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**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Units</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>mobility (n,p)</td>
<td>$\mu(T,N,F)$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SRH lifetime (n,p)</td>
<td>$\tau$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>spont. recomb. coeff.</td>
<td>$B$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Auger coefficient (n,p)</td>
<td>$C$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>optical dielectric constant</td>
<td>$\varepsilon_\infty$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>dc dielectric constant</td>
<td>$\varepsilon_0$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>refractive index</td>
<td>$n(\lambda)$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>absorption coefficient</td>
<td>$\alpha(\lambda)$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>thermal conductivity</td>
<td>$\kappa$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LO phonon energy</td>
<td>$E_{\text{LO}}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>bandgap</td>
<td>$E_g(T)$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>electron affinity</td>
<td>$\chi(T)$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>electron effective mass</td>
<td>$m$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>hole effective mass par.</td>
<td>$A_1- A_6$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>valence split energies</td>
<td>$\Delta_1 - \Delta_3$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>deformation potentials</td>
<td>$a, D_1- D_4$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>elastic constants</td>
<td>$C_{13}, C_{33}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>lattice constant</td>
<td>$a$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>dopant activation energy</td>
<td>$E_a$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>deformation potentials</td>
<td>$D$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*most of these parameters are not exactly known for nitride compounds*

$\Rightarrow$ main source of uncertainty in nitride laser simulations

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### Direct Energy Gap

#### Al$_x$Ga$_{1-x}$N

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

#### In$_x$Ga$_{1-x}$N

$$E_g = 0.77x + 3.42(1-x) - 1.43x(1-x)$$
Wurtzite Band Structure Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Unit</th>
<th>InN</th>
<th>GaN</th>
<th>AlN</th>
</tr>
</thead>
<tbody>
<tr>
<td>electron eff. mass (c-axis)</td>
<td>$m_e^c$</td>
<td>$m_0$</td>
<td>0.11</td>
<td>0.20</td>
<td>0.38</td>
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<tr>
<td>electron eff. mass (transversal)</td>
<td>$m_e$</td>
<td>$m_0$</td>
<td>0.11</td>
<td>0.18</td>
<td>0.25</td>
</tr>
<tr>
<td>hole eff. mass parameter</td>
<td>$A_1$</td>
<td>-</td>
<td>-9.24</td>
<td>-7.24</td>
<td>-3.95</td>
</tr>
<tr>
<td>hole eff. mass parameter</td>
<td>$A_2$</td>
<td>-</td>
<td>-0.50</td>
<td>-0.51</td>
<td>-0.27</td>
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<tr>
<td>hole eff. mass parameter</td>
<td>$A_3$</td>
<td>-</td>
<td>8.88</td>
<td>6.73</td>
<td>3.68</td>
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<tr>
<td>hole eff. mass parameter</td>
<td>$A_4$</td>
<td>-</td>
<td>-3.34</td>
<td>-3.36</td>
<td>-1.84</td>
</tr>
<tr>
<td>hole eff. mass parameter</td>
<td>$A_6$</td>
<td>-</td>
<td>-3.32</td>
<td>-3.35</td>
<td>-1.92</td>
</tr>
<tr>
<td>hole eff. mass parameter</td>
<td>$A_9$</td>
<td>-</td>
<td>-6.08</td>
<td>-4.72</td>
<td>-2.91</td>
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<tr>
<td>direct bandgap</td>
<td>$E_g$</td>
<td>eV</td>
<td>1.89</td>
<td>3.42</td>
<td>6.28</td>
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<tr>
<td>spin-orbit energy</td>
<td>$\Delta_e$</td>
<td>eV</td>
<td>0.001</td>
<td>0.013</td>
<td>0.019</td>
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<tr>
<td>crystal-field energy</td>
<td>$\Delta_d$</td>
<td>eV</td>
<td>0.041</td>
<td>0.042</td>
<td>-0.217</td>
</tr>
<tr>
<td>lattice constant</td>
<td>$a_0$</td>
<td>Å</td>
<td>3.548</td>
<td>3.189</td>
<td>3.112</td>
</tr>
<tr>
<td>elastic constant</td>
<td>$C_{33}$</td>
<td>GPa</td>
<td>200</td>
<td>392</td>
<td>382</td>
</tr>
<tr>
<td>elastic constant</td>
<td>$C_{13}$</td>
<td>GPa</td>
<td>94</td>
<td>100</td>
<td>127</td>
</tr>
<tr>
<td>hydrost. deform. potential ($E_x$)</td>
<td>$a_c$</td>
<td>eV</td>
<td>-4.08</td>
<td></td>
<td></td>
</tr>
<tr>
<td>shear deform. potential</td>
<td>$D_4$</td>
<td>eV</td>
<td>-0.89</td>
<td></td>
<td></td>
</tr>
<tr>
<td>shear deform. potential</td>
<td>$D_6$</td>
<td>eV</td>
<td>4.27</td>
<td></td>
<td></td>
</tr>
<tr>
<td>shear deform. potential</td>
<td>$D_8$</td>
<td>eV</td>
<td>5.18</td>
<td></td>
<td></td>
</tr>
<tr>
<td>shear deform. potential</td>
<td>$D_4$</td>
<td>eV</td>
<td>-2.59</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

