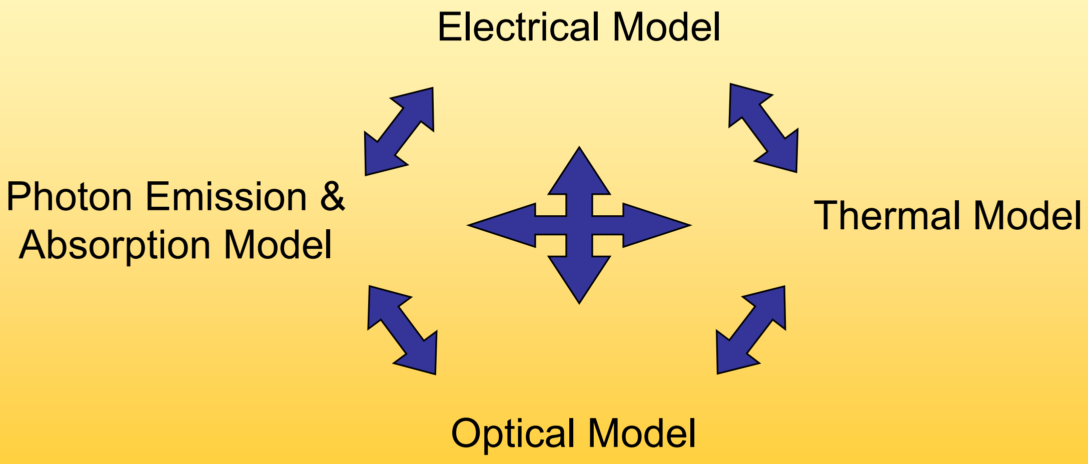
- Dr. Tom Katona, now at S-ET Inc.
- Dr. Simon Li, Crosslight Software Inc.

Outline

1. Nitride Material Properties
2. Light-Emitting Diodes (LED)
3. Laser Diodes (LD)

Optoelectronic Device Physics



Electrical Model

Photon Emission &
Absorption Model

Thermal Model

Optical Model

Nitride Material Parameters

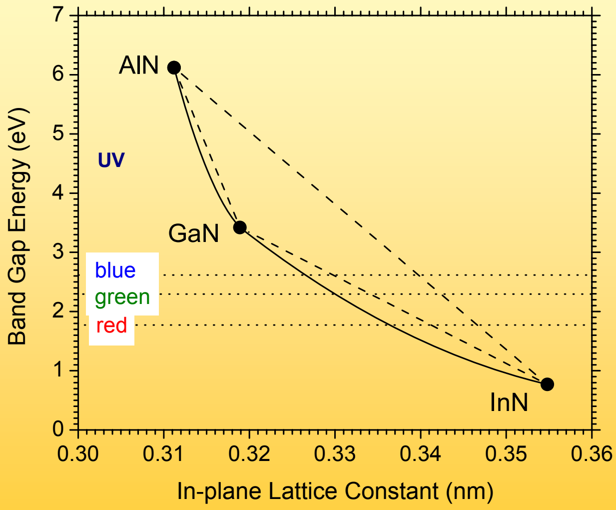
needed: more than 40 material parameters as function of layer composition

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	Δ_1 - Δ_3
dc dielectric constant	ε_o	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



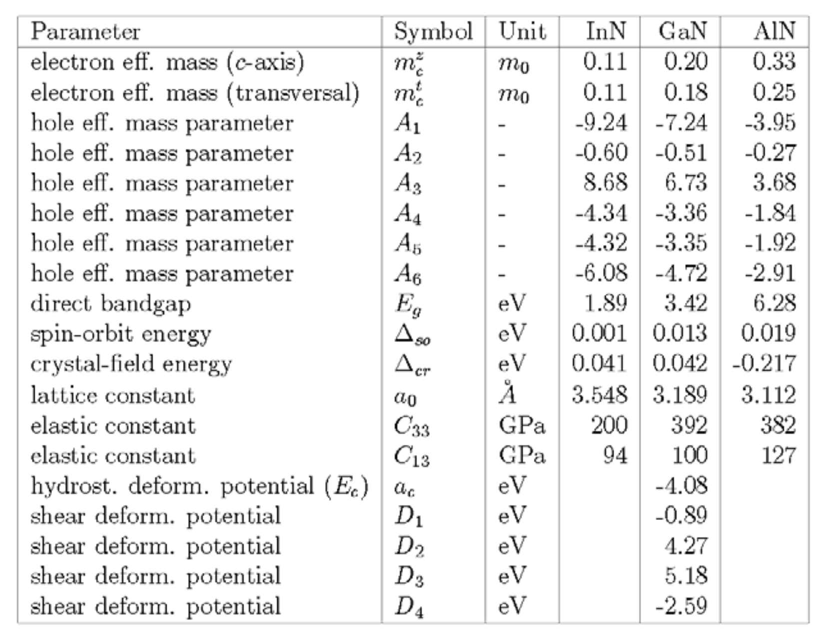
$Al_xGa_{1-x}N$

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

$In_xGa_{1-x}N$

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

Wurtzite Band Structure Parameters



Parameter	Symbol	Unit	InN	GaN	AlN
electron eff. mass (c-axis)	m_c^z	m_0	0.11	0.20	0.33
electron eff. mass (transversal)	m_c^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]

