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

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Outline:

- Introduction
 - Origin of luminescence of InGaN based LED
- Theoretical models for quantum dots
 - Calculation of electronic states of InGaN QD
 - Spontaneous emission
 - Quantum transport mechanism
- Simulation results
- Conclusion



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 luminescence efficiency

External quantum efficiency : more than **12%**

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

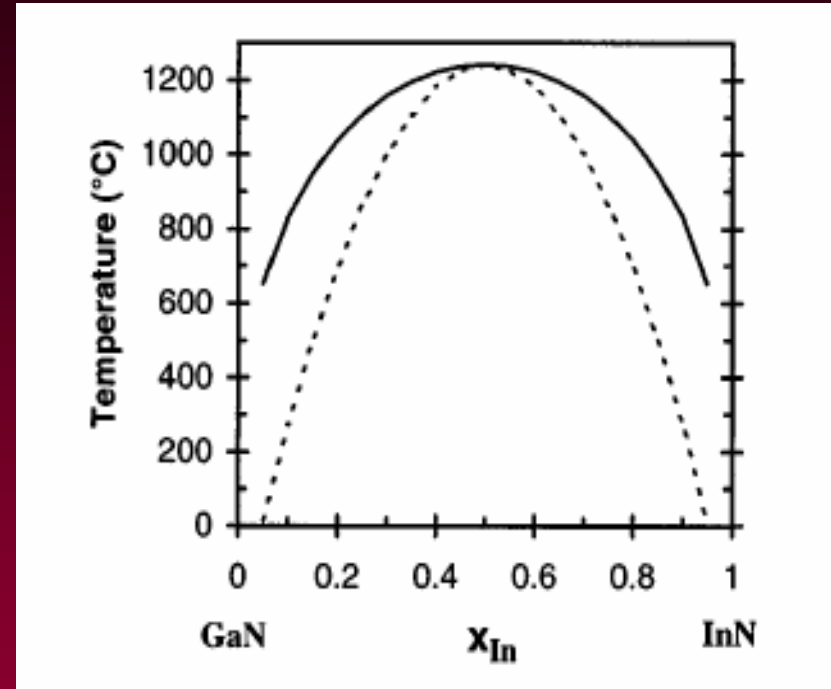
Origin of luminescence of InGaN MQW LED ?????????



Solid phase immiscibility in InGaN alloys

the large difference in Interatomic
spacing between GaN and InN

The binodal and spinodal curve

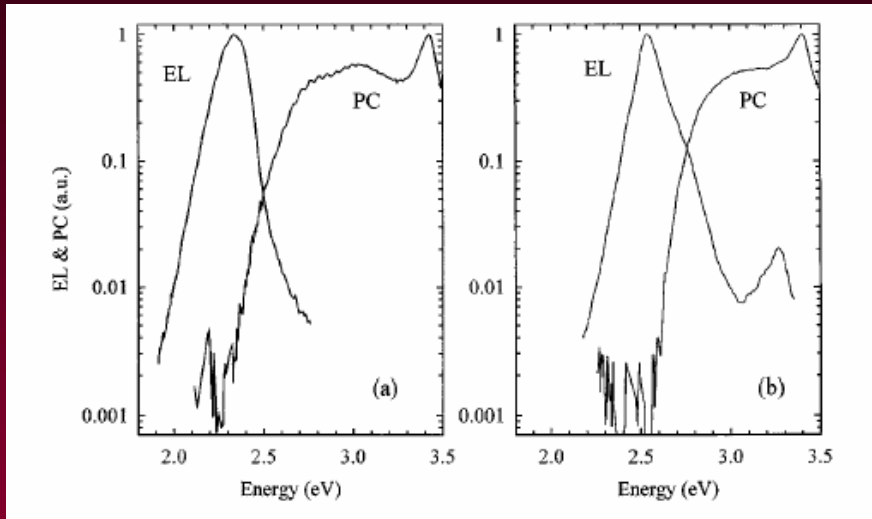


Ho et al. APL. 69. 2701 (1996)

