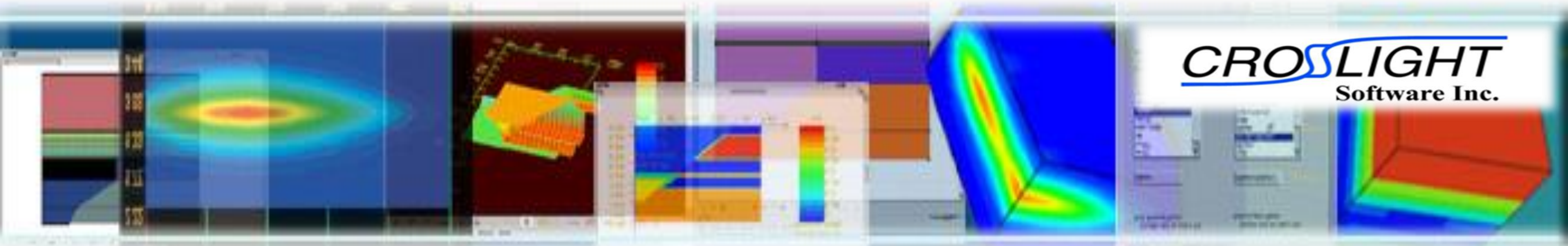


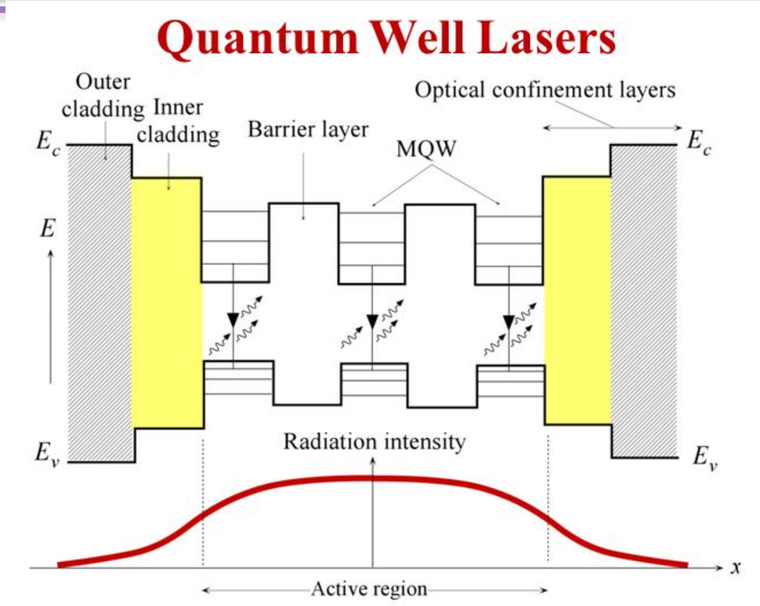
Crosslight Simulation of InGaN MQW LED and Micro-LED

CROSSLIGHT Software Inc.

Contents

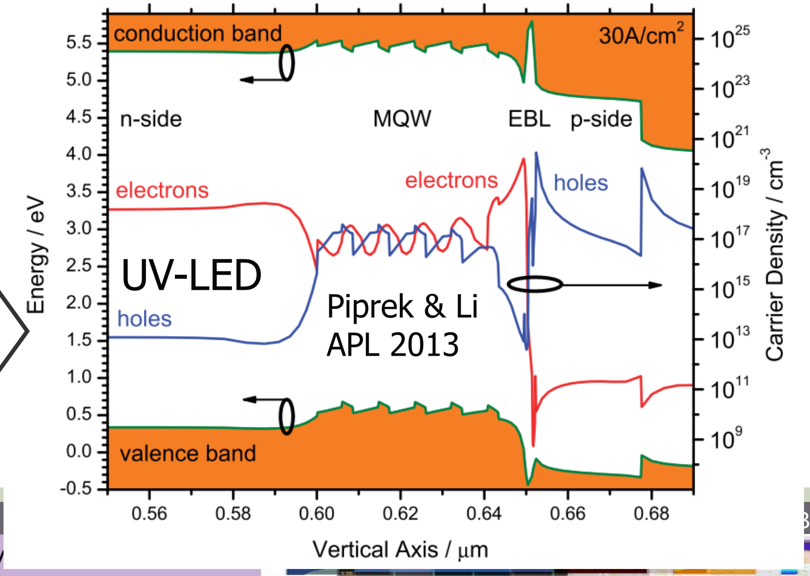
Crosslight: Quantum Simulations

- Use of quantized states in MQW lasers.
- Proposed in 1963
- Nobel Prize in Physics 2000.



Crosslight Software assisted efforts related to Nobel-worthy research.

- GaN p-n junction invented in 1989
- Blue-white GaN LED in 1993
- Nobel Prize in Physics 2014
- UV-LED more recently



Quantum Physics in Semiconductor

$$-\nabla\cdot\left(\frac{\epsilon_0\epsilon_{dc}}{q}\nabla V\right) = -n + p + N_D(1-f_D) - N_A f_A + \sum_j N_{tj}(\delta_j - f_{tj}),$$

Semiconductor eqn.

$$\nabla\cdot J_n - \sum_j R_n^{tj} - R_{sp} - R_{st} - R_{au} + G_{opt}(t) = \frac{\partial n}{\partial t} + N_D\frac{\partial f_D}{\partial t},$$

$$\nabla\cdot J_p + \sum_j R_p^{tj} + R_{sp} + R_{st} + R_{au} - G_{opt}(t) = -\frac{\partial p}{\partial t} + N_A\frac{\partial f_A}{\partial t}.$$

$$J_n = n\mu_n\nabla E_{fn}$$

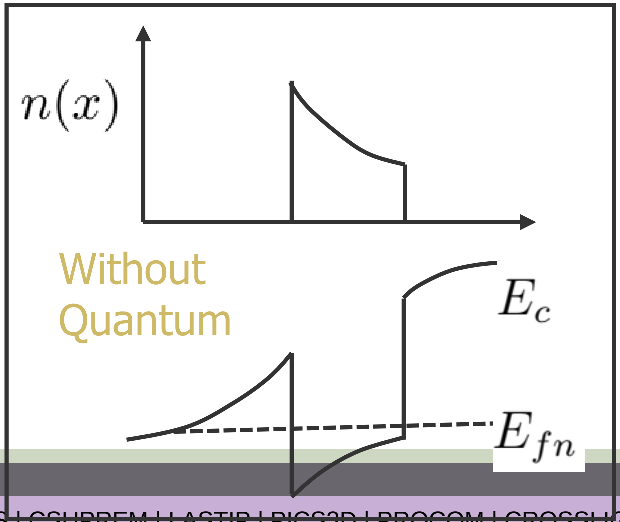
$$J_p = p\mu_p\nabla E_{fp}$$

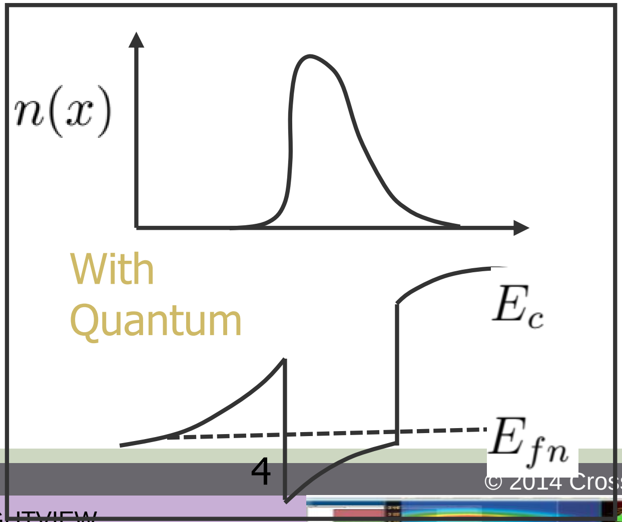
$$H(k)|\psi_i >= E_i(k)|\psi_i >$$

$$n = \sum_j \rho_j^{x0} kTln\left[1 + e^{(E_{fn}-E_j)/kT}\right] + unconfined\ electrons,$$

$$p = \sum_i \rho_i^{x0} kTln\left[1 + e^{(E_i-E_{fp})/kT}\right] + unconfined\ holes,$$

Quantum





Contents

GaN LED simulation capabilities

- Available tools and modules.
- Simulation of IQE droop .
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MQW Models

- K.p theory based MQW model for wurtzite material system.
- Efficient multiple band valley model (HH,LH and CH) with effective mass fit to k.p theory.
- Optionally, manybody gain/spontaneous theory for quantum wells or dots.
- Accurate spectrum model with inhomogeneous broadening using bandgap tail states.
- Spontaneous polarization of surface charges included in self-consistent quantum confinement and transport model.

Transport

- True 2/3D solution of drift-diffusion (DD) equation with option of hot carrier transport.
- Quantum tunneling, quantum capture/escape and direct-flight process included in drift-diffusion model as quantum corrections.
- Heat transport equation self-consistently solved with DD equations.

Light Extraction

- Analytical approach using Green's function [1] offers efficient computation of light extraction efficiency.
- Green's function method to model resonant cavity effect in some LED designs.
- Ray tracing method to compute light extraction in 2 and 3 dimensions.

[1] C. H. Henry, "Theory of spontaneous emission noise

in open resonators and its application to lasers and optical amplifiers,"

J. Lightwave Technol., vol. LT-4, pp. 288--297, March 1986.

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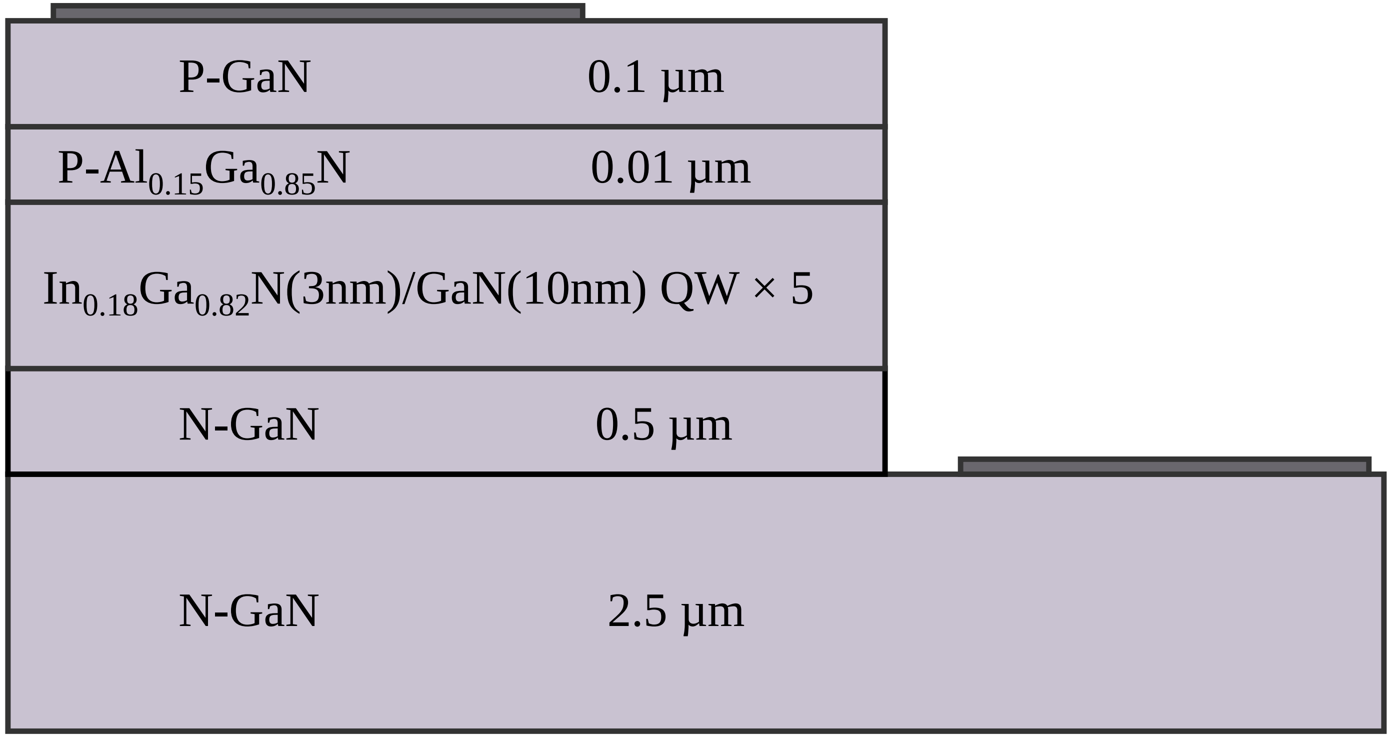
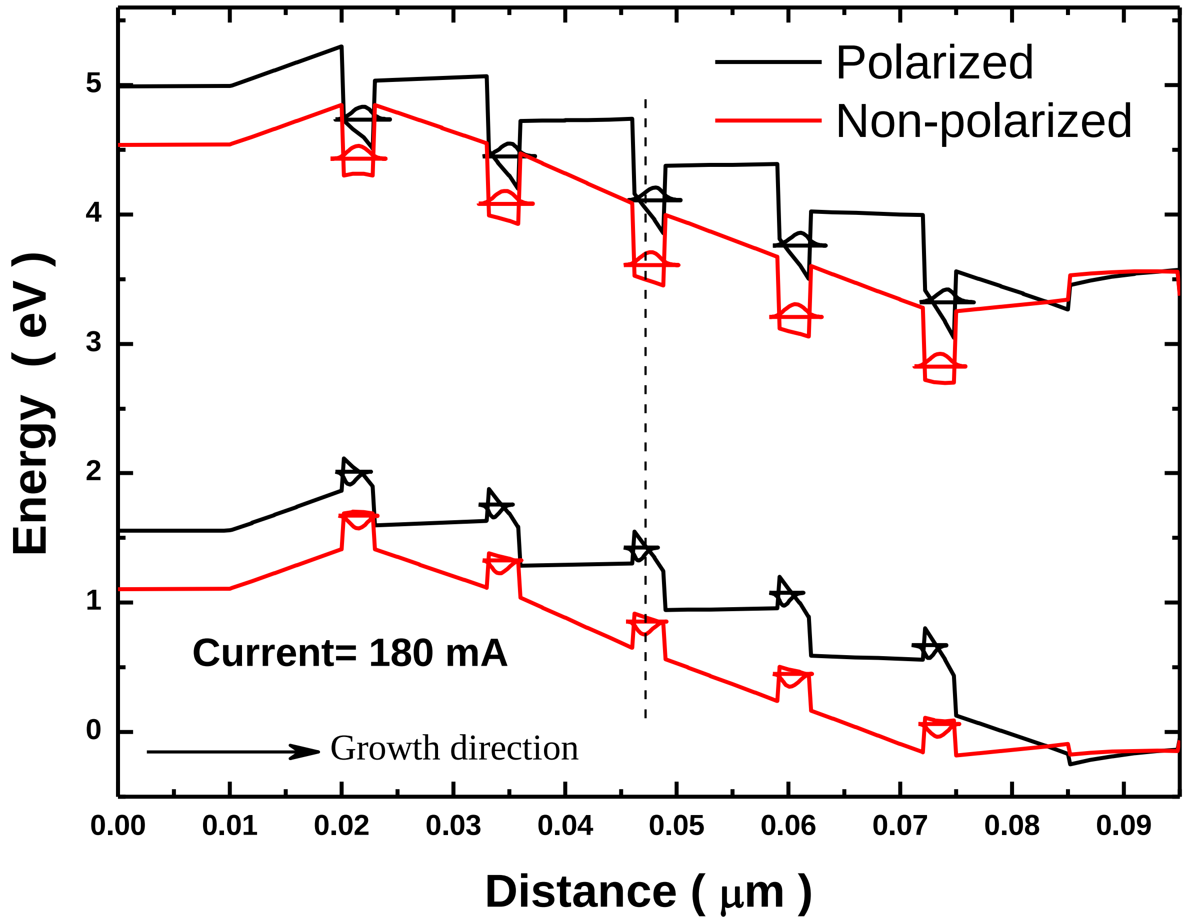
Structure