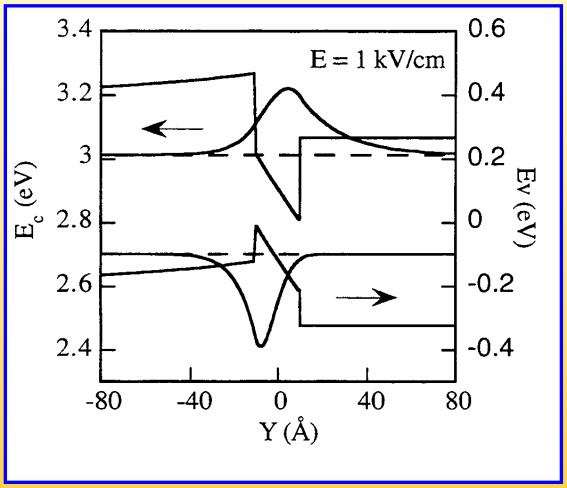
Built-in Polarization

fixed interface charges due to

- spontaneous polarization
- strain induced polarization

quantum well effects

- longer emission wavelength
- less transition strength

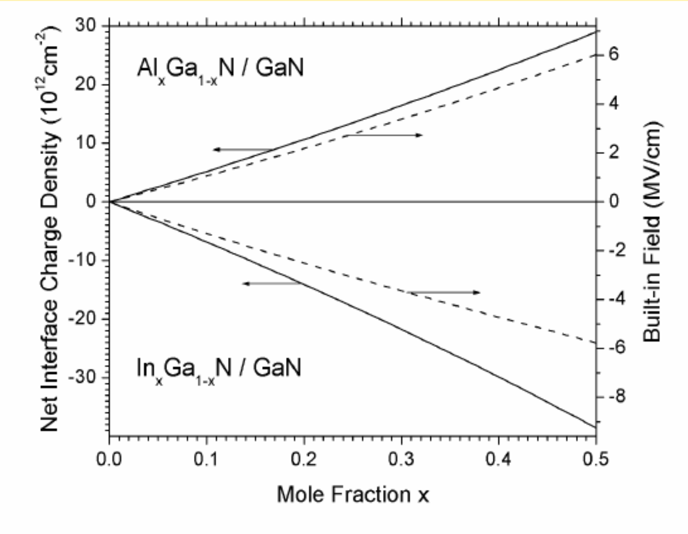


[Fiorentini et al., APL 80, 1204 (2002)]

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

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

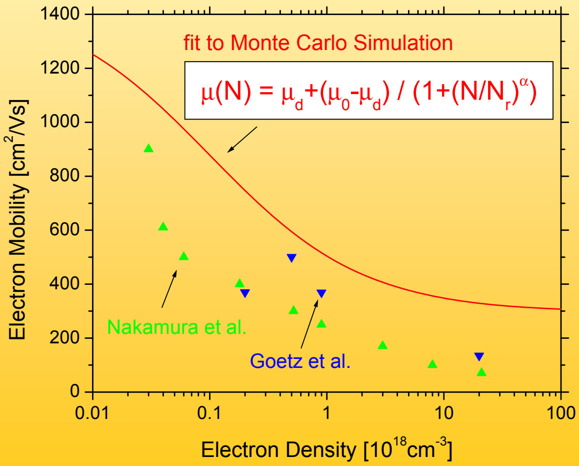


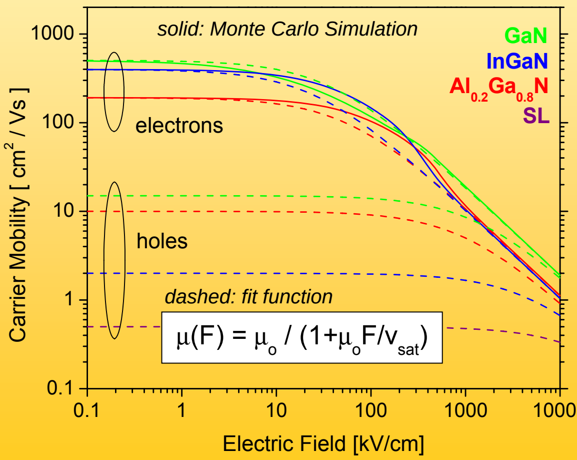
Carrier Mobility μ(N,F,T)

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

doping effect μ(N)

field effect μ(F)





GaN-based Light Emitting Diodes

[Ch. 10 in *Optoelectronic Devises: Advanced Simulation and Analysis*, ed. J. Piprek, Springer 2005]

Ultraviolet LED Design

AlGaN Multi-Quantum Well (MQW) Structure

Parameter Unit	d (nm)	N_{dop} (1/cm^3)	μ (cm^2/Vs)	n_{r} —	κ_{L} (W/cmK)
p-GaN	5	1×10^{18}	10	2.77	1.3
p-AlGaN 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$_{0.10}$Ga$_{0.90}$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$_{0.10}$Ga$_{0.90}$N well	5	—	300	2.79	0.2
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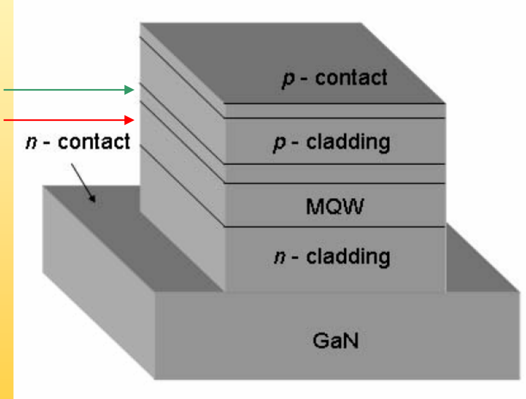
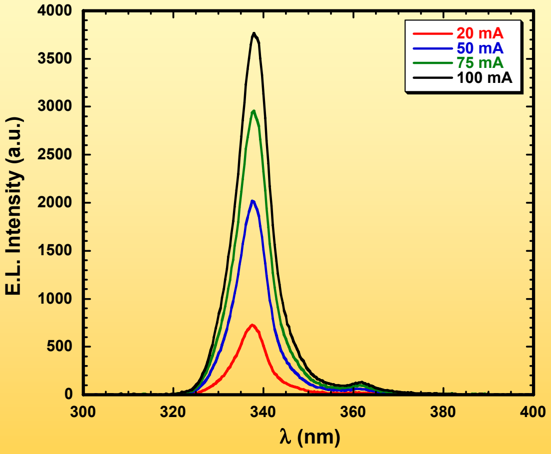
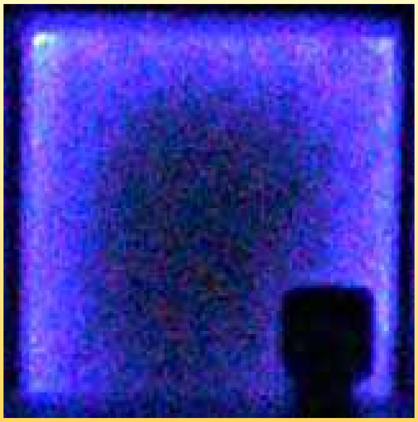
n-AlGaN SL cladding	126	2×10^{18}	10	2.48	0.2
n-GaN contact layer	500	2×10^{18}	200	2.77	1.3