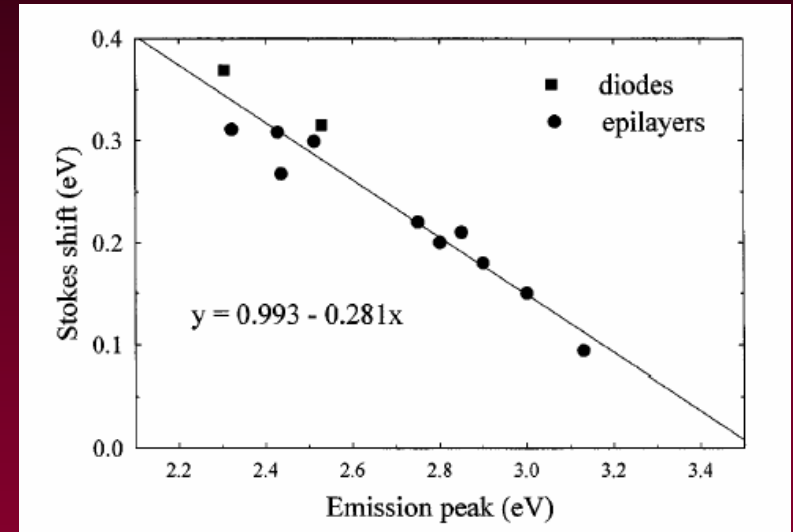
InGaN region with high In content



Donnell et al. PRL, 82, 237 (1999)

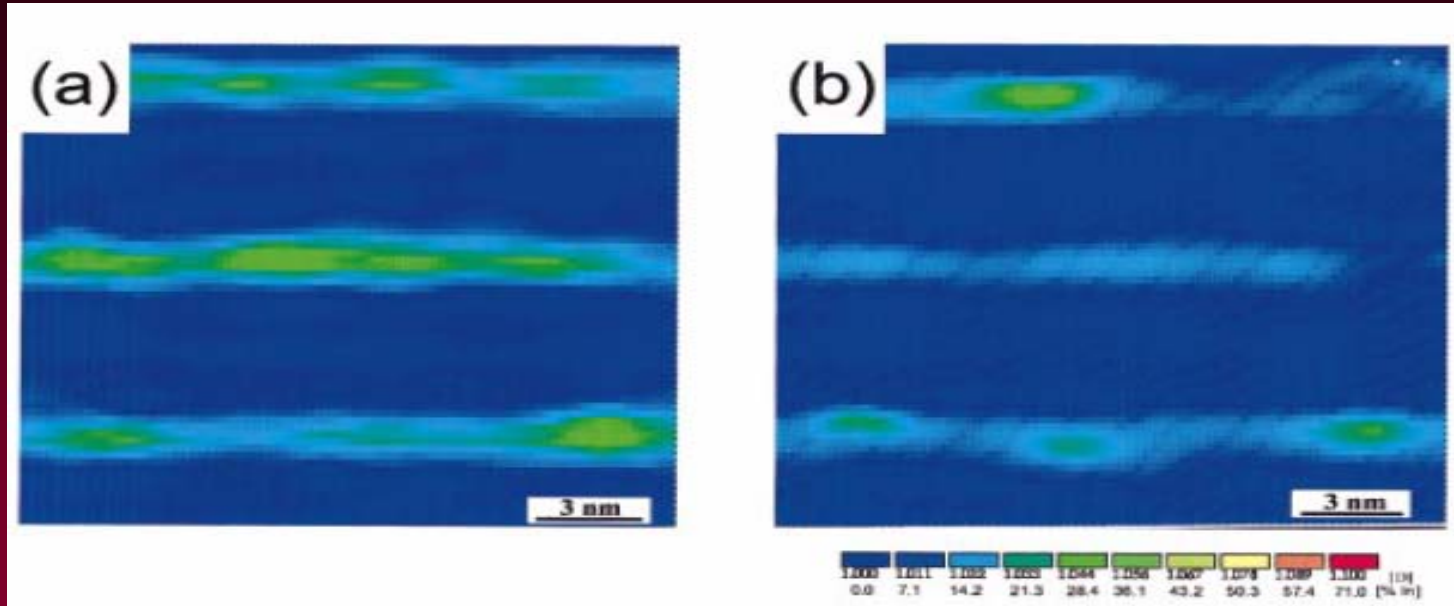


EL and PC spectra form green and blue
inGaN based LED



Stokes shift plotted against emissin peak energy
for inGaN based LED

Large Stokes shift shows origin of luminescence
comes from InGaN quantum dots with high In content



