Simulation of InGaN/GaN multiple quantum well light-emitting diodes with Quantum Dot electrical and optical effects

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Outline:

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Introduction

InGaN based MQW LED: traffic signals, full-color displays, back lighting in liquid-crystal displays, replacement for conventional incandescent and fluorescent light bulbs in near future.

Blue, green and white LED has a high luminescent efficiency.

External quantum efficiency: more than 12%.

Threading dislocation density: $10^8 - 10^{12}\text{cm}^{-2}$.

Origin of luminescence of InGaN MQW LED: ????????
Solid phase immiscibility in InGaN alloys

the large difference in Interatomic spacing between GaN and InN

The binodal and spinodal curve

InGaN region with high In content

Ho et al. APL. 69. 2701 (1996)
EL and PC spectra form green and blue inGaN based LED

Stokes shift plotted against emission peak energy for inGaN based LED

Large Stokes shift shows origin of luminescence comes from InGaN quantum dots with high In content
InGaN quantum dots: 3~5 nm
In content 35%

HRTEM images for blue InGaN LED  
Musikhin et al  APL, 80, 2099 (2002)
The mechanism of luminescence in InGaN-based MQW LEDs

the radiative recombination within the In-rich quantum dots

Numerical simulation is an effective method to study and optimize the characteristics of optoelectronic devices

There is few simulation considering the QD origin of luminescence for InGaN-based MQW LEDs

Simulate In$_{0.22}$Ga$_{0.78}$N/GaN MQW green LED by APSYS software based on Quantum Dot model
Theoretical models for quantum dots

1. Quantum dot structure

A certain density of QDs is assumed to be embedded in InGaN quantum well.
QD structure is approximated by a disk-like high indium cylinder surrounded by QW material with lower indium composition to form a dot/well complex system.

**InGaN QD parameters:**

- **In content:** 0.56
- **QW In content:** 0.22
- **Size:** height 1.5nm, diameter 3.6nm and 5nm
2. Calculation of electronic states of QD

\[
\left[-\frac{\hbar^2}{2m^*}\left(\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) + \frac{\partial^2}{\partial z^2}\right) + V(r, z)\right] \varphi(r, z) = E \varphi(r, z)
\]  

(1)

Disk like shape dot/well system

cylindrical coordinates to describe QD potential distribution of electron and hole.

Energy band diagram of an InGaN quantum dot in a quantum well
Confined dot levels for InGaN quantum dots with height of 1.5nm, diameter of 3.6nm and 5.0nm

the interband transition between confined dot levels close to the bottom of dot potential is responsible for the LED emission
3. Spontaneous emission

In dot/well system, spontaneous emission comes from two parts:

**QD**

\[
\begin{align*}
\rho_{qd}^{sp}(E) &= \sum_{i,j} \sum_{s} \frac{q^2 n_r E M_b^2 N_{qd}(s)}{\pi \varepsilon_0 m_0^2 \hbar^2 c_0 t_{complx}} \left| \left\langle \varphi_{is} | \varphi_{js} \right\rangle \right|^2 G_s(E - E_{ij}) f_c(1 - f_v) \\
\end{align*}
\]

**QW**

\[
\begin{align*}
\rho_{qw}^{sp}(E) &= \sum_{i=j} \left( \frac{2 \pi}{\hbar} \right) \left| H_{ij} \right|^2 f_j(1 - f_i) D(E) \rho_{ij}
\end{align*}
\]

Total spontaneous emission determined by:

\[
\begin{align*}
\rho_{qd}^{sp}(E) &= \rho_{qw}(E) + \rho_{qd}(E)
\end{align*}
\]
4. Quantum transport mechanism

Non-equilibrium quantum transport model

1) fly directly over the small QDs

2) escaping from the deep QD potential before being thermalized
Simulation results

Stokes shift is 370meV

QD emission in our green LED

photocurrent is from the inter-subband transition in InGaN quantum wells

EL, PC spectrum and simulated absorption spectrum based on MQW model with In content of 0.22
Experimental EL
Simulated EL based on MQW Model
Simulated EL based on QD Model

Calculated and experimental EL spectrum

Experiment: 2.35-2.40eV
MQW model: 2.67eV
QD model: good agreement with experiment
QD model with Quantum Transport close to experiment

The I-V characteristics of InGaN-based LED
MQW model
QD model without Q.Trans

90% ~ 100% which is overestimated

QD model with Q.Trans

close to experiment

The IQE of InGaN-based LED

It indicates that quantum transport mechanism plays an important role in the InGaN-based MQW LED
Conclusion

1) QD model with Q.Trans. accurately accounts for the experimental data of InGaN based LED

2) Quantum dot emission and non-equilibrium quantum transport played very important roles in the InGaN-based MQW LEDs

3) The simulation allows us to understand better for the quantum states effect in the device performance

4) With our more delicate model, one may be able to optimize the InGaN-based LEDs performance
Thank you for your attention!