[Thomas Katona, PhD Thesis, UCSB 2003]

UV Emission Measurement



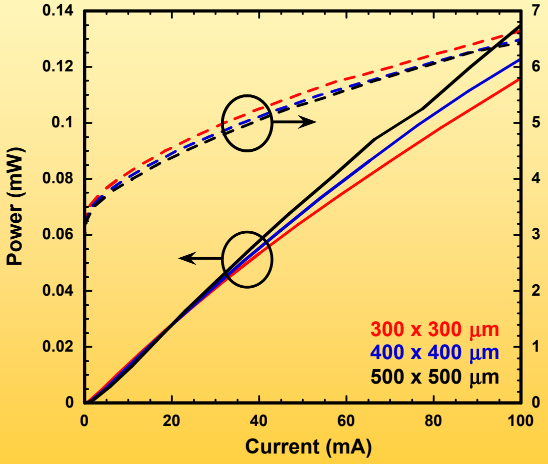


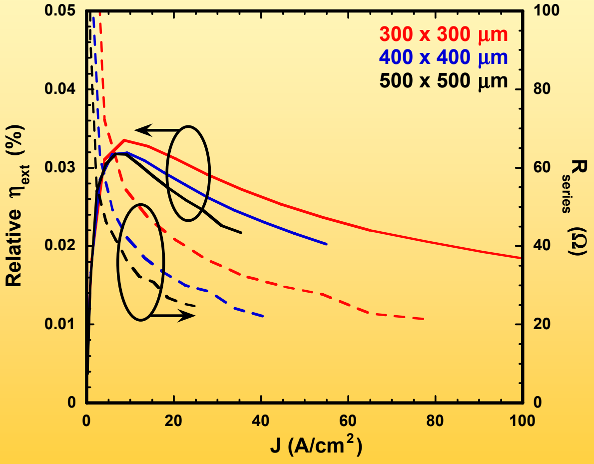
λ_{peak} = 338 nm FWHM = 8nm

Power Measurements

Max Power = 0.135 mW at 100mA DC

Max Quantum Efficiency = 0.033%





LED Simulation

three-dimensional physics-based model

Drift-Diffusion model (incl. thermionic emission)
for electrons n(x,y) and holes p(x,y)

Spontaneous emission spectrum
from wurtzite kp band structure
of strained quantum wells

Internal temperature T(x,y)
from heat flux equation

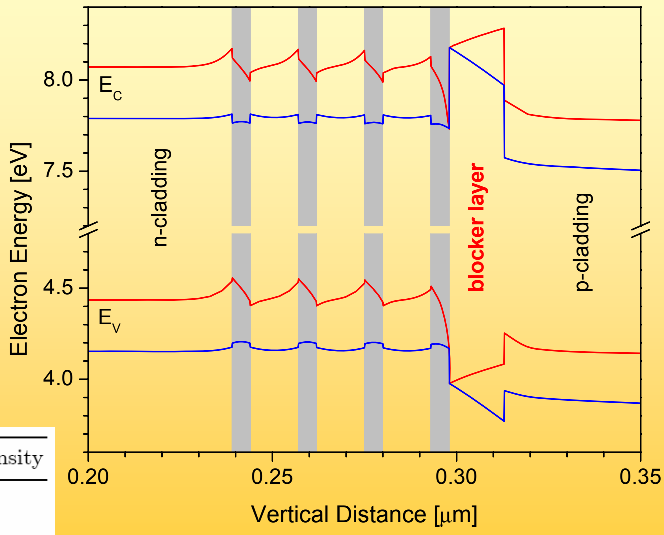
Ray tracing model for light extraction
from every source point

APSYS by Crosslight Software

MQW Band Diagram

$Al_{0.3}Ga_{0.7}N$ blocker layer:

bandgap adjusted
from 4.1 eV to 4.5 eV



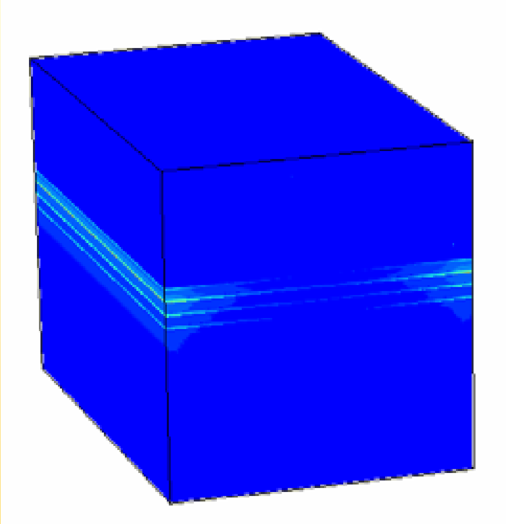
grey – quantum wells
blue – no polarization charges