Size: 300 μm × 300 μm

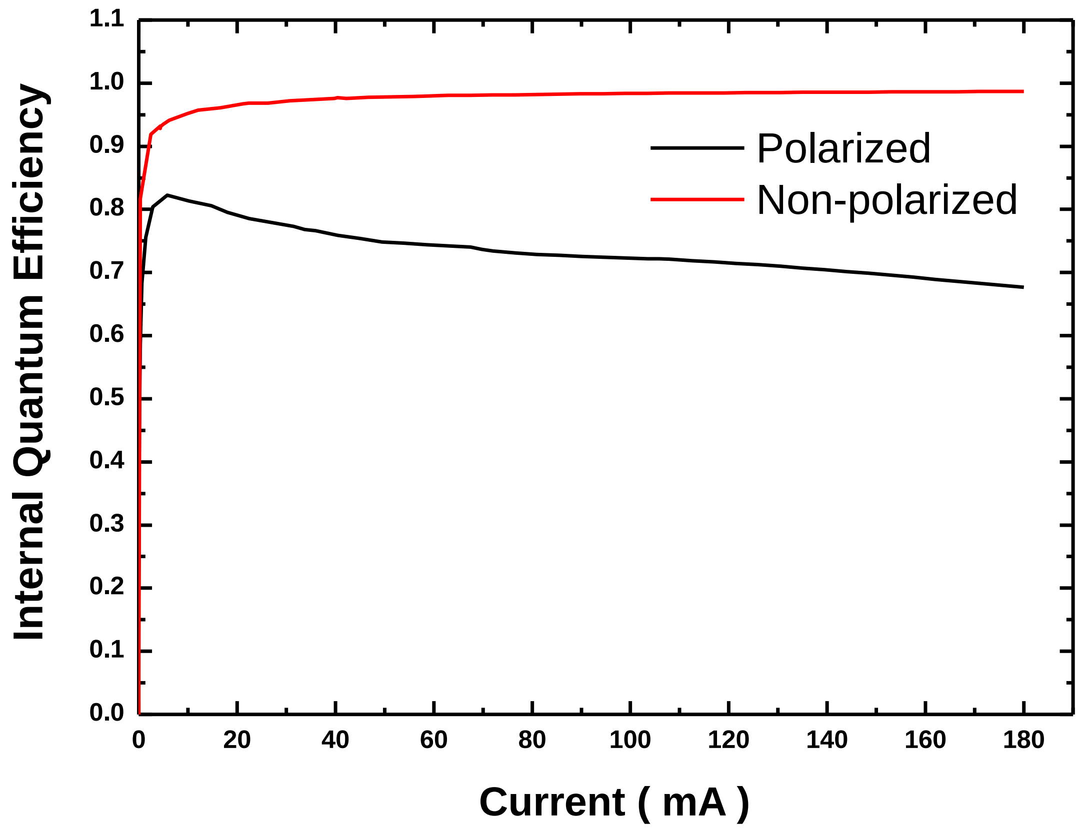
Lifetimes of carriers (τ) in the five QWs along the growth direction are assumed to be 30ns, 35ns, 40ns, 45ns and 50ns, respectively, because the quality of QWs improves (with less defects) with more QWs.
The polarization charge set on the QW interfaces is 50% of the theoretical value calculated based on the Ref. Appl. Phys. Letts, 80, 1204(2002). This represents screening.

Band Diagram



Polarization field tilts the energy band and induces the spatial separation of the electron and hole wave functions.

IQE Curve



Polarization charges in the MQW structure play an important role leading to the low luminous efficiency of InGaN/GaN MQW LEDs.

Qualitative analysis of IQE

Spontaneous emission: B * n^2 (enhanced by QD?)

Non-radiative SRH loss: A * n

Non-radiative Auger loss: C * n^3

Current overflow loss: D * n^f f=?

Non-equilibrium flying-over/escape: E * n^g g=?

Temperature dependence of all of above

Schools of thoughts to explain IQE droop:

1) Overflow caused by polarization field (RPI-Piprek).
2) Auger (Lumileds).
3) Combination: overflow + non-equilibrium escape (Crosslight).
4) Quantum dot or dot like DOS exists: initial high IQE decreases after dots are filled up (IQE).

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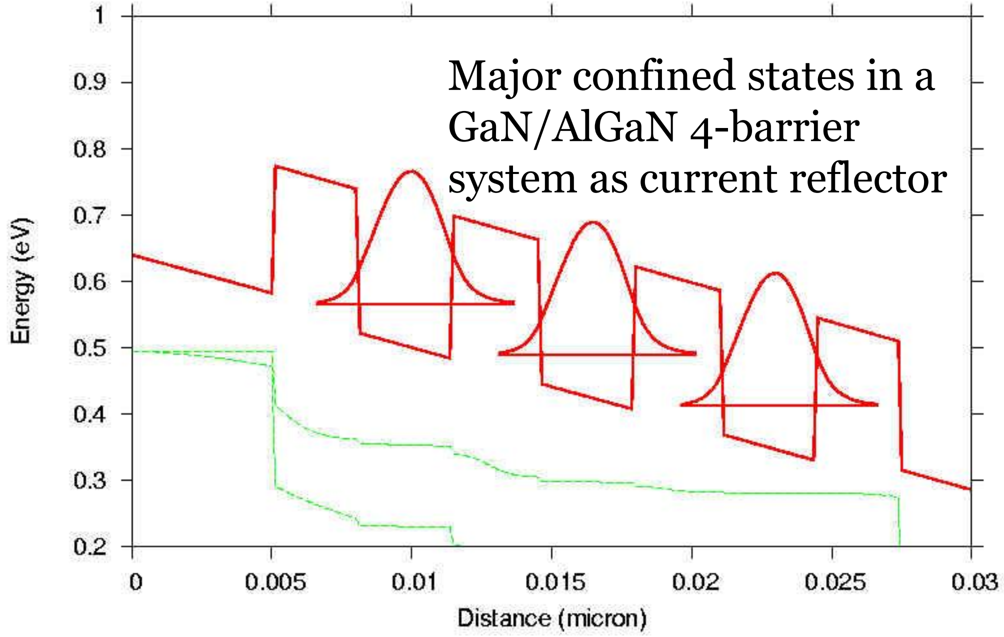
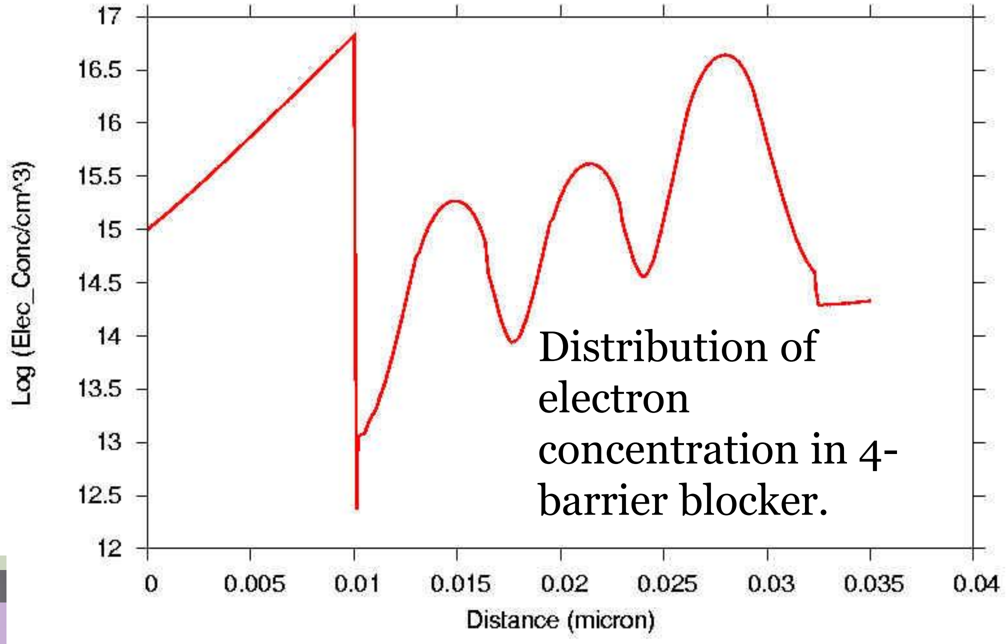
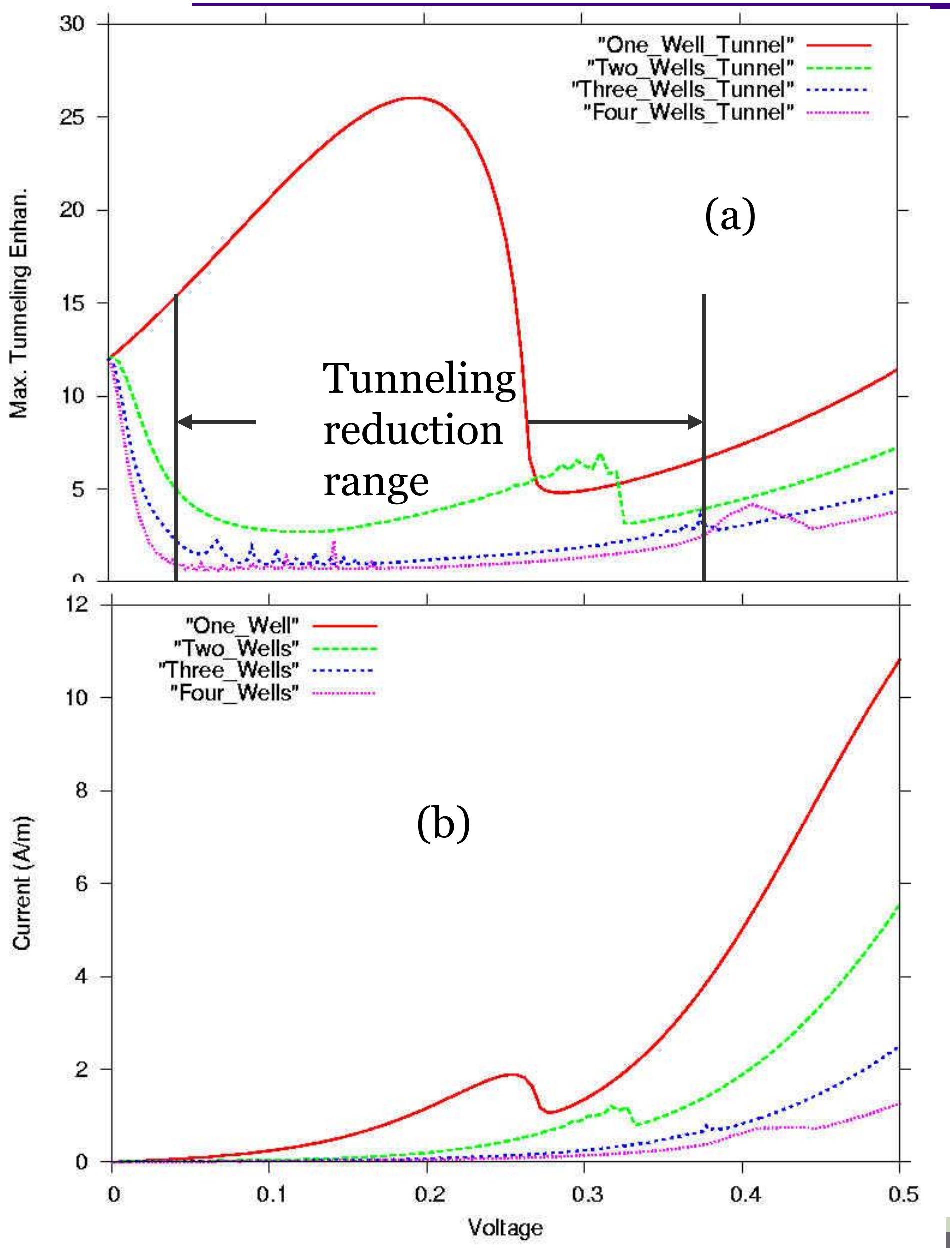
Use of superlattice





- LED design may take advantage of quantum interference effect to reduce or enhance current transport.
- Superlattice may act as a DBR mirror to reflect or block leakage current.
- Previous example of GaAlInN-LED shows strong desire to block leakage current.
- Consider quantum tunneling behavior for a superlattice (SL) consisting of two to five barriers of GaN/AlGaN.