HRTEM images for blue InGaN LED Musikhin et al APL,80,2099(2002)

InGaN quantum dots: 3~5 nm
In content 35%



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

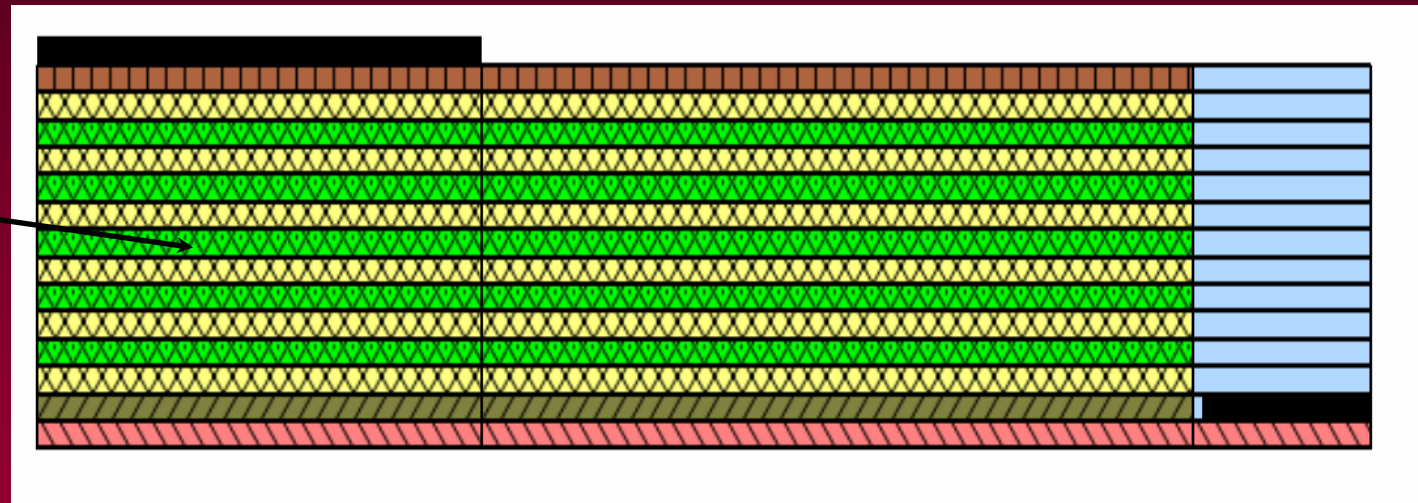
Simulate $\text{In}_{0.22}\text{Ga}_{0.78}\text{N}/\text{GaN}$ MQW green LED
by APSYS software based on Quantum Dot model