Polarization charges

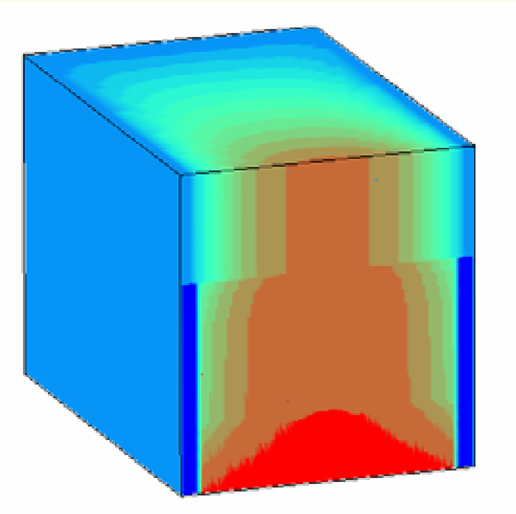
Interface	Built-in Charge Density
$GaN/Al_{0.16}Ga_{0.84}N$	$+6.88 \times 10^{12} cm^{-2}$
$Al_{0.16}Ga_{0.84}N/Al_{0.10}Ga_{0.90}N$	$-2.73 \times 10^{12} cm^{-2}$
$Al_{0.10}Ga_{0.90}N/Al_{0.16}Ga_{0.84}N$	$+2.73 \times 10^{12} cm^{-2}$
$Al_{0.10}Ga_{0.90}N/Al_{0.30}Ga_{0.70}N$	$+9.89 \times 10^{12}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