Formation of SL reflector



(a) Maximum tunneling enhancement factor (quantum correction to drift-diffusion) as a function bias showing a large bias range with reduction in tunneling current due to quantum interference effects, as superlattice (SL) size increases to larger than three wells.

(b) Total leakage current through the SL reflector shows strong leakage reduction as SL size increases.

➔ Conclusion: superlattice is effective in leakage current blocking.

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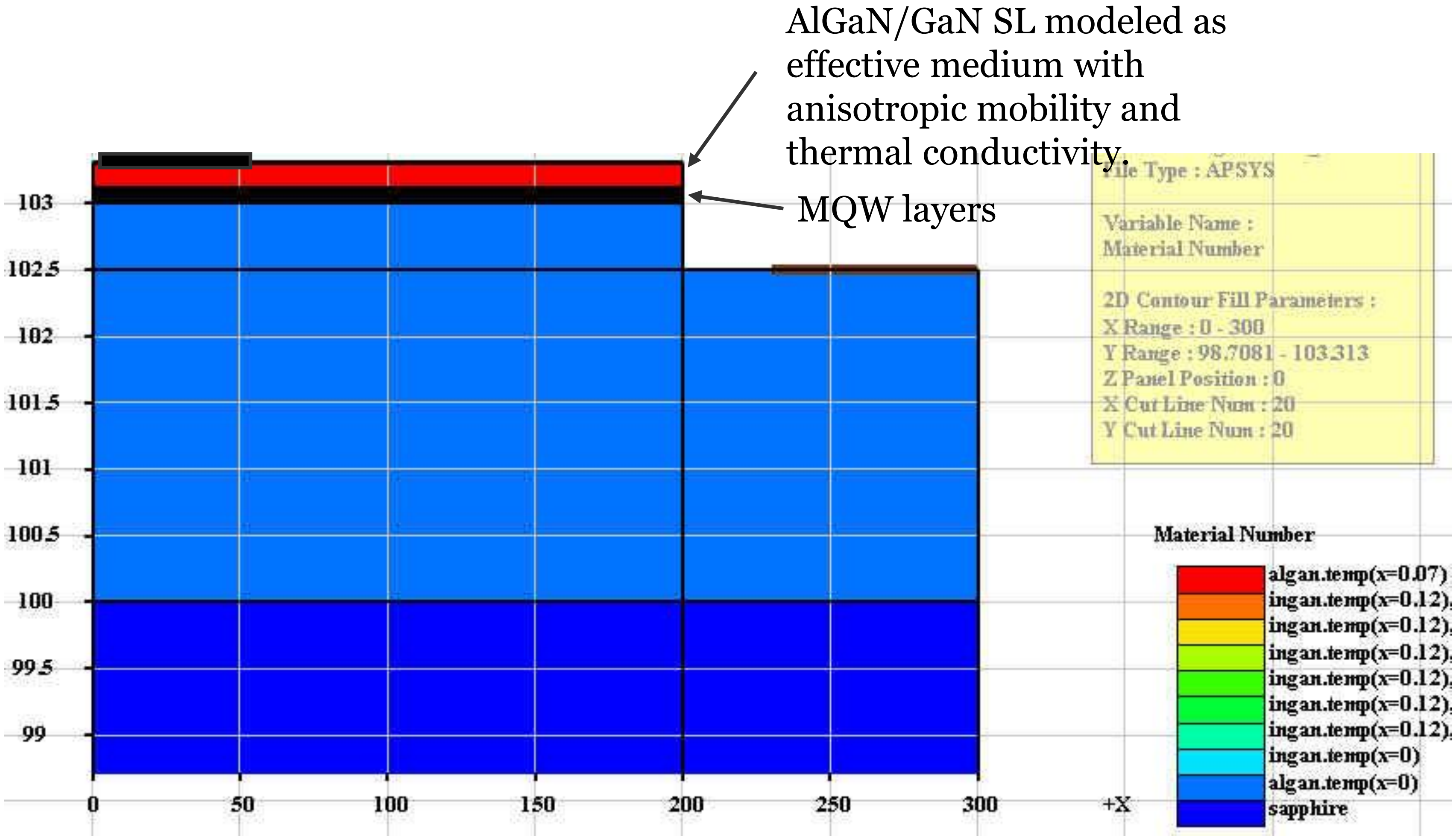
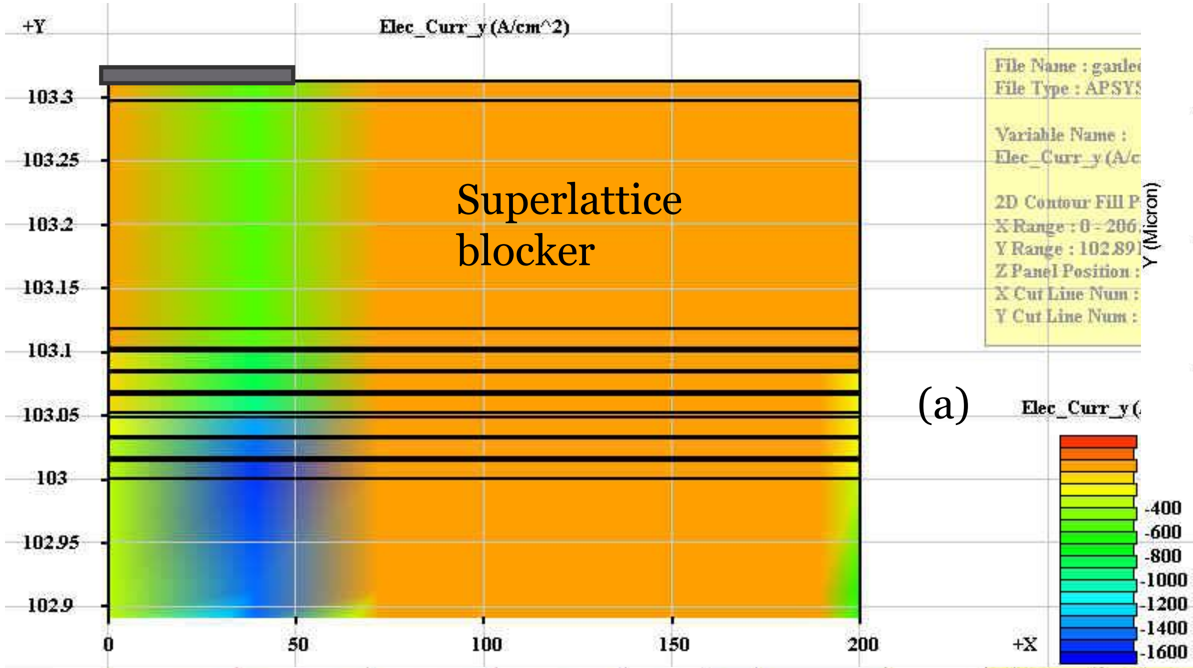
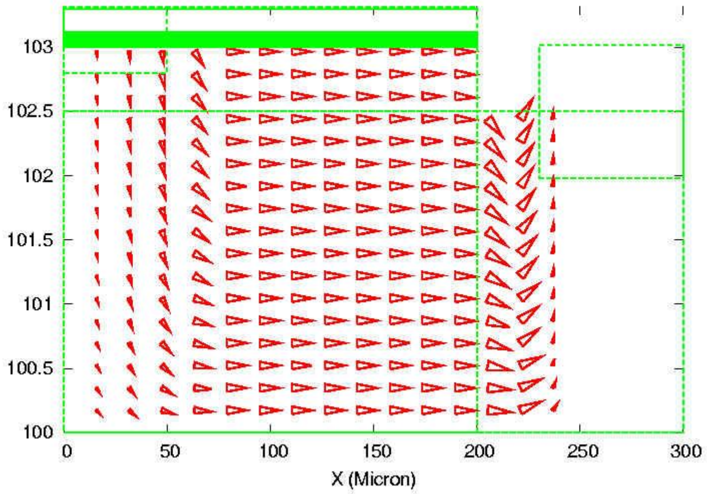
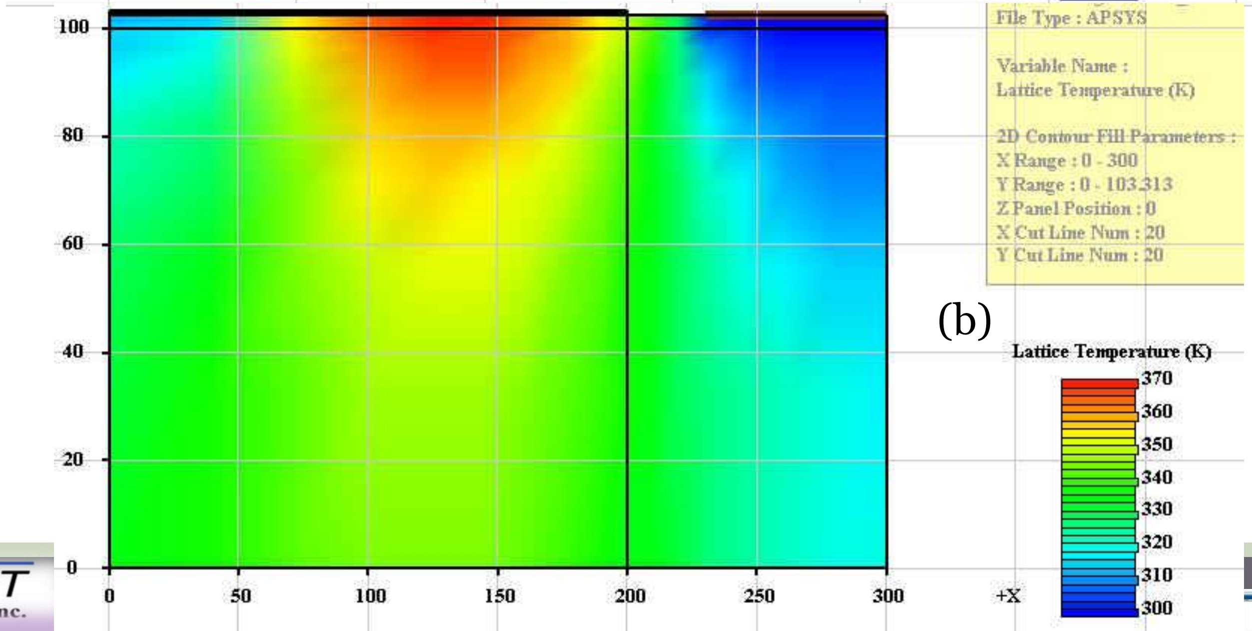
A Common InGaN LED



Current crowding and self-heating



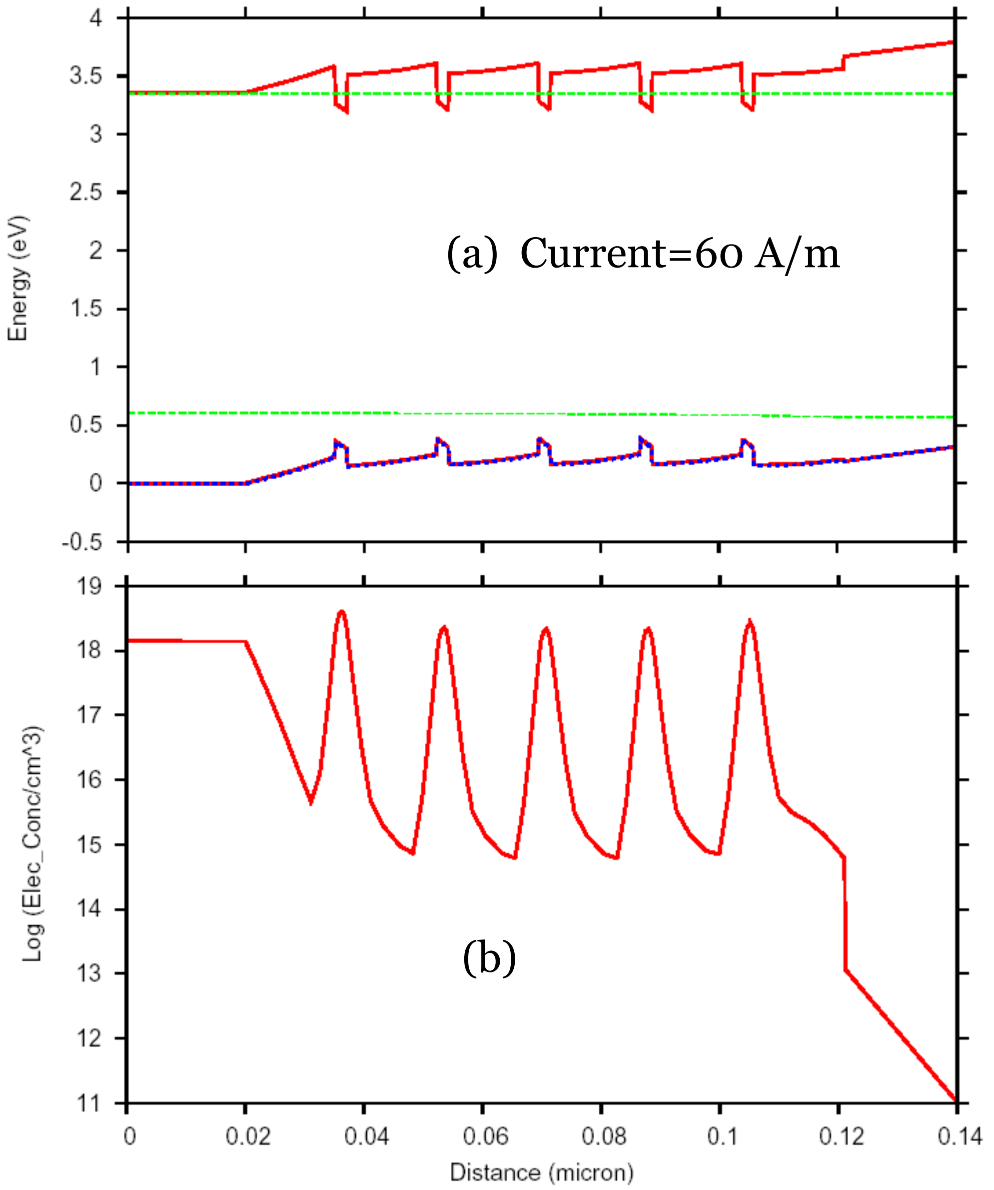




(a) Y-component electron current flow diagram shows vertical current crowding near the top contact. Also, about 30 percent current overflow leakage is observed at high injection.

