Interplay of screening and band gap renormalization effects in near UV InGaN light emitting diodes

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Outline

- introduction into near UV LEDs
- theoretical model
- calculated band profiles and luminescence peak wavelengths for different barrier compositions of near UV MQW active region
- fabrication of near UV LEDs and experimental setup
- measured luminescence spectra and peak wavelength dependence
- conclusions
Introduction

- many applications for UV light sources but conventional mercury lamps bulky, expensive, toxic ⇒ need for LEDs based on (Al,In,Ga)N
- nitrides grown along c-axis suffer from spontaneous and piezoelectric polarization
- active region of conventional visible LEDs:
  - compressively strained InGaN QWs separated by InGaN barriers, where difference of indium contents > 5%
  - strong piezoelectric polarization effects
- active region of near UV LEDs:
  - indium content in QW < 3%
    ⇒ aluminum containing barriers needed for sufficient carrier confinement
  - additional spontaneous polarization effects
Polarization of c-plane Al$_x$In$_y$Ga$_{1-x-y}$N/GaN

zero total polarization discontinuity to (In)GaN achievable by adding small amount of In to AlGaN $\implies$ ‘polarization matching’
Theoretical model

Schrödinger equation: \( 8 \times 8 \, k \cdot p \) Hamiltonian taking into account 3 uppermost valence bands and lowest conduction band, doubly degenerated

\[
H\left(E^*_c, E^*_v, k_\parallel, \frac{d}{dz}\right) \Psi_n(k_\parallel, z) = E_n(k_\parallel) \Psi_n(k_\parallel, z)
\]

renormalization of bulk band edges

\[
E^*_c = E_c - e\phi_H - \frac{1}{2}V_{xc} \left(\frac{n+p}{2}\right)
\]
\[
E^*_v = E_v - e\phi_H + \frac{1}{2}V_{xc} \left(\frac{n+p}{2}\right)
\]

\(V_{xc}\) exchange–correlation potential in local density approximation

\(\phi_H\) Hartree potential from Poisson equation

\[
-\varepsilon_0 \text{div} \left(\varepsilon_r \text{grad} \phi_H\right) = e(p - n + N_D^+ - N_A^-) - \text{div} \left(P_{sp} + P_{pz}\right)
\]

luminescence: free carrier theory with sech–type of broadening

Band gap renormalization (BGR) \( \Delta E_g = -V_{xc} \)

\[ V_{xc} = \zeta N^{1/3} \text{ (exchange only)} \]

Binet:
\[ \zeta = 2.1 \times 10^{-8} \text{ eVcm} \]

Yoshikawa:
\[ \zeta = 4.27 \times 10^{-8} \text{ eVcm} \]

\( \approx 10 \text{ nm} \) ‘red’ shift of band gap wavelength due to BGR at \( \lambda = 375 \text{ nm} \)

R. Zimmermann, Many-Particle Theory of Highly Excited Semiconductors, Leipzig, Germany: Teubner, 1987
M. Yoshikawa et al. J. Appl. Phys. 86, 4400, 1999
Near UV multi quantum well active region

100 nm p-GaN
10 nm p-Al$_{0.23}$Ga$_{0.77}$N electron blocking
7 nm Al$_x$In$_y$Ga$_{1-x-y}$N barrier
3.5 nm In$_{0.02}$Ga$_{0.98}$N QW
7 nm Al$_x$In$_y$Ga$_{1-x-y}$N barrier
10 nm n-Al$_{0.23}$Ga$_{0.77}$N hole blocking
100 nm n-GaN
Conduction band profiles at $U_F = 3.32$ V
Calculated luminescence peak vs. carrier density

- GaN barriers ‘red’ shift of luminescence peak wavelength
- \( \text{In}_{0.04}\text{Al}_{0.16}\text{Ga}_{0.84-x}\text{N} \) barriers
  \( x < 0.04 \) ‘blue’ shift of peak wavelength, decreases with increasing \( x \)
  \( x = 0.04 \) constant peak wavelength
Screening of polarization charges vs. BGR

$\text{Al}_{0.16}\text{In}_{0.04}\text{Ga}_{0.80}\text{N}$

- no BGR: ‘blue’ shift due to the increasing compensation of the polarization charges by the injected charged carriers
- no polarization: ‘red’ shift due to shrinkage of the band gap
Fabrication and experimental setup

- growth by metal organic vapor phase epitaxy (MOVPE) on 2-inch (0001) sapphire substrates*
- standard LED processing technology
- 100 μm × 100 μm p-contact area
- electro luminescence measured on wafer through substrate using a calibrated Si photodetector
- pulse duration 1 μs and repetition frequency 50 Hz (duty cycle 0.00005) to avoid self-heating

Measured luminescence spectra at $I = 0.26 \, \text{A}$

- short-wavelength slope influenced by absorption in GaN layers
- small ripples due to interference effects
- luminescence peaks determined by Gaussian fits
Measured peak wavelength versus injection current

- Dependence of wavelength shifts on barrier composition as simulated
- Different order of peak wavelengths
- Measured wavelength shifts are smaller than simulated ones
Conclusions

- dependence of luminescence properties of near UV LEDs on barrier composition investigated theoretically and experimentally
- both band gap renormalization and screening of polarization charges contribute to wavelength shifts
- good correspondence of theoretical and experimental results
- composition of the barriers and the associated strain and polarization are important parameters in LED optimization
Band profiles versus barrier composition \((U = 0 \text{ V})\)

\[
\begin{align*}
\text{GaN} & : & E_F \\
\text{Al}_{0.16}\text{Ga}_{0.84}\text{N} & : & E_F \\
\text{Al}_{0.16}\text{In}_{0.02}\text{Ga}_{0.82}\text{N} & : & E_F \\
\text{Al}_{0.16}\text{In}_{0.04}\text{Ga}_{0.80}\text{N} & : & E_F
\end{align*}
\]
Result of simulation by APSYS (J. Piprek)

\[ I_{\text{max}} = 0.5 \, \text{A}, \ \Delta I = 0.05 \, \text{A} \]