3D Simulation Results

Internal Emission Rate



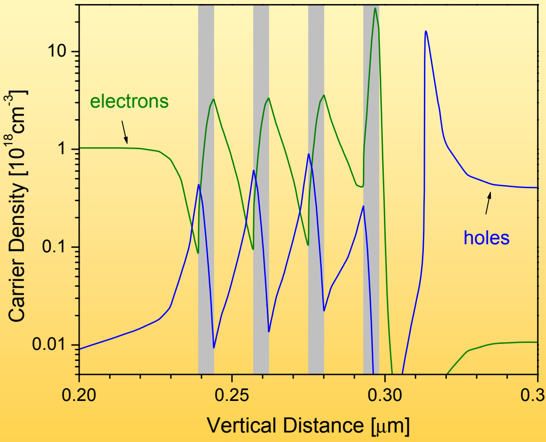
Vertical Current Density



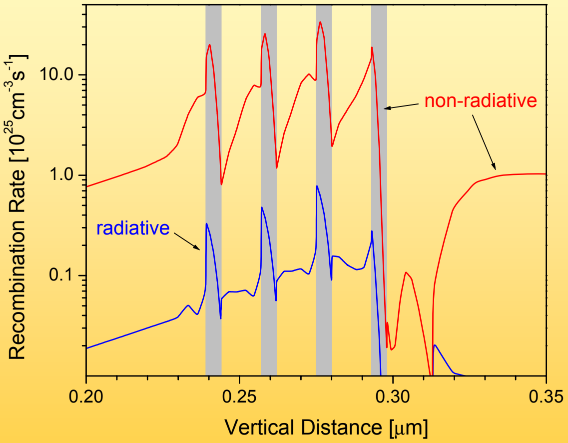
current = 100 mA,   bias= 6.5 V

Carrier Recombination

Carrier Density



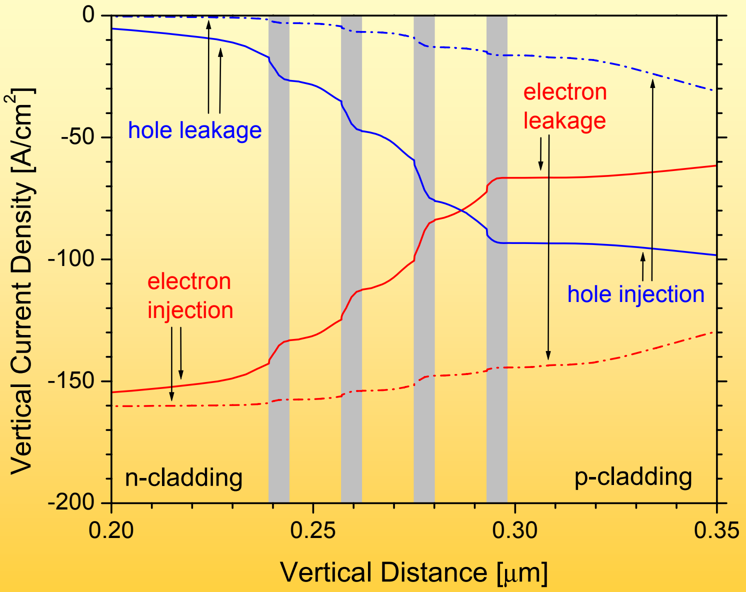
Recombination Rate



electron – hole separation in QW

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

Carrier Leakage from MQW



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

LED Efficiency

Quantum efficiency

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

detected eff. η_{det} = 0.035 %

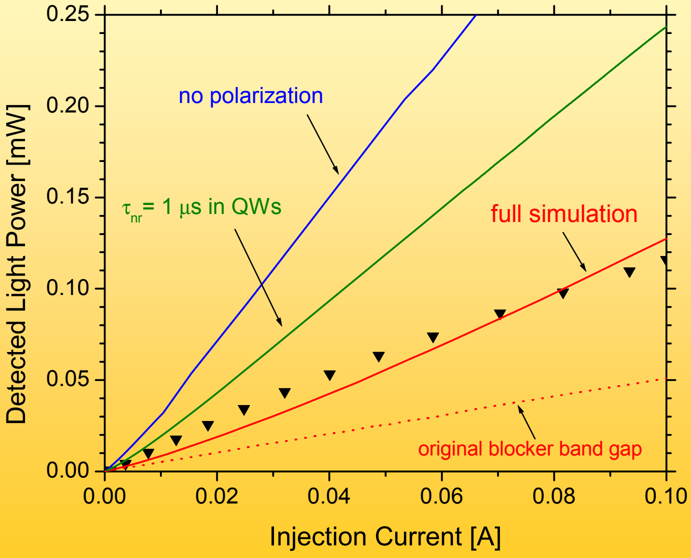
internal eff. η_{int} = 1.0 %

optical eff. η_{opt} = 4.5 %

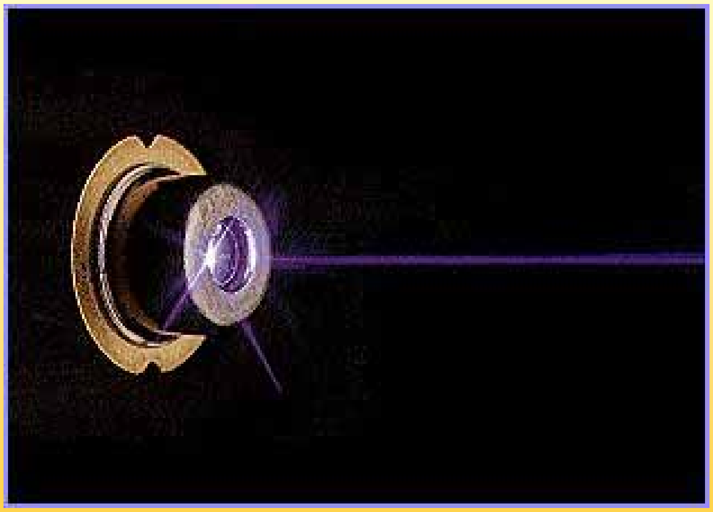
capture eff. η_{ext} = 82 %

triangles: measurement

Light vs. Current



GaN-based Laser Diode

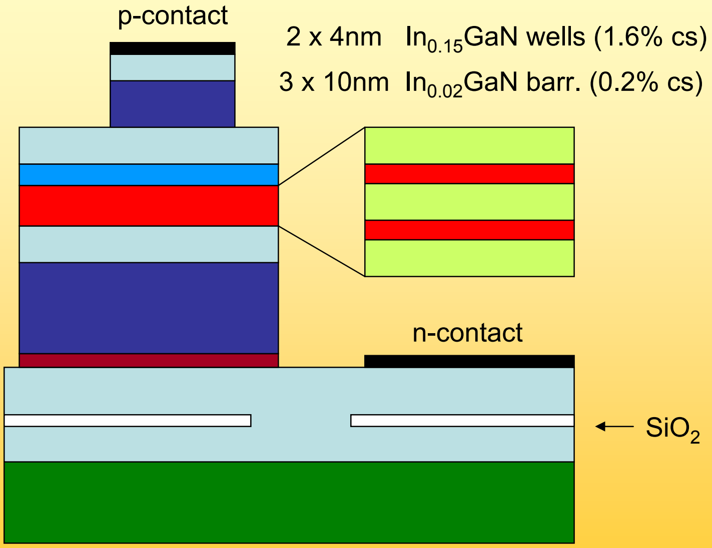


[Ch. 9 in *Semiconductor Optoelectronic Devises: Introduction to Physics and Simulation*
by J. Piprek, Academic Press, 2003]

Rigde-Waveguide Laser Diode

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

30nm	GaN	contact
600nm	AlGaN-SL	cladding
100nm	GaN	waveguide
20nm	AlGaN	barrier
38nm	InGaN	active
100nm	GaN	waveguide
1200nm	AlGaN-SL	cladding
100nm	InGaN	compliance
3000nm	GaN	ELOG substrate
	Sapphire	substrate



2 x 4nm $In_{0.15}GaN$ wells (1.6% cs)
3 x 10nm $In_{0.02}GaN$ barr. (0.2% cs)

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

Laser Simulation

two-dimensional physics-based model

Drift-Diffusion model (incl. thermionic emission)
for electrons n(x,y) and holes p(x,y)

Strained-QW gain g(λ,n,p,T,x,y)
from wurtzite kp band structure

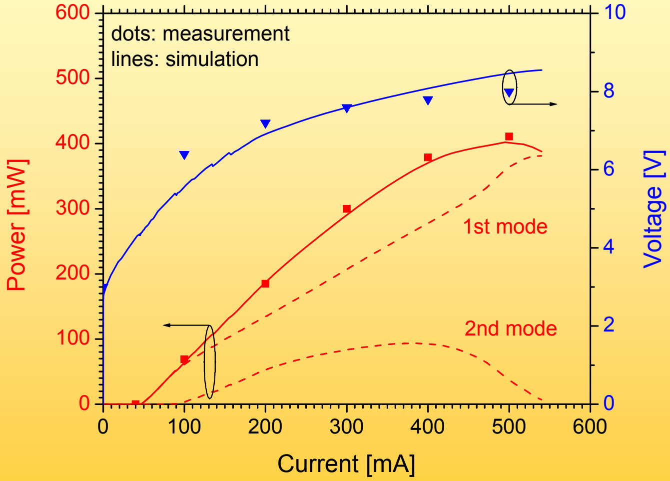
Internal temperature T(x,y)
from heat flux equation