(b) Temperature distribution shows heating occurs mostly between the electrodes.

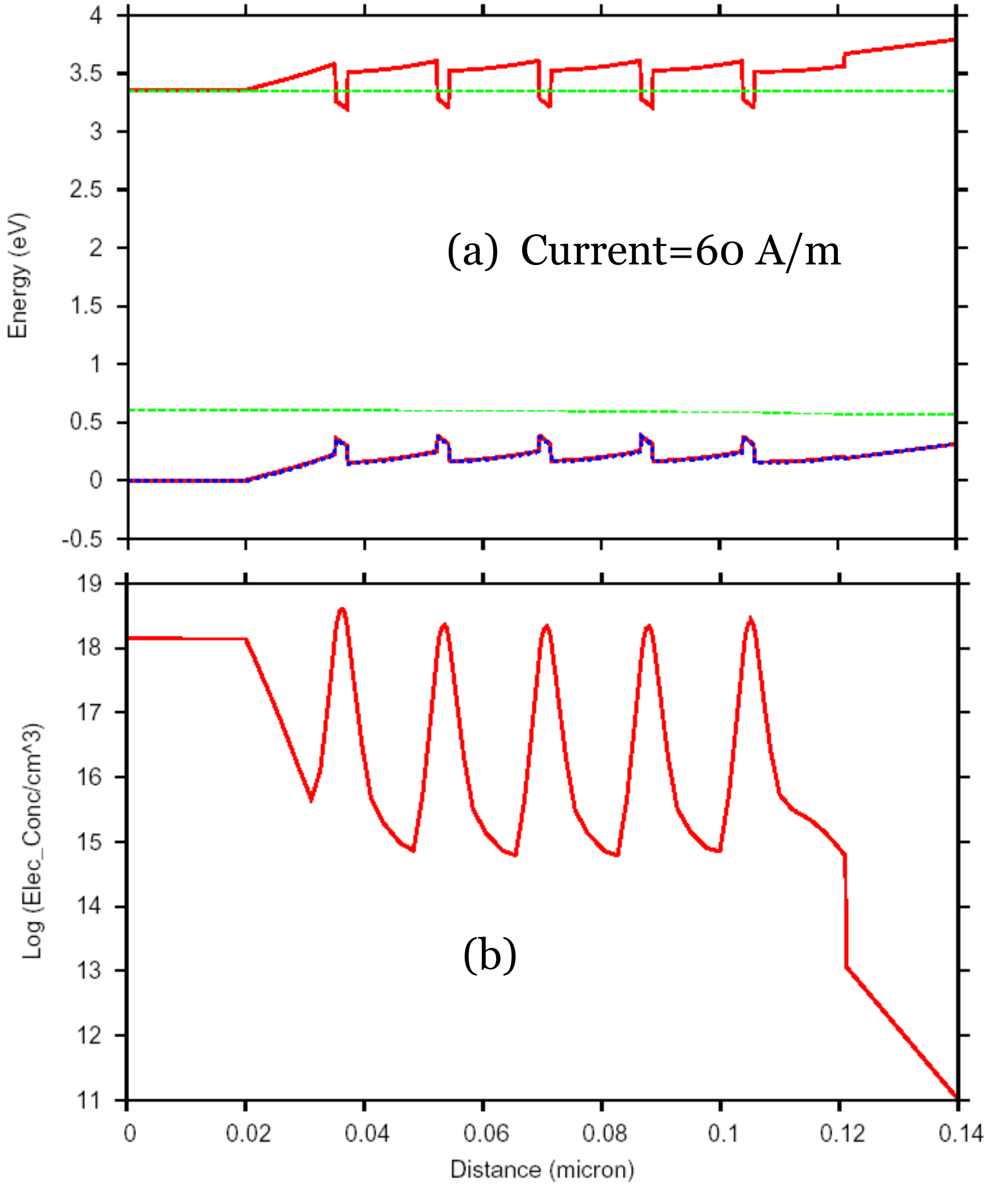
Piezo effects



(a) Band diagram of MQW region with Piezo surface charge. Potential distortion can be reduced if well width is small.

(b) Distribution of electron concentration corresponding to the above band diagram.

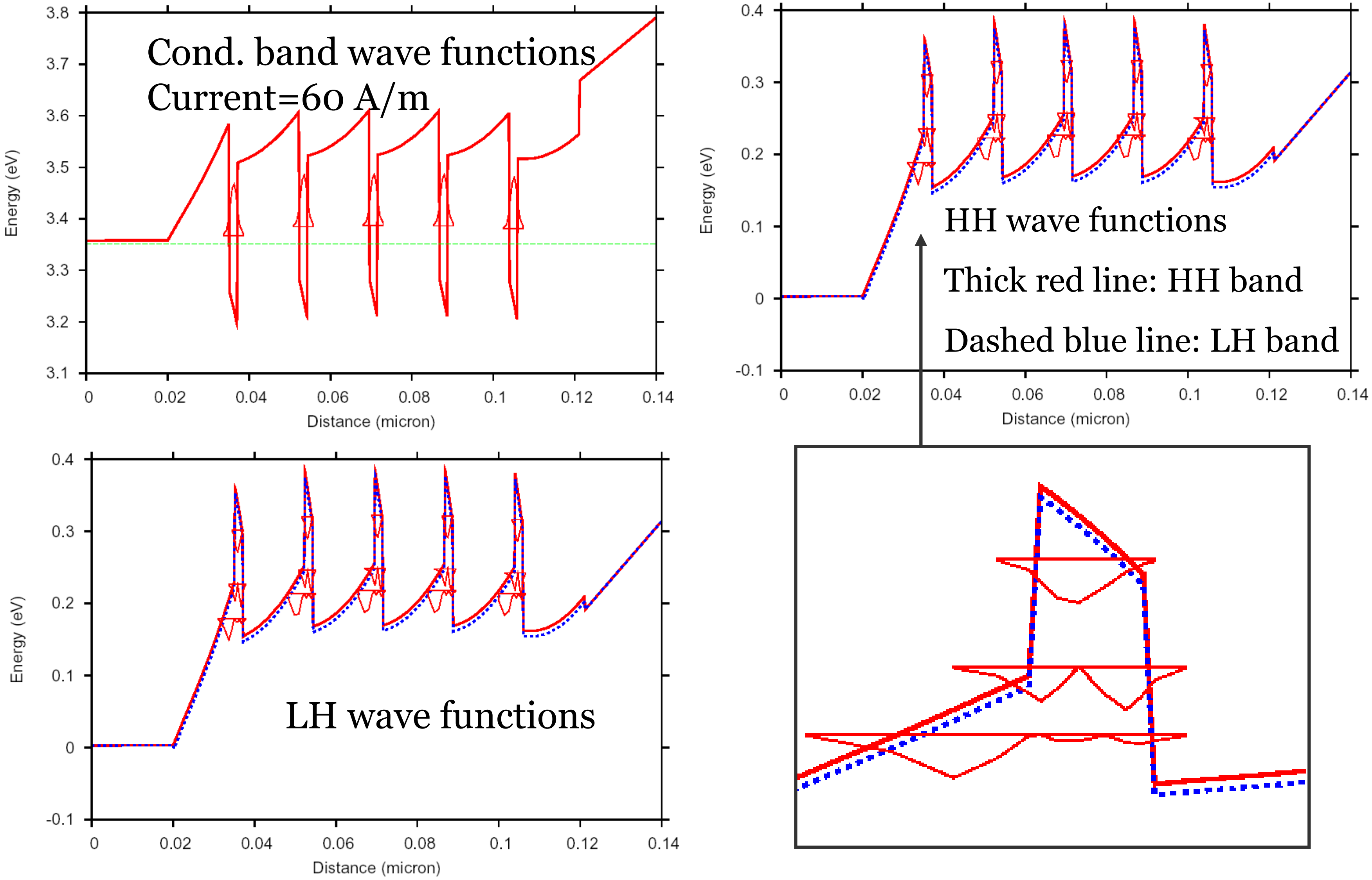
Piezo effects



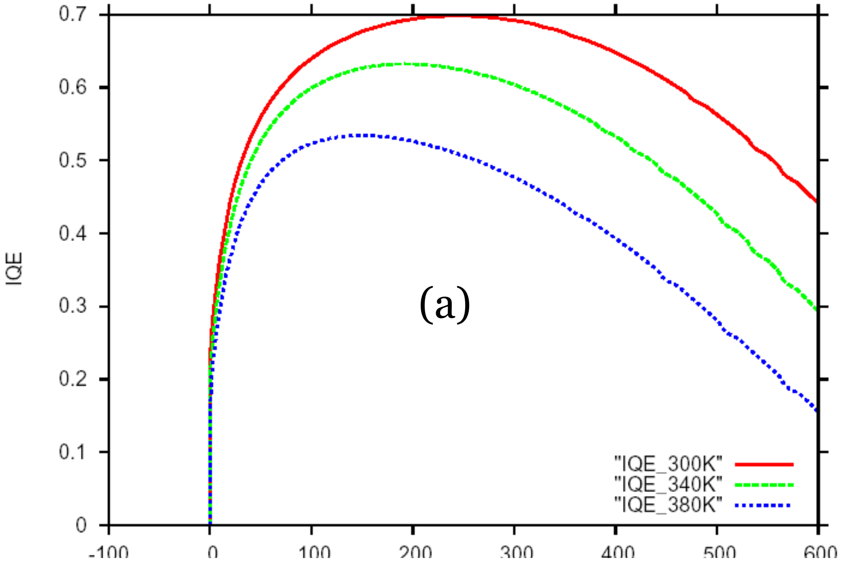
(a) Band diagram of MQW region with Piezo surface charge. Potential distortion can be reduced if well width is small.

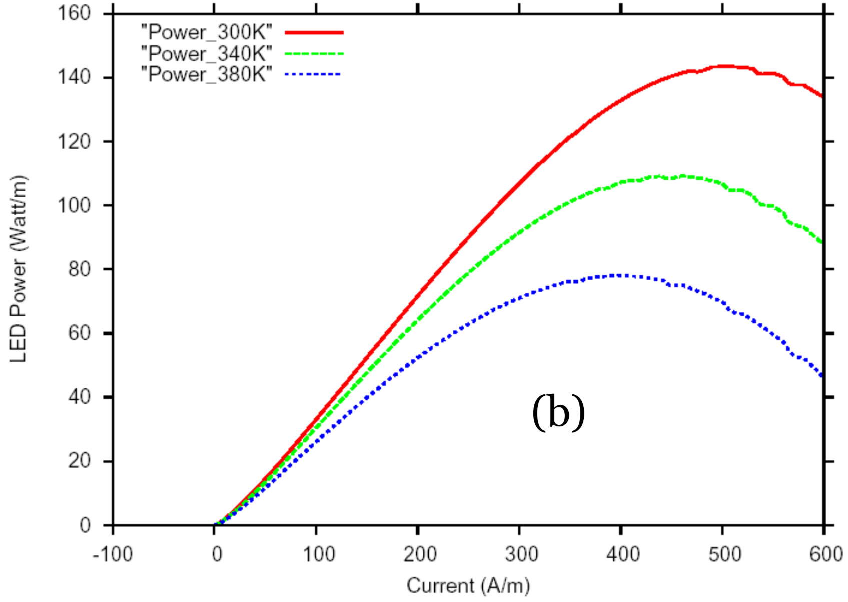
(b) Distribution of electron concentration corresponding to the above band diagram.

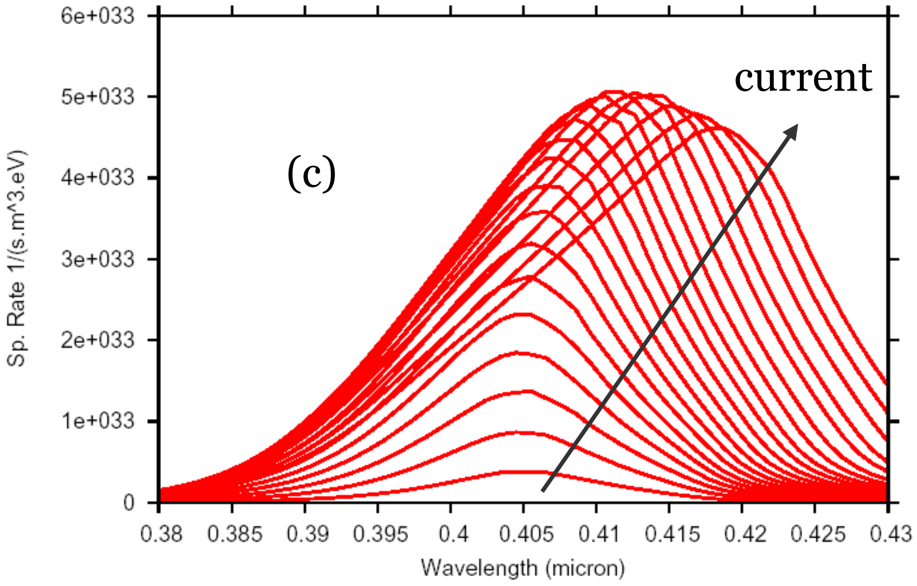
A close look at wave functions



Performance





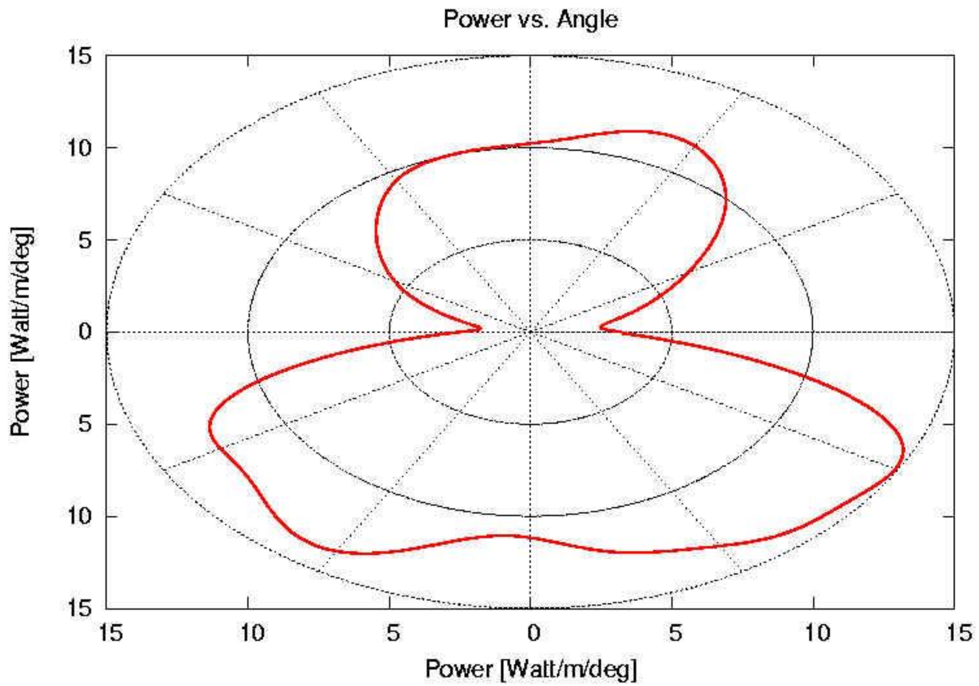


(a) IQE showing decrease at high injection condition due to thermal reduction of spontaneous emission rate.