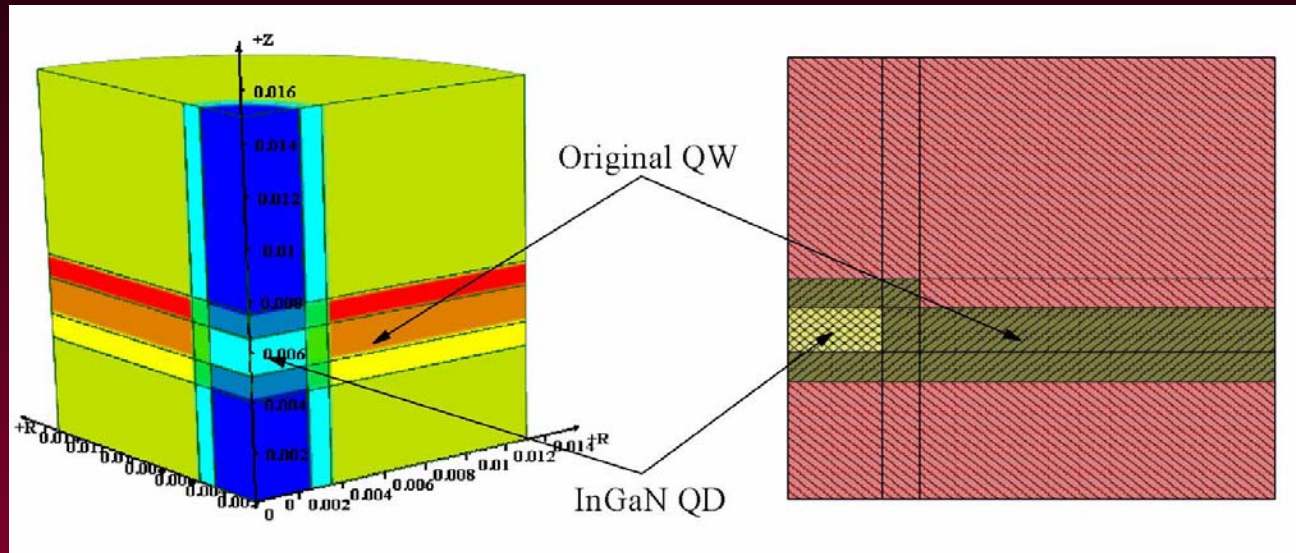
Theoretical models for quantum dots

1. Quantum dot structure

InGaN MQW
with InGaN QDs



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

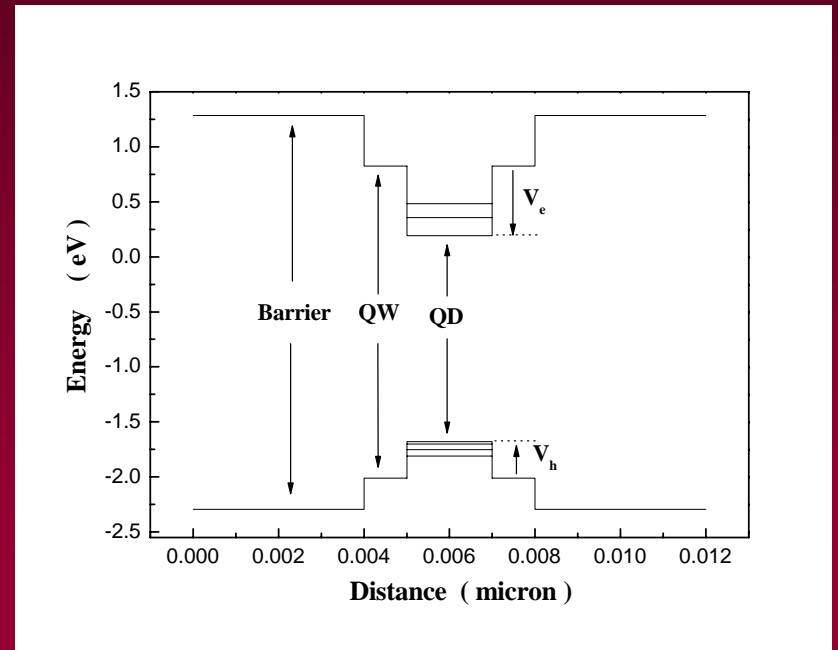


2. Calculation of electronic states of QD

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

Disk like shape dot/well system

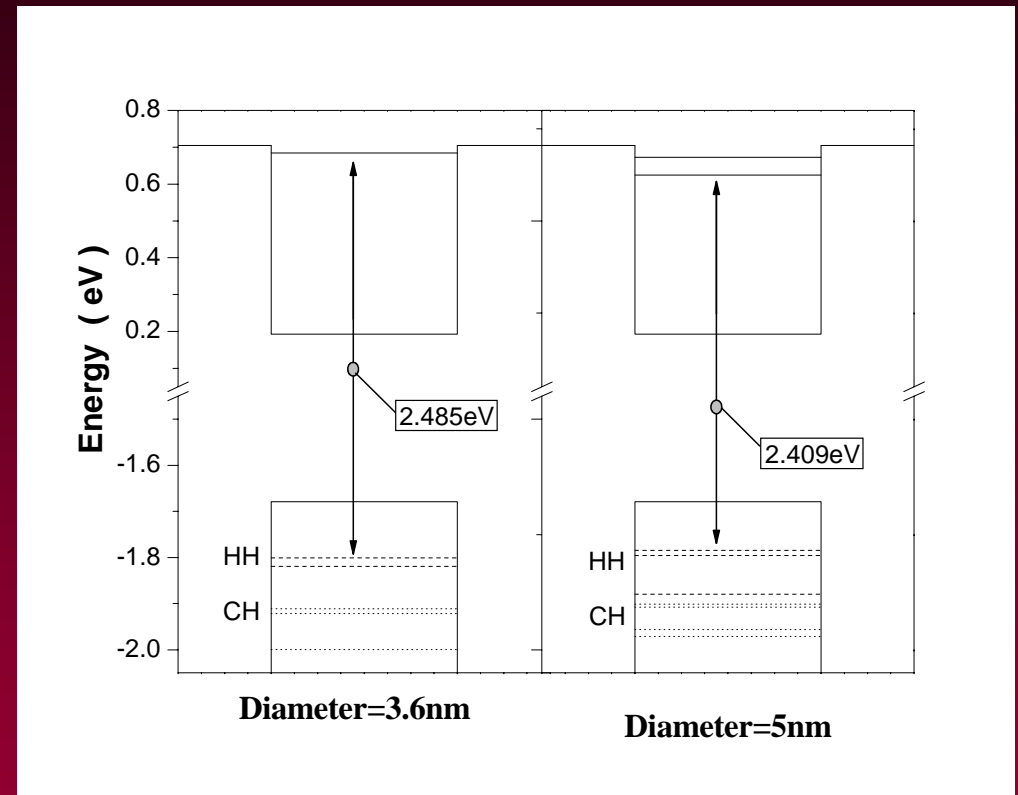
cylindrical coordinates to describe QD
potential distribution of electron and hole.



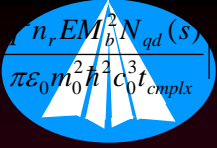
Energy band diagram of an InGaN quantum dot in a quantum well



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 part:

QD

$$r_{qd}^{sp}(E) = \sum_s \sum_{i,j} \frac{q^2 n_r EM_b^2 N_{qd}(s)}{\pi \epsilon_0 m_0^2 \hbar^2 c_0^3 t_{cplx}} \left| \langle \varphi_{is} | \varphi_{js} \rangle \right|^2 G_s(E - E_{ijs}) f_c(1 - f_v) \quad (2)$$

QW

$$r_{qw}^{sp}(E) = \sum_{i=j} \left(\frac{2\pi}{\hbar} \right) |H_{ij}|^2 f_j'(1 - f_i') D(E) \rho_{ij} \quad (3)$$

Total spontaneous emission determined by:

$$r_{2d}^{sp}(E) = r_{qw} r_{qw}^{sp}(E) + r_{qd}^{sp}(E) \quad (4)$$



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



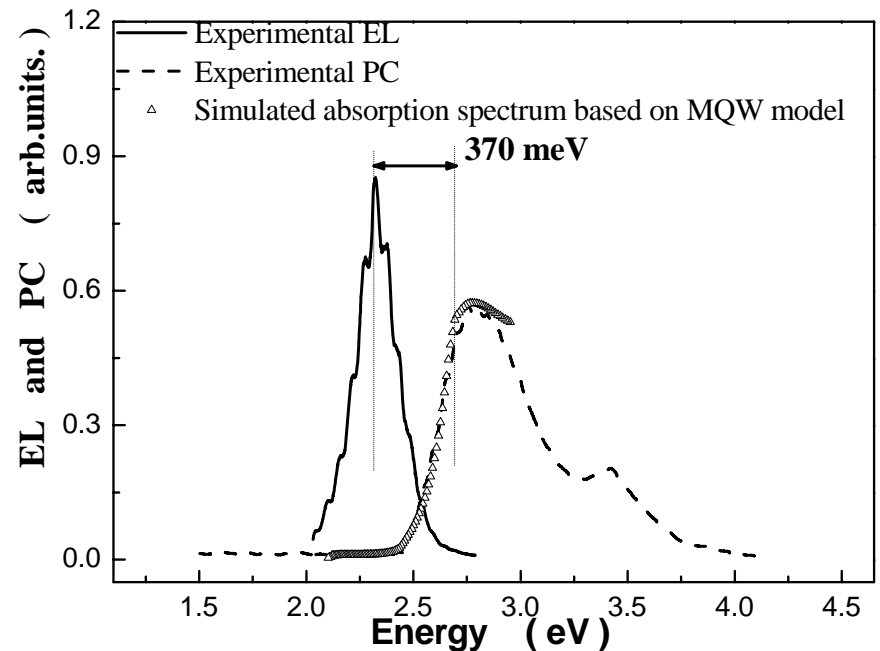
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Simulation results