[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

[Florentini et al., APL 80, 1204 (2002)]
### Polarization Field

The polarization field can be expressed as:

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

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

**PROBLEM:** Mg acceptor \( E_A > 0.17 \) eV  
hole mobility < 15 cm\(^2/\)Vs  
hole conductivity constant

**doping effect \( \mu(N) \)**

\[ \mu(N) = \mu_d + (\mu_0 - \mu_d) \frac{1}{1 + (N/N_r)\alpha} \]

**field effect \( \mu(F) \)**

\[ \mu(F) = \frac{\mu_0}{1 + \mu_0 F/\nu_{sat}} \]
GaN-based Light Emitting Diodes

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

Ultraviolet LED Design

**AlGaN Multi-Quantum Well (MQW) Structure**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$d$ (nm)</th>
<th>$N_{dop}$ ($1/cm^2$)</th>
<th>$\mu$ ($cm^2/Vs$)</th>
<th>$\tau$</th>
<th>$\kappa_L$ (W/cmK)</th>
</tr>
</thead>
<tbody>
<tr>
<td>p-GaN</td>
<td>5</td>
<td>$1 \times 10^{18}$</td>
<td>10</td>
<td>2.77</td>
<td>1.3</td>
</tr>
<tr>
<td>p-AlGaN SL cladding</td>
<td>126</td>
<td>$4 \times 10^{17}$</td>
<td>0.5</td>
<td>2.48</td>
<td>0.2</td>
</tr>
<tr>
<td>p-Al$<em>{0.5}$Ga$</em>{0.7}$N blocker</td>
<td>15</td>
<td>$1 \times 10^{17}$</td>
<td>5</td>
<td>2.02</td>
<td>0.1</td>
</tr>
<tr>
<td>i-Al$<em>{0.10}$GaN$</em>{0.90}$N well</td>
<td>5</td>
<td>300</td>
<td>2.79</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>n-Al$<em>{0.16}$Ga$</em>{0.84}$N barrier</td>
<td>13</td>
<td>$2 \times 10^{18}$</td>
<td>185</td>
<td>2.48</td>
<td>0.2</td>
</tr>
<tr>
<td>i-Al$<em>{0.10}$GaN$</em>{0.90}$N well</td>
<td>5</td>
<td>300</td>
<td>2.79</td>
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<td>300</td>
<td>2.79</td>
<td>0.2</td>
<td></td>
</tr>
</tbody>
</table>

UV Emission Measurement

$\lambda_{\text{peak}} = 338$ 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

- \( \text{Al}_{0.3}\text{Ga}_{0.7}\text{N} \) blocker layer:
  bandgap adjusted from 4.1 eV to 4.5 eV