(b) Thermal roll-off of P-I curve estimated from ray tracing extraction of optical power.

(c) EL(300K) spectrum from zero to 600 A/m, with 30 A/m increment per curve. Please note that the initial blue shift is due to band-filling while the red shift at high injection is due to bandgap reduction at higher temperatures.

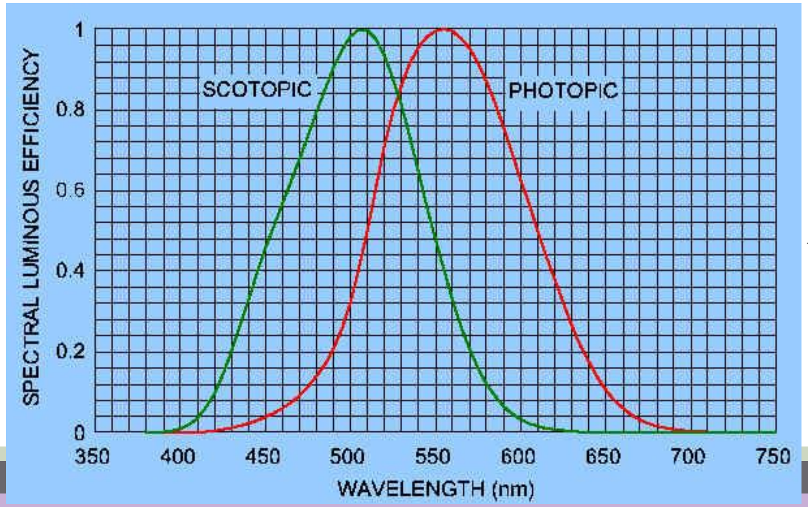
Power vs. angle from ray-tracing



Conversion of 2D raytracing power density into Lumen:

Lumen=(Watt/m/degree) x (180/pi) x (LED length) x (1/2) x (683) x (Spectral luminous efficiency)

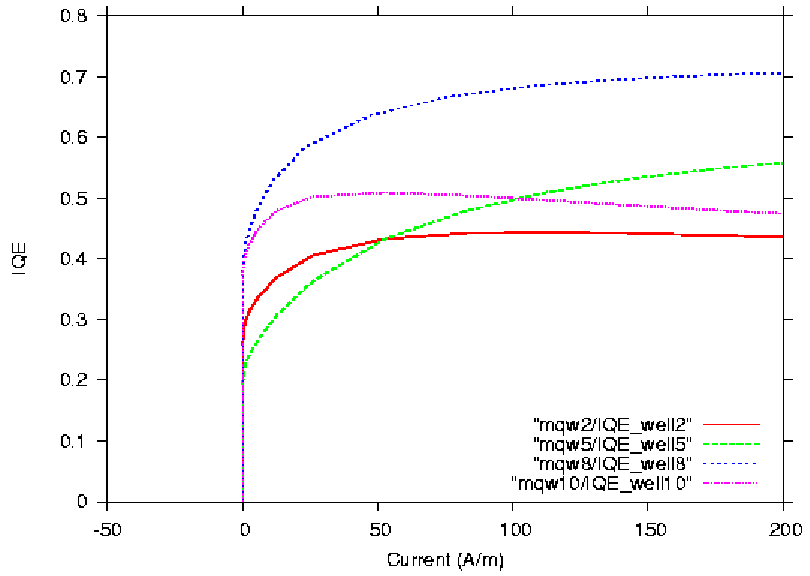
Factor of ½ above ensures integral over 4pi stereo-radian equals the total light source power.

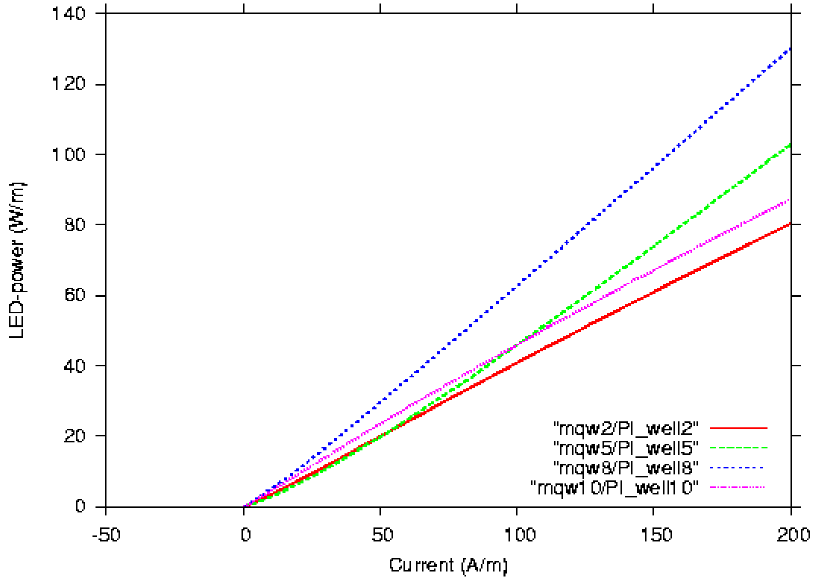


Photopic=day time eye sensitivity adapted data

Scotopic=night time eye sensitivity adapted data

Quantum well number variation





MQW region is isolated as a 1D structure for a special study of quantum well variation.

LED performance versus well depends on competition of various loss mechanisms: overflow, non-radiative and light extraction.

Accurate simulation depends on inclusion of a number physical models: piezo charge, quantum transport, interband optical transition and light extraction.

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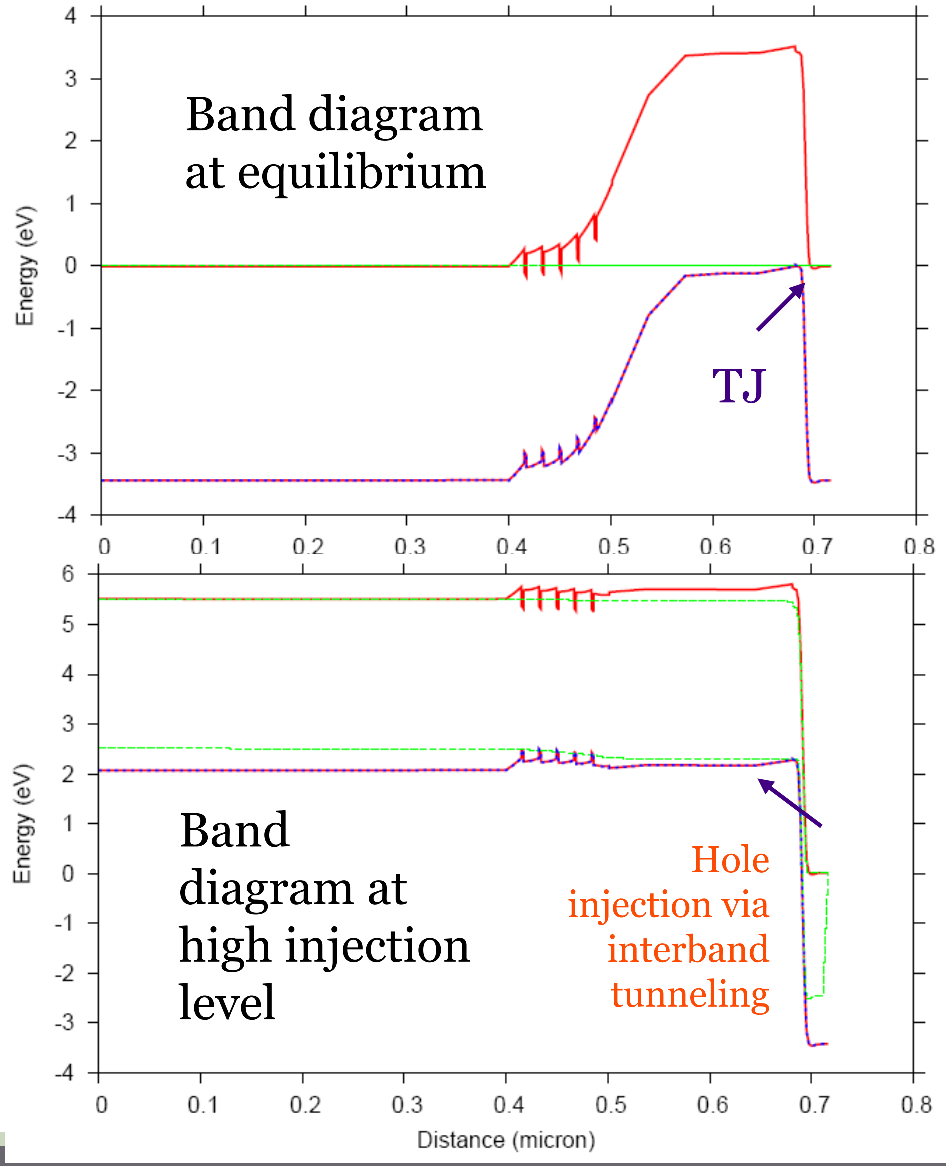
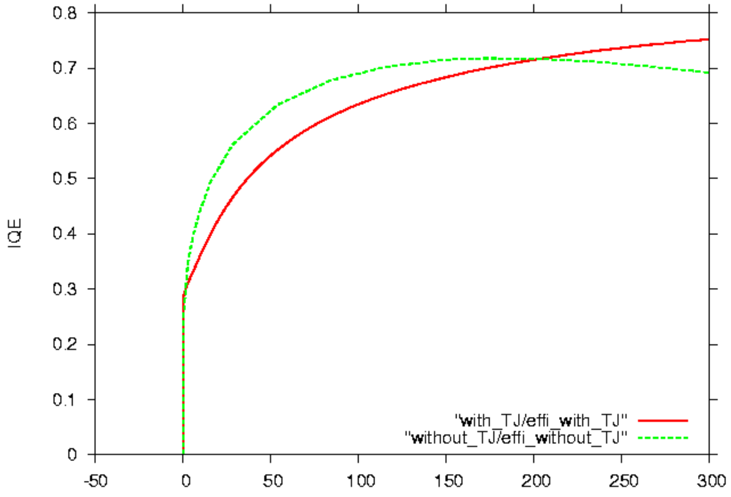
Tunnel junction contact design

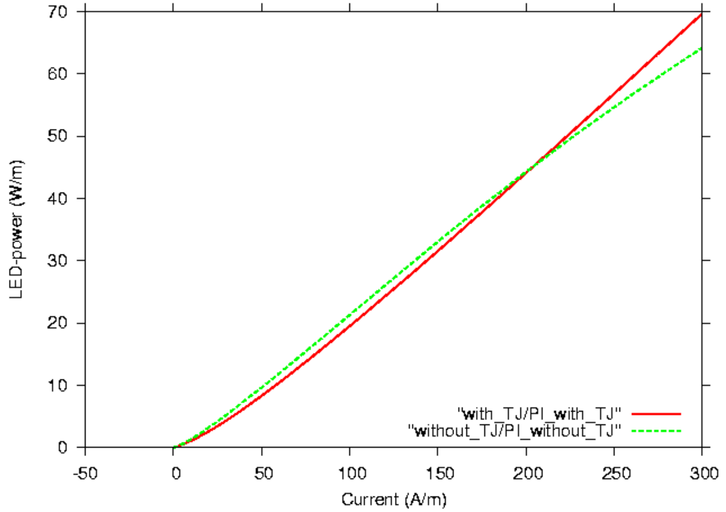


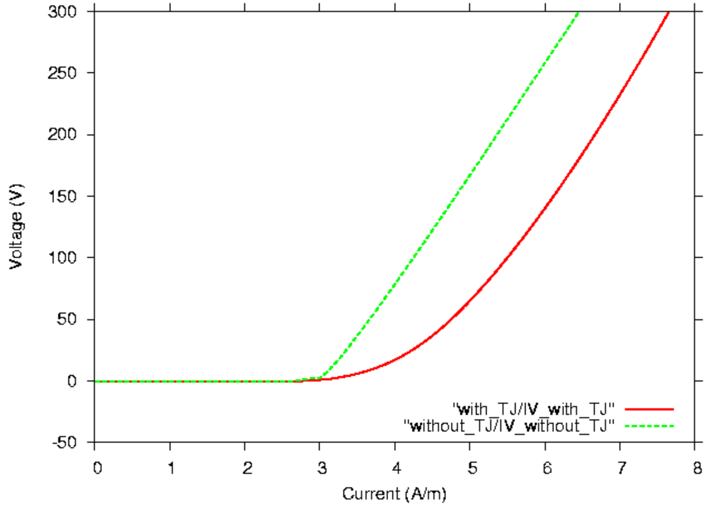
p-GaN's conductivity is low and thus carrier crowding is a limiting factor in GaN LEDs. Tunnel junction (TJ) can be used to supply holes efficiently to the p-type region by electron tunneling effects. S.R. Jeon et al., "Lateral current spreading in GaN-based light-emitting diodes utilizingtunnel contact junctions," Appl. Phys. Lett. vol. 78, No. 21, p3265, 2001