Stokes shift is 370meV

QD emissin in our green LED

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



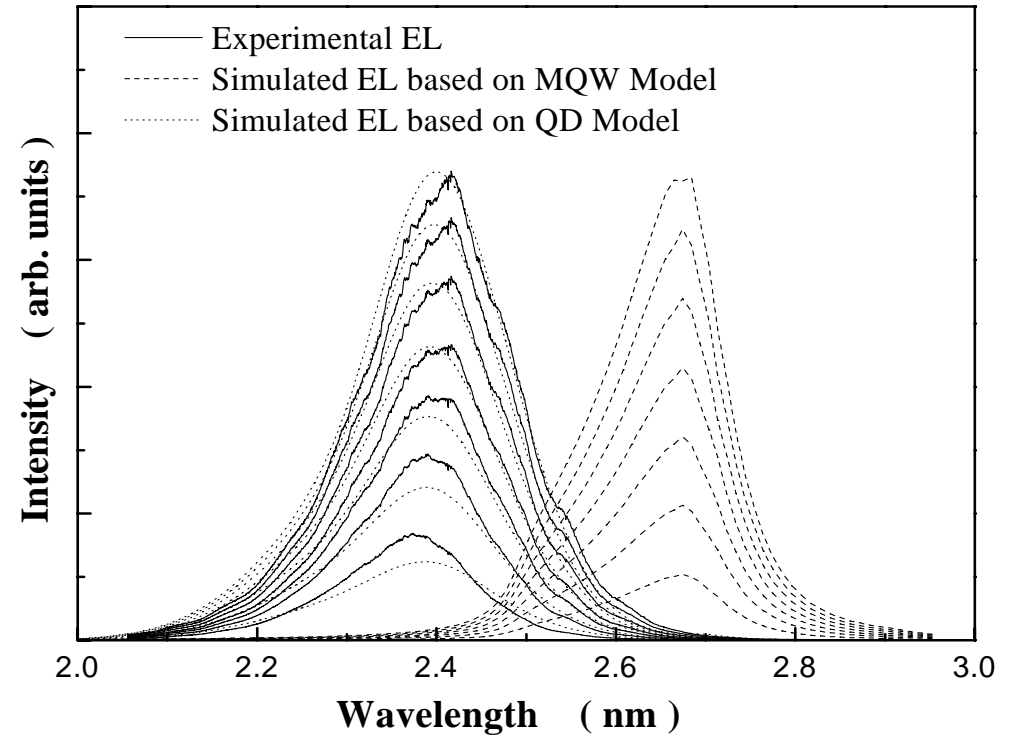
EL, PC spectrum and simulated absorption spectrum based on MQW model with In content of 0.22