Transversal optical mode intensity W(x,y)
from effective index method

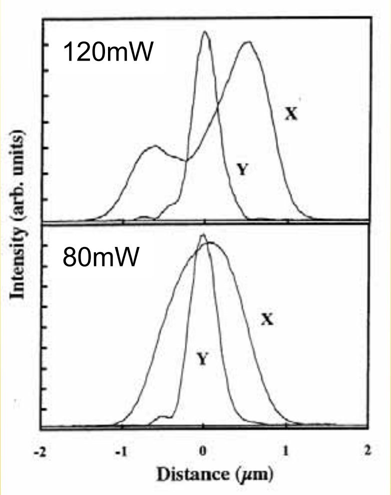
LASTIP by Crosslight Software

Comparison to Measurements

CW simulation vs. measurement



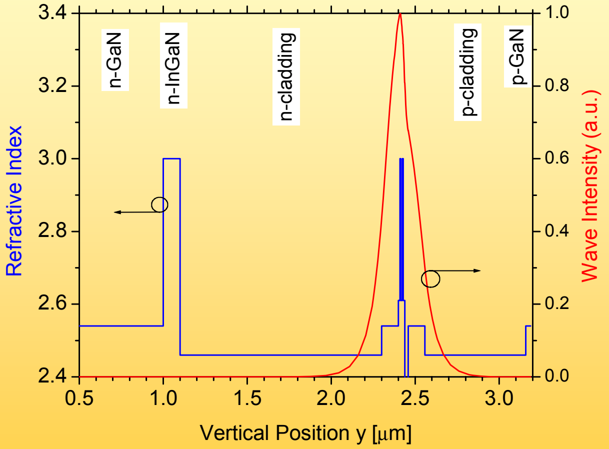
measured near-field



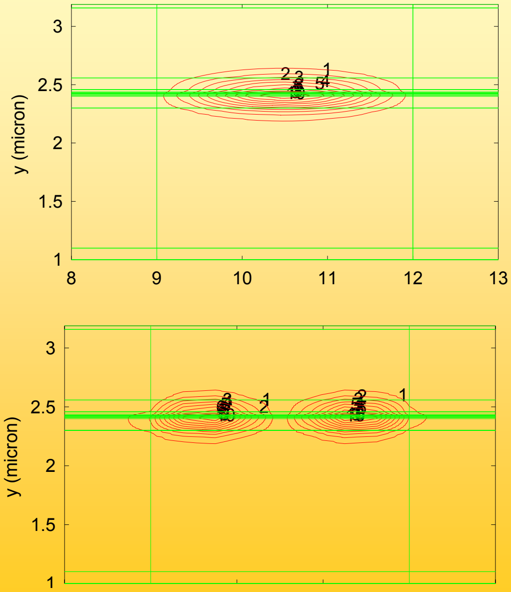
fit parameters α_i = 12 cm^{-1} τ_{SRH} = 0.5 ns (QW) R_{th} = 75 K/W

Optical Modes

vertical profile of index and mode



near field profile



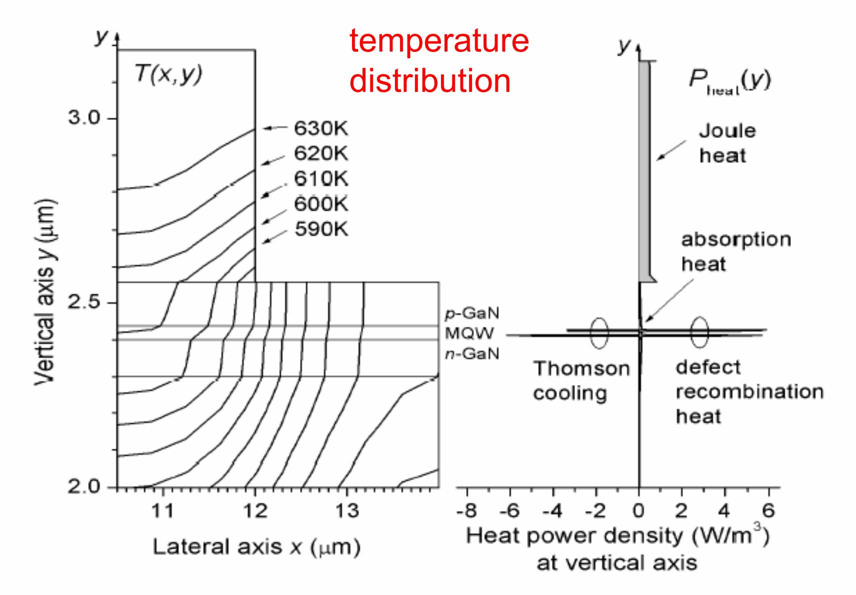
optical confinement factor
= 0.015 per quantum well

Self-Heating

thermal resistance:

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

external
R_{th}= 30 K/W

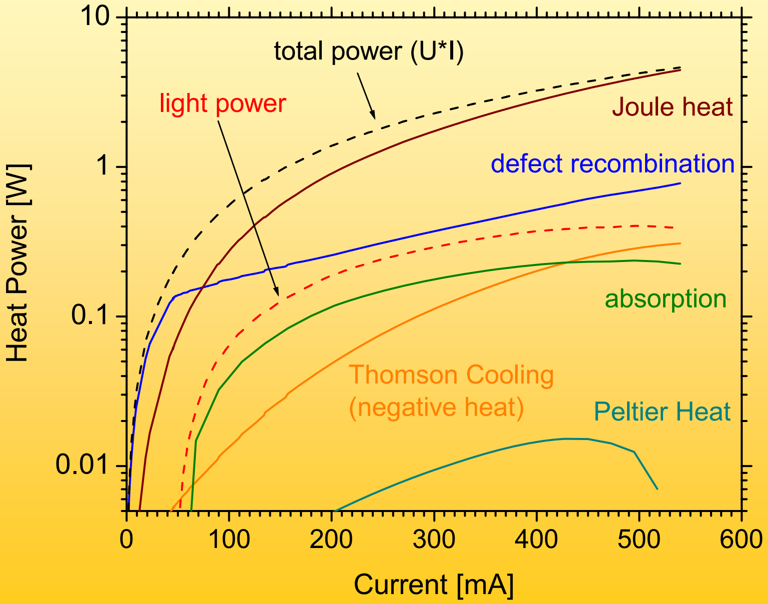


temperature distribution

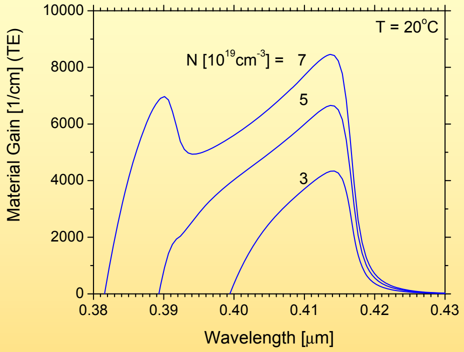
heat power profile at laser axis

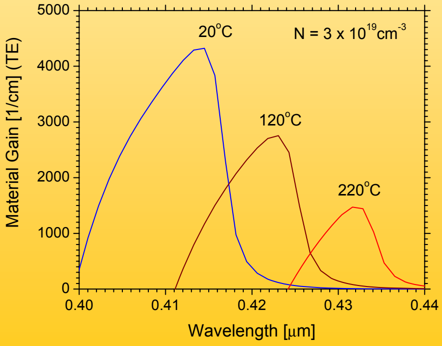
Heat Sources

heat power contributions vs. current



Optical Gain





considered:

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

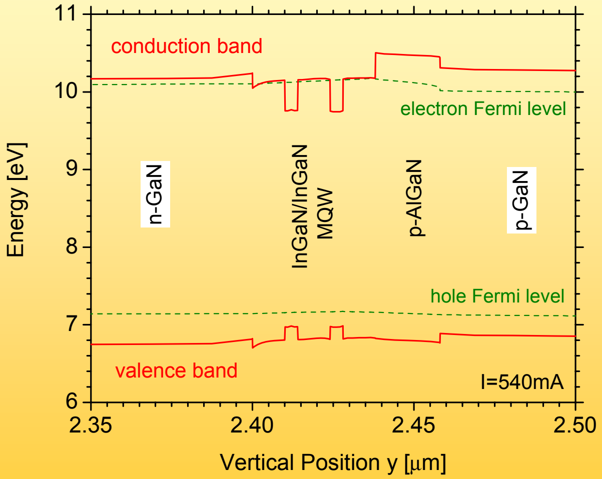
$$\Delta E_g = (-\,4.5 \times 10^{-8}\ \text{eVcm})\ N^{1/3}$$

- thermal band gap shrinkage:

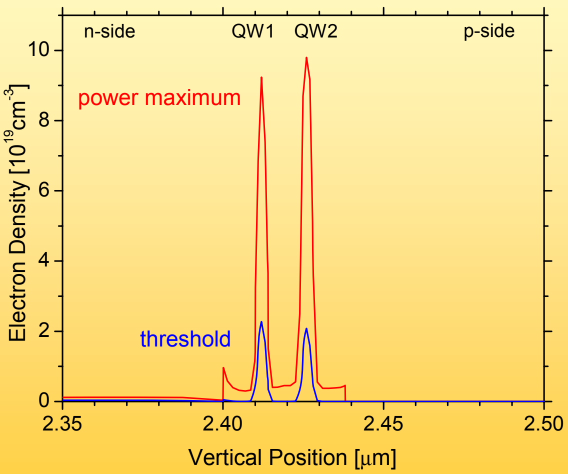
$dE_g/dT = -\,0.6$ meV/K
$d\lambda_e/dT = 0.09$ nm/K

Quantum Well Active Region

energy band diagram
at power maximum



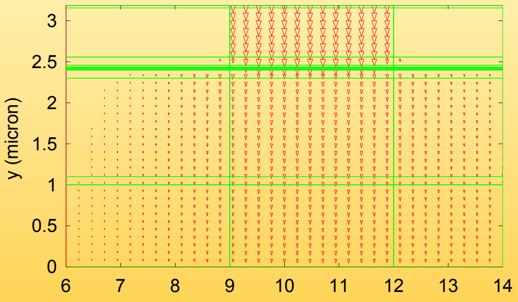
QW carrier density profile



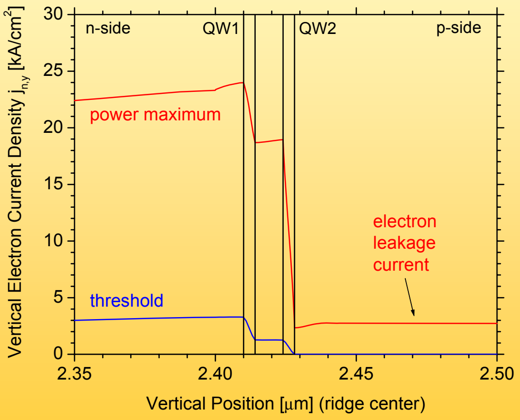
band offset $\Delta E_c / \Delta E_v = 0.7 / 0.3$