Tunnel junction enhances carrier spreading



Compared with conventional LED, the turn-on voltage is higher with TJ. Note that at high injection, the IQE of with_TJ device does not roll over, because TJ also acts as electron blocking layer





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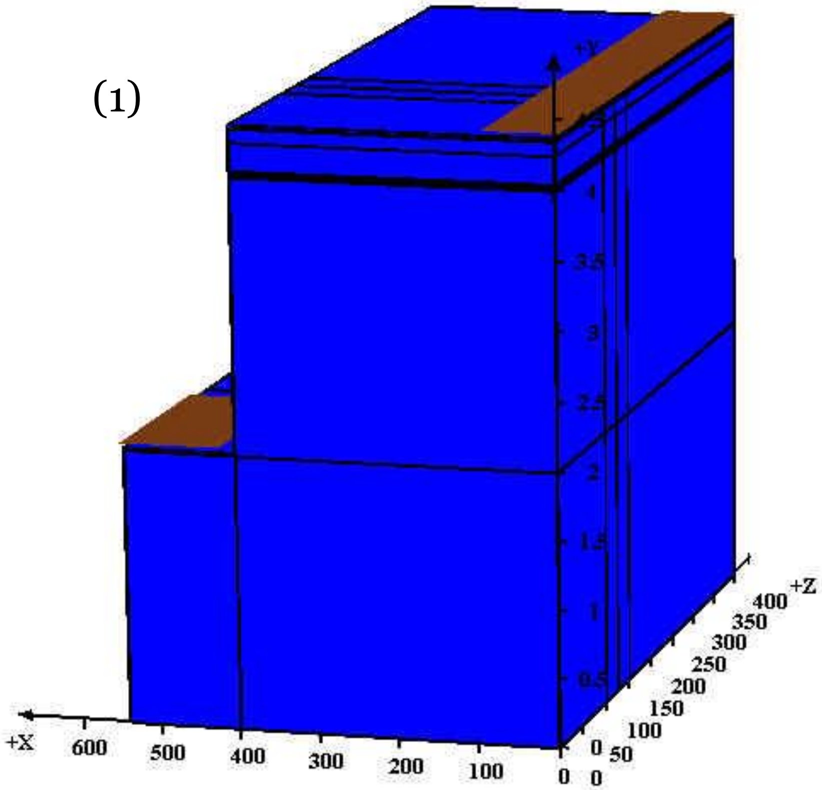
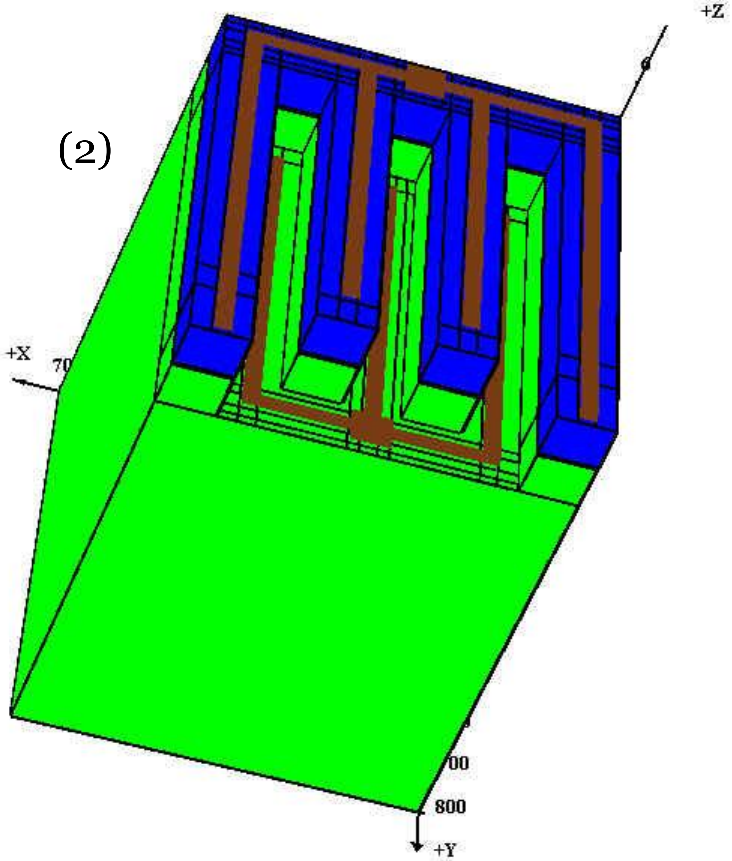
Two 3D configurations

(1)



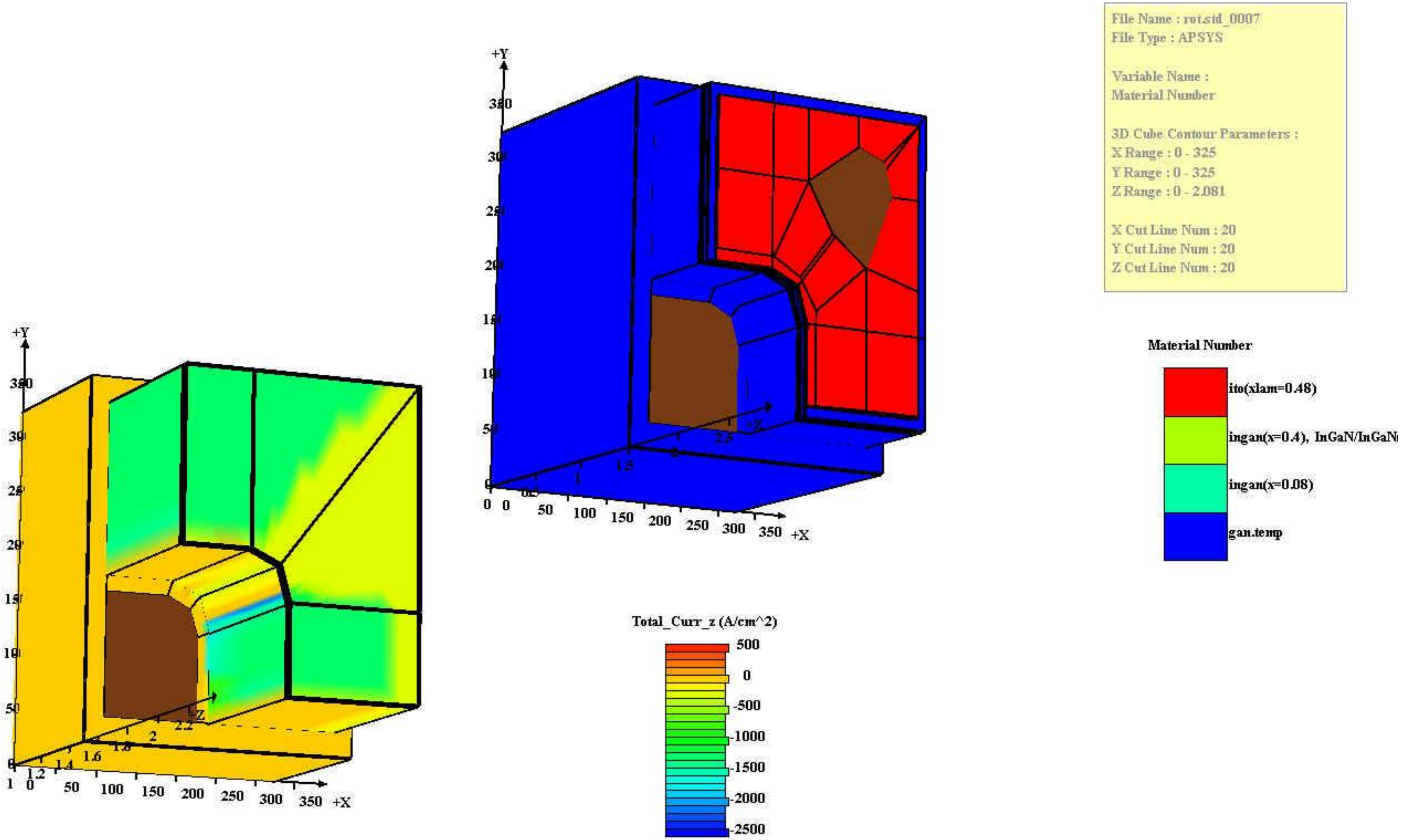
(2)



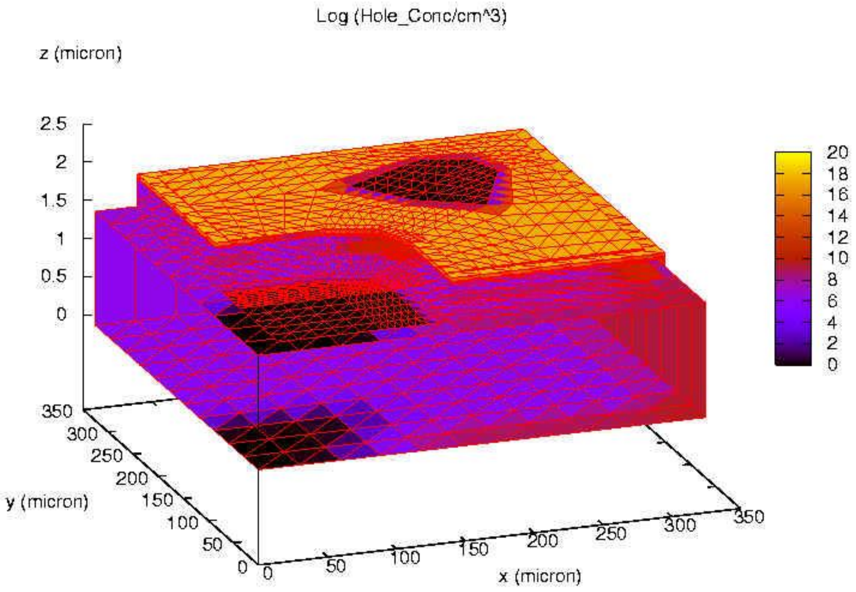
(1) Quantum wells parallel to x-z plane. Advantages: easy to convert 2D simulation set up files into 3D; More detailed analysis of physical variable over x-y planes.

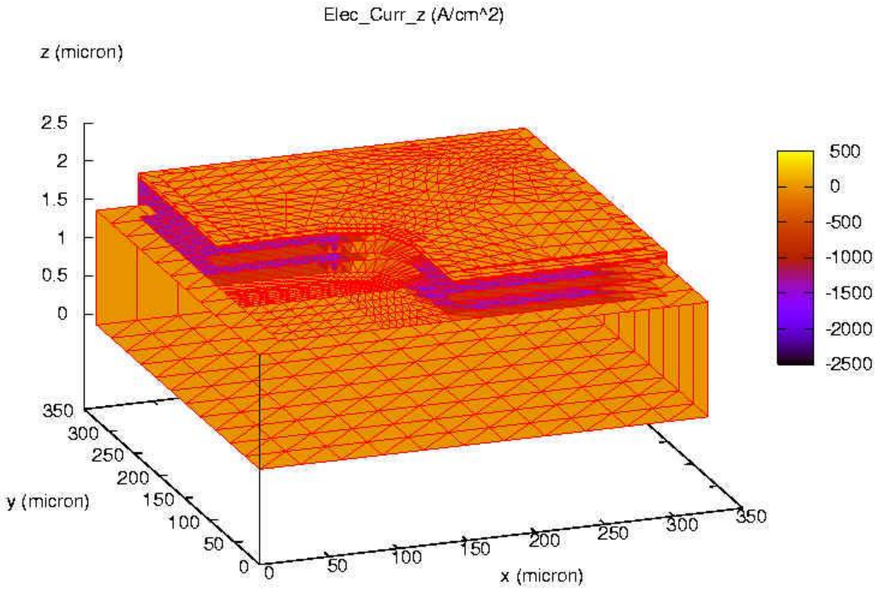
(2) Quantum wells parallel to x-y plane. Advantages: easy to set up structure with complicated geometry within single layers. More efficient numerically to compute spreading effects parallel to layers, assuming the same total number of mesh points.