Experiment 2.35-2.40eV

MQW model 2.67eV

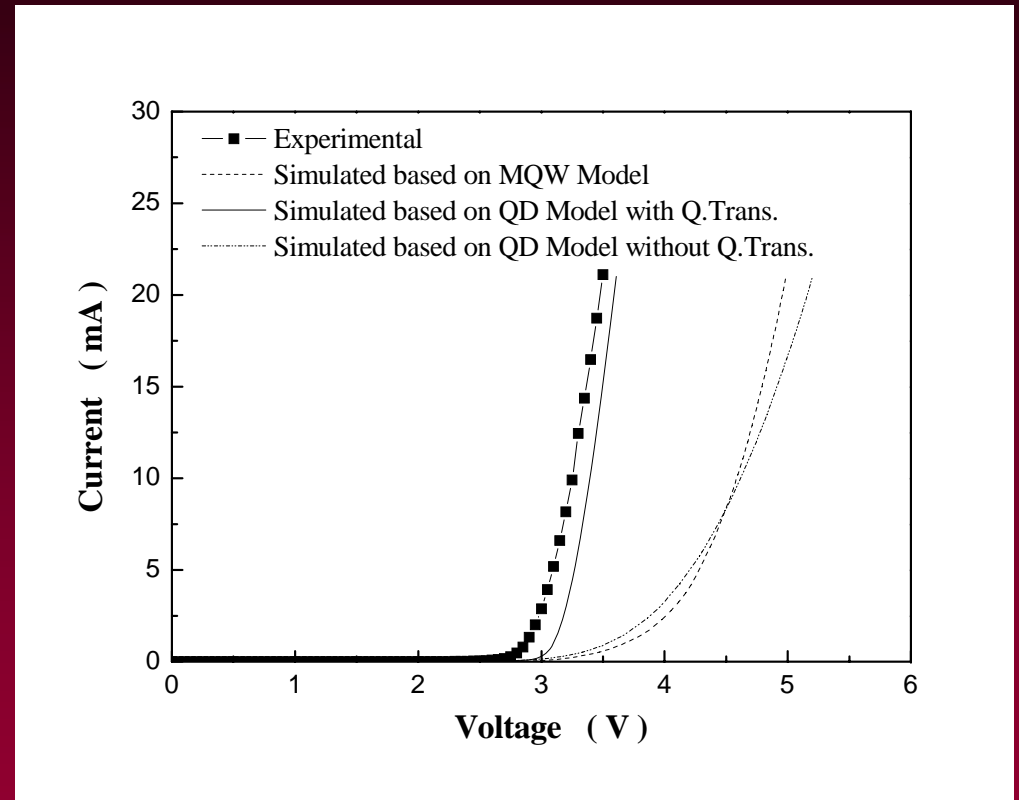
QD model
good agreement with experiment



Calculated and experimental EL spectrum



QD model with Quantum Transport
close to experiment



The I-V characteristics of InGaN-based LED



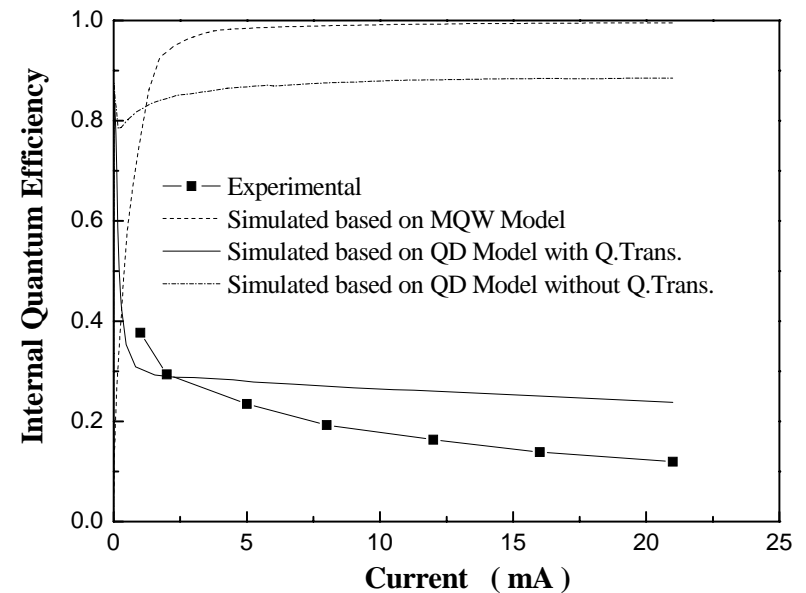
MQW model

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



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Thank you for your attention!