<table>
<thead>
<tr>
<th>Interface</th>
<th>Built-in Charge Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{GaN/Al}<em>{0.16}\text{Ga}</em>{0.84}\text{N} )</td>
<td>( +6.88 \times 10^{12} \text{cm}^{-2} )</td>
</tr>
<tr>
<td>( \text{Al}<em>{0.16}\text{Ga}</em>{0.84}\text{N/Al}<em>{0.10}\text{Ga}</em>{0.90}\text{N} )</td>
<td>( -2.73 \times 10^{12} \text{cm}^{-2} )</td>
</tr>
<tr>
<td>( \text{Al}<em>{0.10}\text{Ga}</em>{0.90}\text{N/Al}<em>{0.16}\text{Ga}</em>{0.84}\text{N} )</td>
<td>( +2.73 \times 10^{12} \text{cm}^{-2} )</td>
</tr>
<tr>
<td>( \text{Al}<em>{0.10}\text{Ga}</em>{0.90}\text{N/Al}<em>{0.30}\text{Ga}</em>{0.70}\text{N} )</td>
<td>( +9.89 \times 10^{12} \text{cm}^{-2} )</td>
</tr>
<tr>
<td>( \text{Al}<em>{0.30}\text{Ga}</em>{0.70}\text{N/Al}<em>{0.16}\text{Ga}</em>{0.84}\text{N} )</td>
<td>( -7.16 \times 10^{12} \text{cm}^{-2} )</td>
</tr>
<tr>
<td>( \text{Al}<em>{0.16}\text{Ga}</em>{0.84}\text{N/GaN} )</td>
<td>( -6.88 \times 10^{12} \text{cm}^{-2} )</td>
</tr>
</tbody>
</table>

Polarization charges

- grey – quantum wells
- blue – no polarization charges
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: $E_{\text{block}} = 4.5$ eV, dashed lines: $E_{\text{block}} = 4.1$ 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

$\tau_n = 1 \, \mu$s in QWs

full simulation

no polarization

original blocker band gap

NUSOD '06 Tutorial MA2, Joachim Piprek 9/11/06
GaN-based Laser Diode

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

Ridge-Waveguide Laser Diode


ridge width = 3\(\mu\)m, cavity length = 450 \(\mu\)m, 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 $g(\lambda,n,p,T,x,y)$ 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  $\alpha_i = 12 \text{ cm}^{-1}$  $\tau_{\text{SRH}} = 0.5 \text{ ns (QW)}$  $R_{th} = 75 \text{ K/W}$
**Optical Modes**

- Vertical profile of index and mode
- Near field profile

Optical confinement factor = 0.015 per quantum well

**Self-Heating**

Thermal resistance:

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

External \( R_{th} = 30 \text{ K/W} \)

Temperature distribution

Heat power profile at laser axis
Heat Sources

Heat power contributions vs. current

- Joule heat
- Defect recombination
- Thomson Cooling (negative heat)
- Peltier Heat
- Light power
- Absorption

Optical Gain

- 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:

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

$$\frac{d\lambda_e}{dT} = 0.09 \text{ nm/K}$$
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.

Current Loss [mA]

Lasing Power: 0 (thr.) 420mW

Optimization: Facet Coating

Facet reflectance (front / back)

P\textsubscript{max} = 480 mW

R = 0.02 / 0.95

R = 0.18 / 0.95

dots: measurement, lines: simulation

Output Power (front) [mW]

Current [mA]
Optimization: Heat Sinking

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

\[ P_{\text{max}} = 770 \text{ mW} \]

\[ R_{\text{th}} = 45 \text{ K/W} \]

\[ R_{\text{th}} = 75 \text{ K/W} \]

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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

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 (Gunta/Bertazzi/Parola/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/Osinski)
18. Optical properties of edge-emitting lasers: measurement and simulation (Schwarz/Witzmann)
19. Electronic properties of InGaN vertical-cavity lasers (Piprek/Li/Forbes/Nakamura)
20. Optical design of vertical-cavity lasers (Nakwaski/Czyszczanowski/Sarzala)
21. GaN nanowire lasers (Maslov/Ning)

_to be published in January 2007_