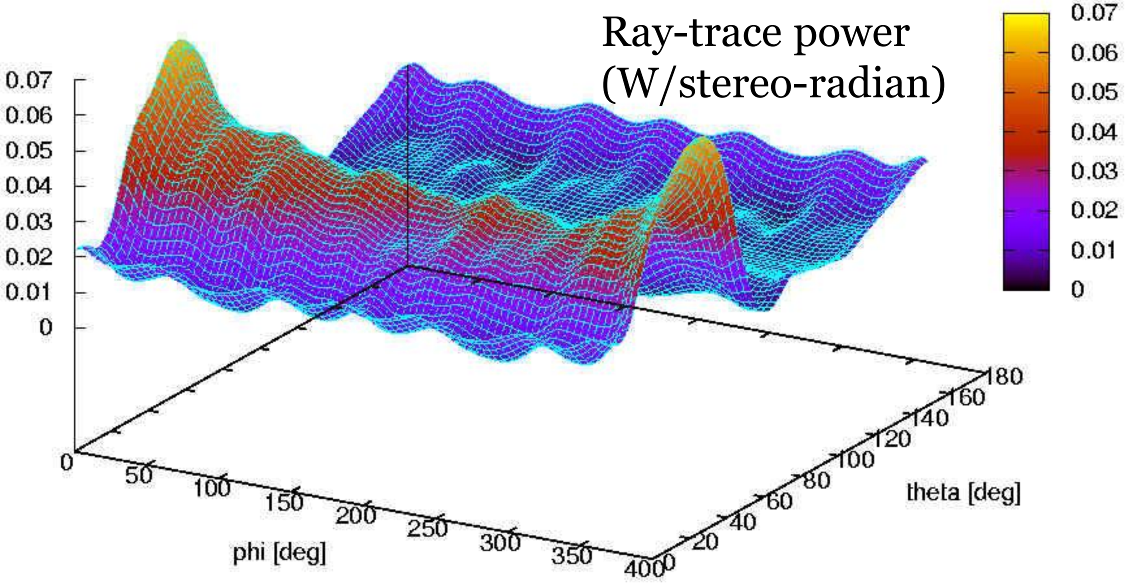
LED with ITO electrode

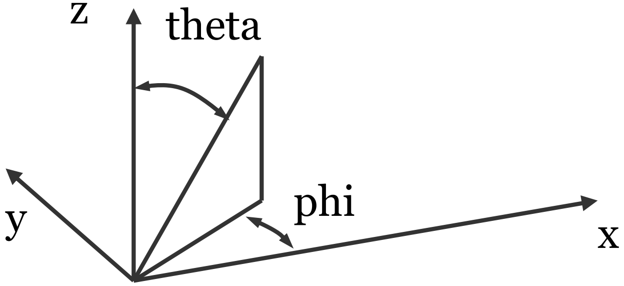


More 3D results



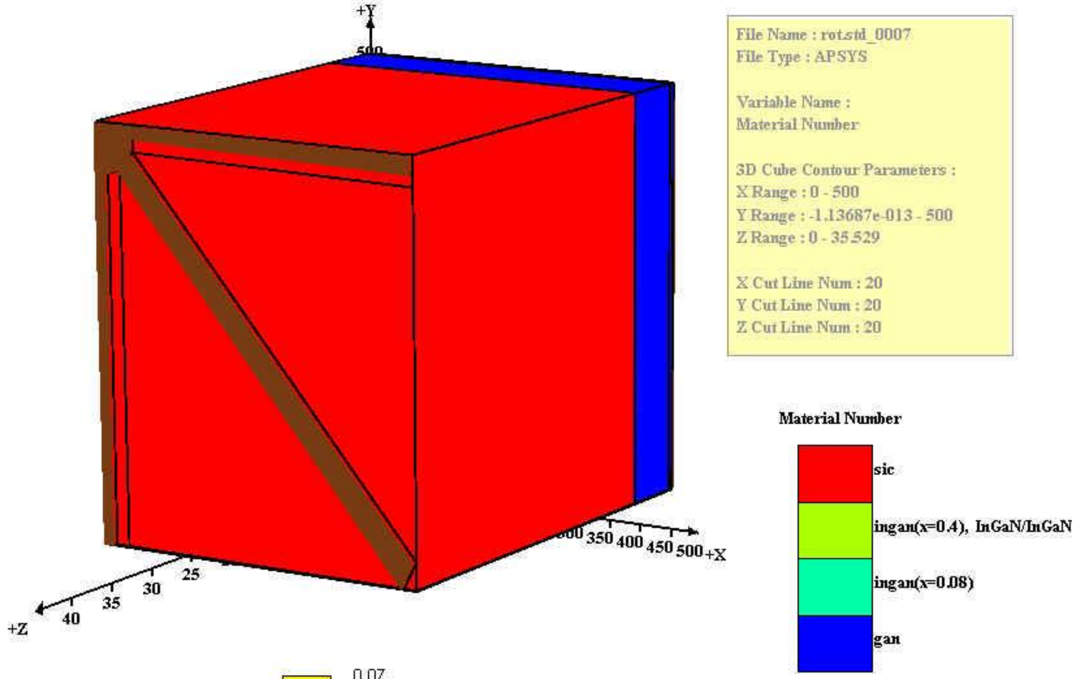




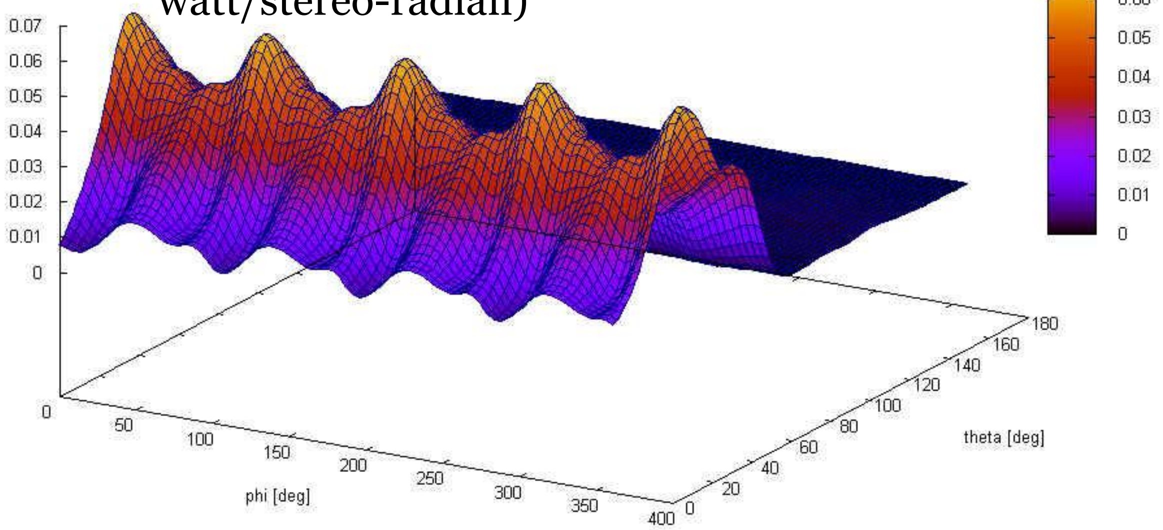


3D mirror boundaries

LED with star-shaped electrode: simulate only ¼ of device with ray-tracing mirror boundaries at x=0 and y=500 um.



3D ray-tracing power including mirror images (in watt/stereo-radian)



➔ Substantial savings in computation time achieved using mirror boundaries since computation cost scales non-linearly with mesh size.

LED Capability Summary

- The APSYS software has incorporated numerous advanced modules for GaN based LED simulation and design.
- Rigorous theoretical approaches may be used in all levels of modeling ranging from many-body quantum well theory to 3D transport and ray-tracing.
- Flexible simulator construction enables various modules to be turned on/off depending on design requirements.
- Self-consistent integration of various modules within APSYS enables all-in-one simulation approach.

Contents

Advanced Topics

- Modeling dislocations and V-shaped pits
- Multiple quantum barrier analysis
- Hot Auger carrier non-local transport model

Introduction: effects of V-pit dislocation

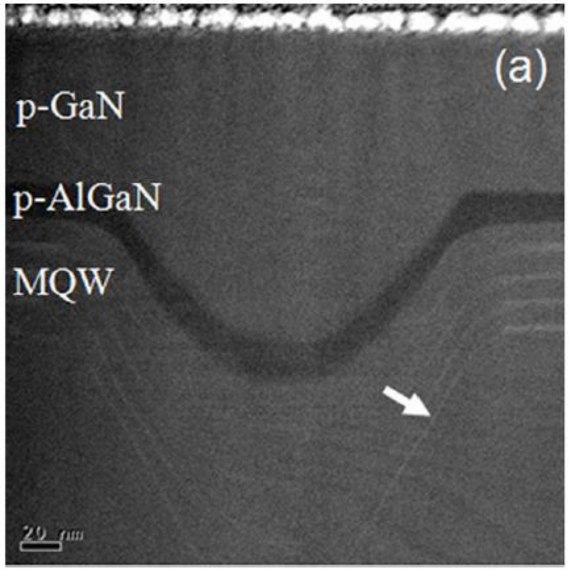
Distortion of MQW makes the QW width smaller and effective bandgap larger at the pit.

Emission at shorter wavelength at the V-pit.

Expulsion of electrical current away from the V-pit to suppress non-radiative recombination of LED.

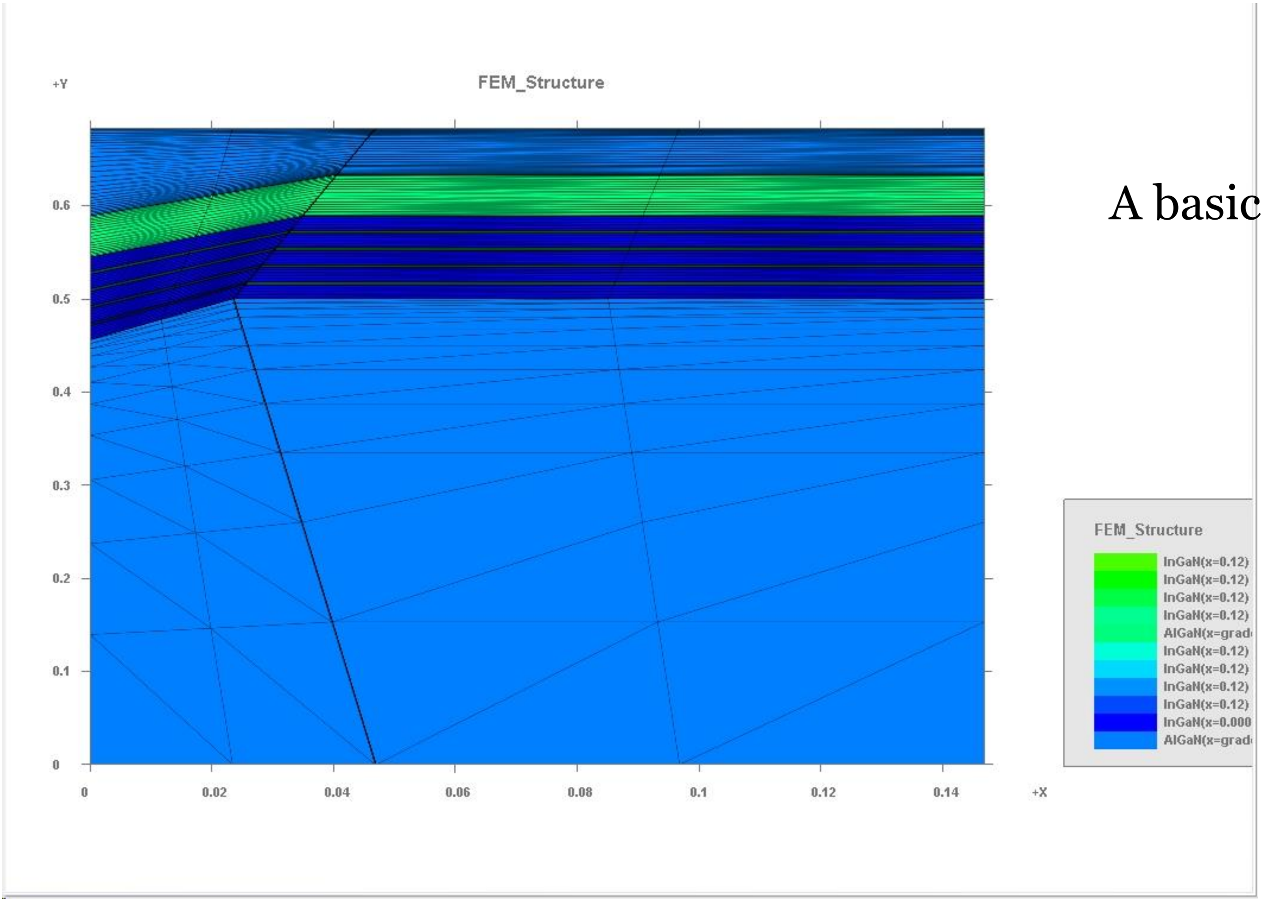
Appl. Phys. Lett. **102**, 251123 (2013)

251123-2 Han *et al.*



Upgraded LayerBuilder (Ver. 2015 or later)

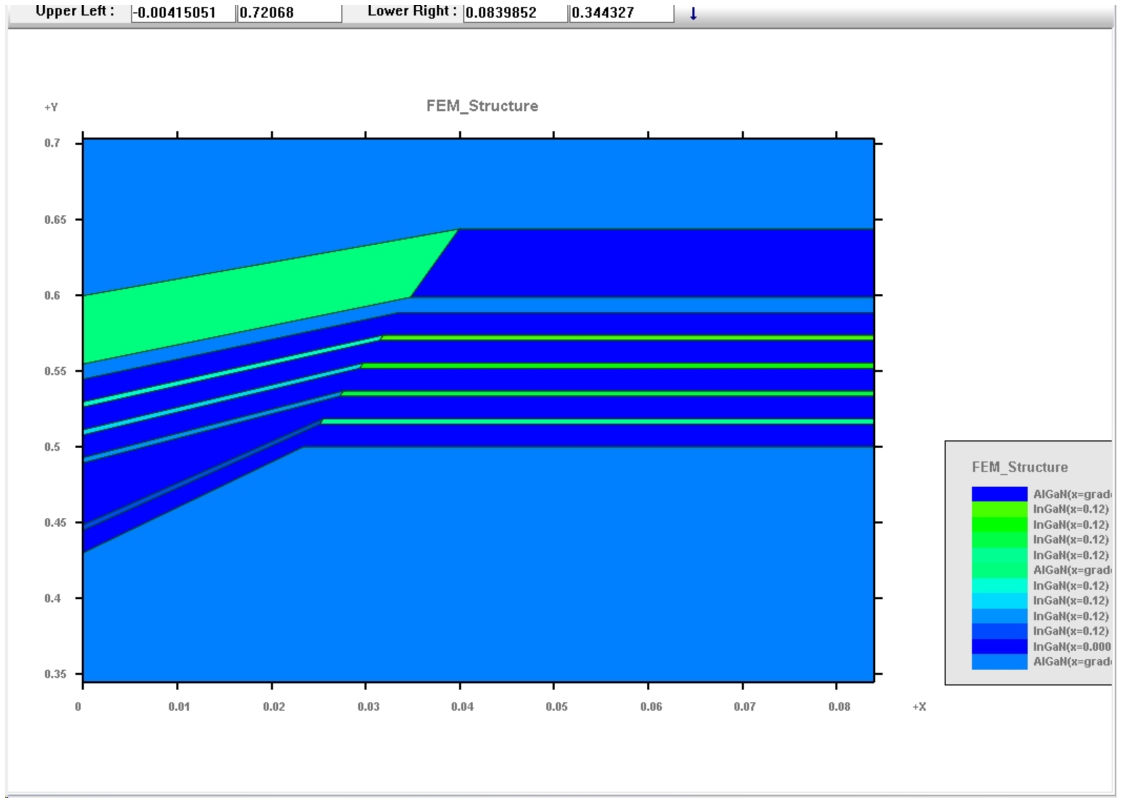
Makes it easy to set up mesh for the MQW within the V-pit without compromising celebrated models such as quantum transport, quantum confinement, k.p-based band structure, radiative recombination models, etc…