Leakage Current

2D current flow

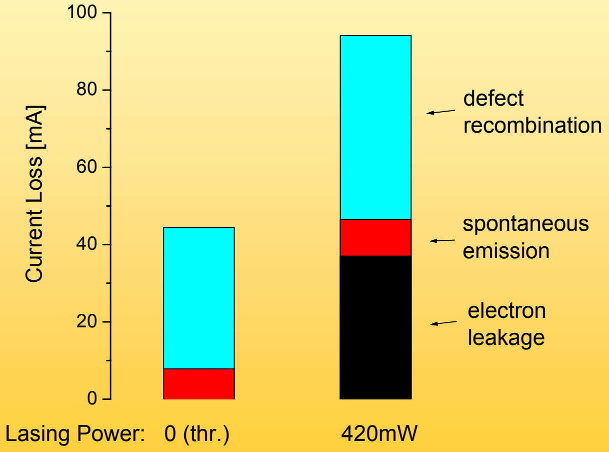


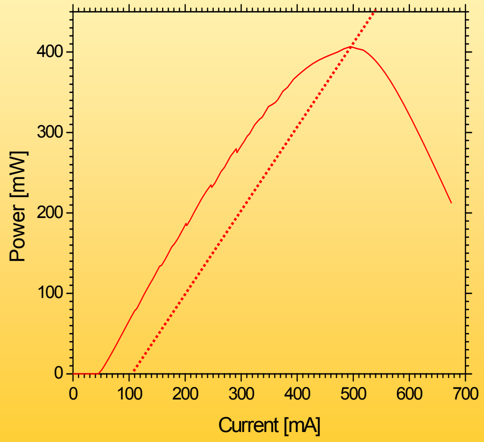
1D electron current profile



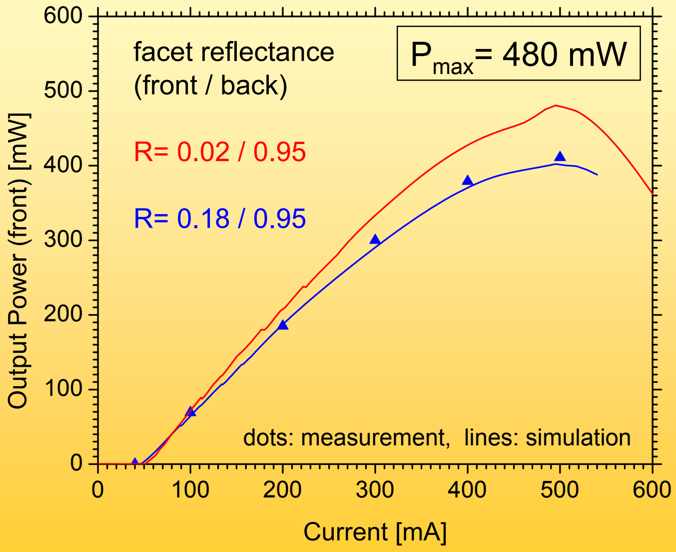
Carrier Loss Comparison

vertical electron leakage into p-region
limits maximum lasing power



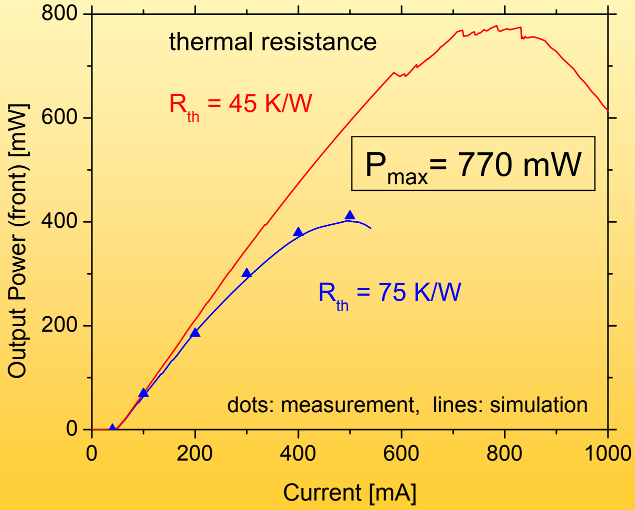


Optimization: Facet Coating

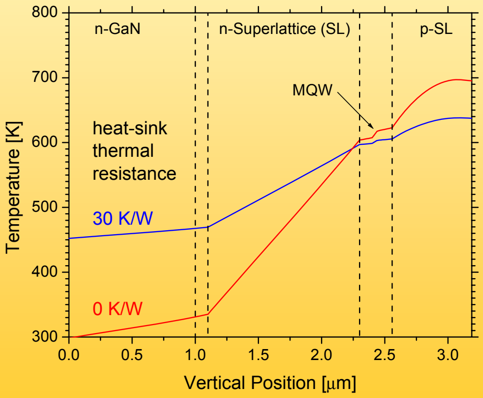


Optimization: Heat Sinking

removed heat-sink (sapphire) thermal resistance (30 K/W)



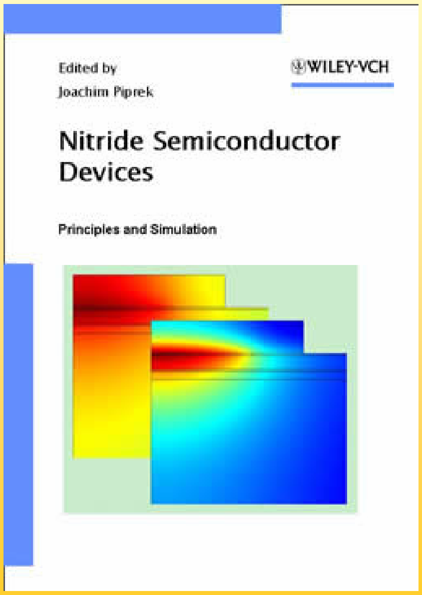
temperature profile
at maximum power



Summary

1. **GaN (opto)electronics creates new opportunities and challenges for device simulation**
2. **Realistic results possible with careful consideration of material properties**

Further Reading



Edited by
Joachim Piprek

WILEY-VCH

Nitride Semiconductor Devices

Principles and Simulation

Part 1: Material Properties

1. Introduction (Piprek)
2. Electron bandstructure parameters (Vurgaftman/Meyer)
3. Spontaneous and piezoelectric polarization: basic theory vs. practical recipes (Bernardini)
4. Transport parameters for electrons and holes (Bellotti/ Bertazzi)
5. Optical constants of bulk nitrides (Goldhahn / Buchheim/Schley/Winzer/Wenzel)
6. Intersubband absorption in AlGaN quantum wells (Gunna/Bertazzi/Paiella/Bellotti)
7. Interband transitions in InGaN quantum wells (Hader/ Moloney/ Thränhardt/ Koch)
8. Electronic and optical properties of quantum wells with (1010) crystal orientation (Park/Chuang)
9. Carrier scattering in quantum-dot systems (Jahnke)

Part 2: Devices

10. AlGaN/GaN high electron mobility transistors (Palacios / Mishra)
11. Intersubband optical switches for optical communications (Suzuki)
12. Intersubband electroabsorption modulator (Holmström)
13. Ultraviolet light emitting diodes (Kuo/ Yen/ Chen)
14. Visible light emitting diodes (Karpov)
15. Light-emitting diodes for the generation of white light (Linder/Eisert/Jermann/Berben)
16. Fundamental characteristics of edge-emitting lasers (Hatakoshi)
17. Resonant internal transverse-mode coupling in InGaN/GaN/AlGaN lasers (Smolyakov/Osiński)
18. Optical properties of edge-emitting lasers: measurement and simulation Schwarz Witzigmann)
19. Electronic properties of InGaN vertical-cavity lasers (Piprek/ Li/ Farrell/DenBaars/Nakamura)
20. Optical design of vertical-cavity lasers (Nakwaski/Czyszanowski/Sarzala)
21. GaN nanowire lasers (Maslov/Ning)

to be published in January 2007