



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

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..translating ideas into innovation





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 $Al_x ln_y Ga_{1-x-y} N/GaN$



zero total polarization discontinuity to (In)GaN achievable by adding small amount of In to AlGaN \implies 'polarization matching'





Theoretical model*

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

$$\mathbf{H}\left(E_{\mathsf{c}}^{*}, E_{\mathsf{v}}^{*}, \boldsymbol{k}_{||}, \frac{d}{dz}\right) \Psi_{n}(\boldsymbol{k}_{||}, z) = E_{n}(\boldsymbol{k}_{||}) \Psi_{n}(\boldsymbol{k}_{||}, z)$$

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 ϕ_{H} Hartree potential from Poisson equation

$$-\varepsilon_0 \operatorname{div} \left(\varepsilon_{\mathsf{r}} \operatorname{grad} \phi_{\mathsf{H}} \right) = e(p - n + N_{\mathsf{D}}^+ - N_{\mathsf{A}}^-) - \operatorname{div} \left(\boldsymbol{P}_{\mathsf{sp}} + \boldsymbol{P}_{\mathsf{pz}} \right)$$

luminescence: free carrier theory with sech-type of broadening

* H. Wenzel, Opt. Quant. Electron. 38, 953, 2006





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



R. Zimmermann, Many-Particle Theory of Highly Excited Semiconductors, Leipzig, Germany: Teubner, 1987

- F. Binet et al. Phys. Rev. B 60, 4715, 1999
- M. Yoshikawa et al. J. Appl. Phys. 86, 4400, 1999





Near UV multi quantum well active region



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Conduction band profiles at $U_F = 3.32$ V







Calculated luminescence peak vs. carrier density



- GaN barriers 'red' shift of luminescence peak wavelength
- In_xAl_{0.16}Ga_{0.84-x}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 Al_{0.16}In_{0.04}Ga_{0.80}N polarisation + BGR 370 wavelength \(\lambda / nm) no polarisation 365 360 no BGR 10 20 30 40 n carrier density N / 10¹⁸ cm⁻³

- 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
- $100 \ \mu m \times 100 \ \mu m$ 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

A. Knauer et al. Proc. SPIE 6797, 677970X-1, 2007





Measured luminescence spectra at I = 0.26 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

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Band profiles versus barrier composition (U = 0 V)





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Result of simulation by APSYS (J. Piprek) $I_{max} = 0.5 \text{ A}, \Delta I = 0.05 \text{ A}$