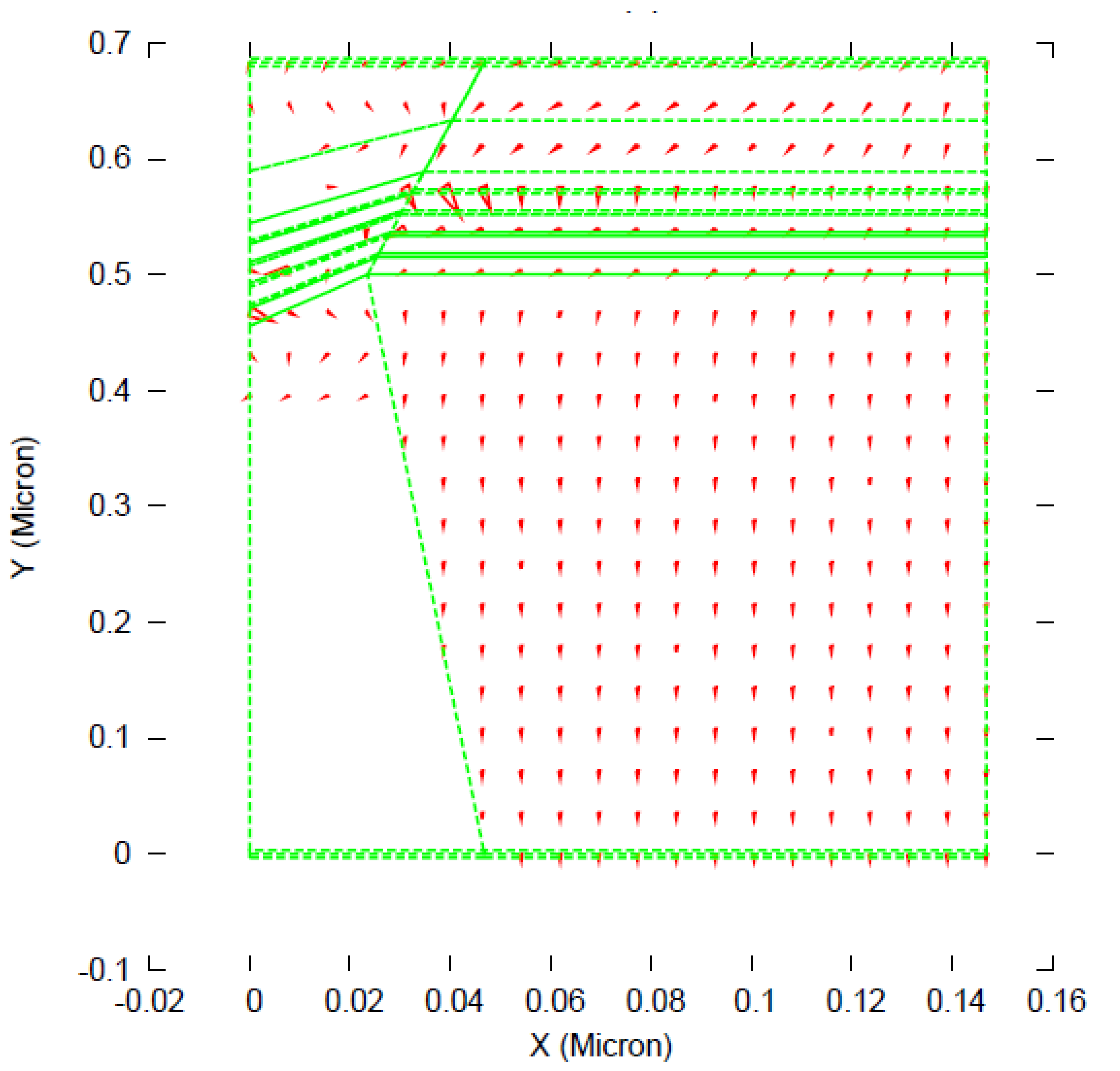
A basic V-pit example.

A more complicated V-pit example

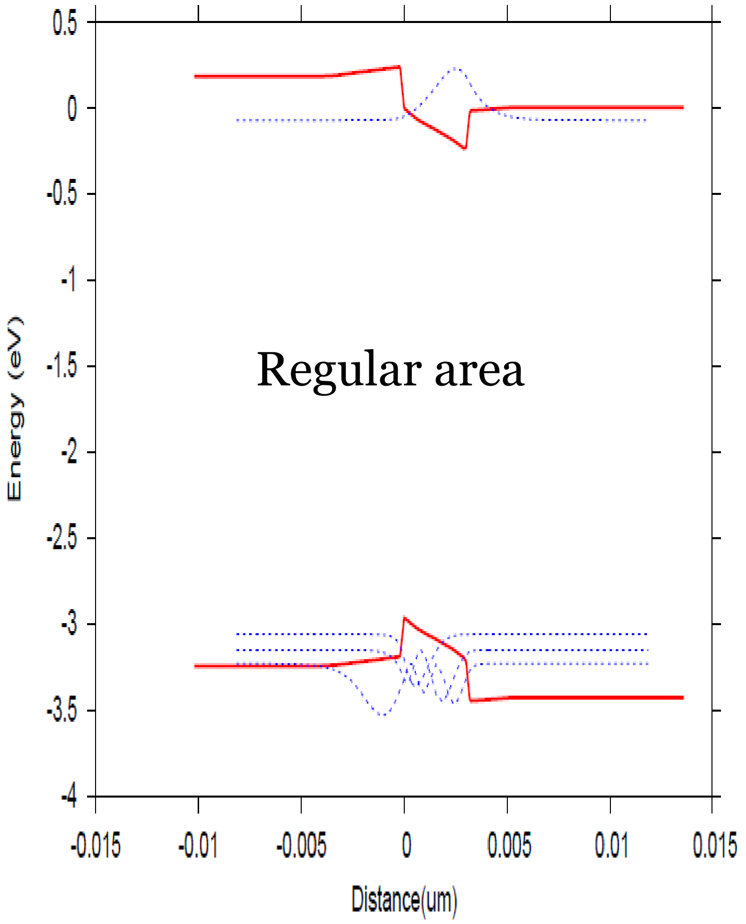
It is possible to use multiple columns to construct a V-pit with smooth shape.
Also possible to use CSUPREM to deposit and etch to form such shapes.

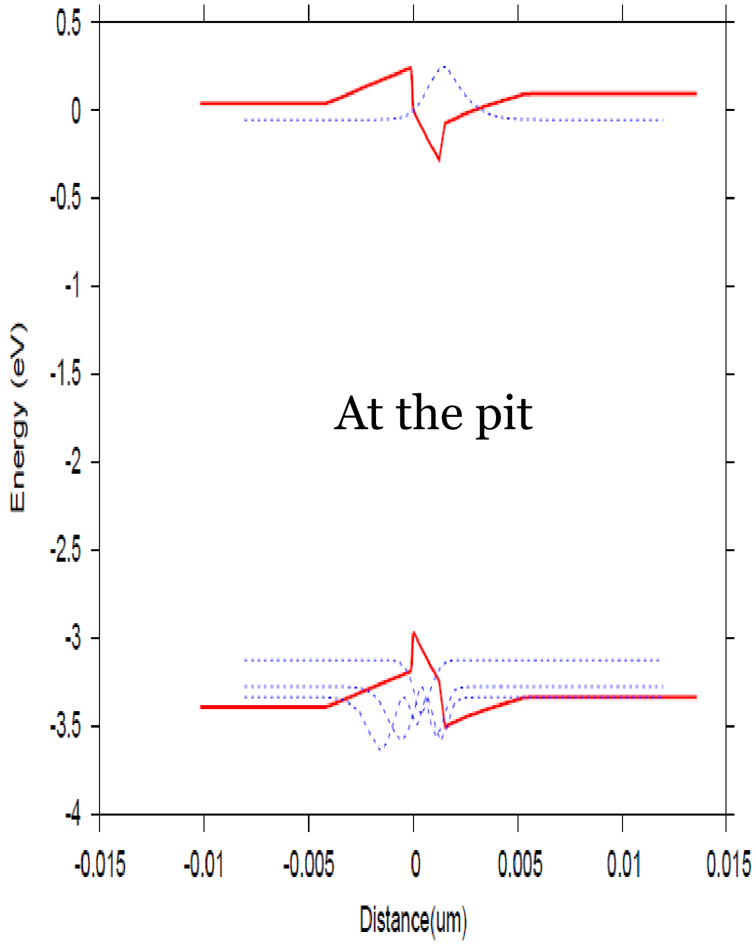


Distribution of current flow:

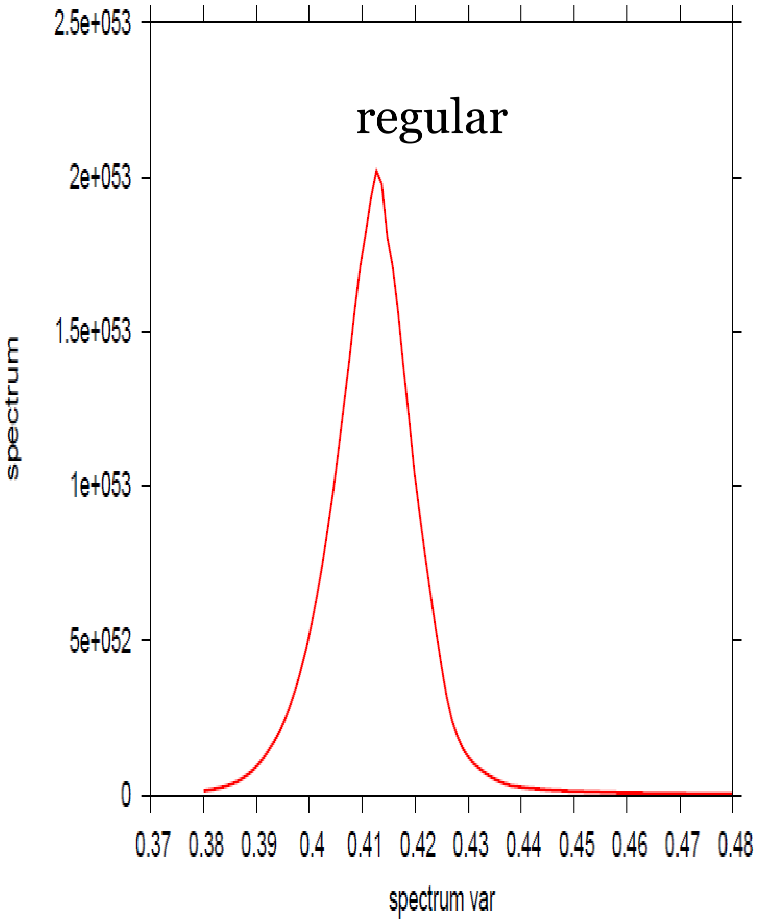


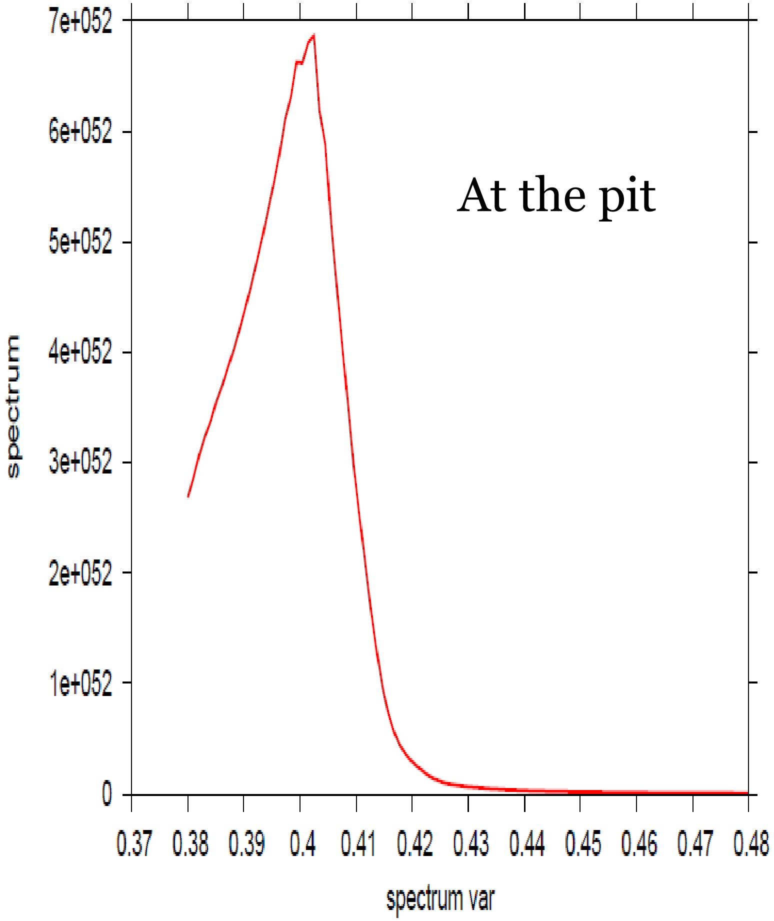
Different quantum confinement at the pit



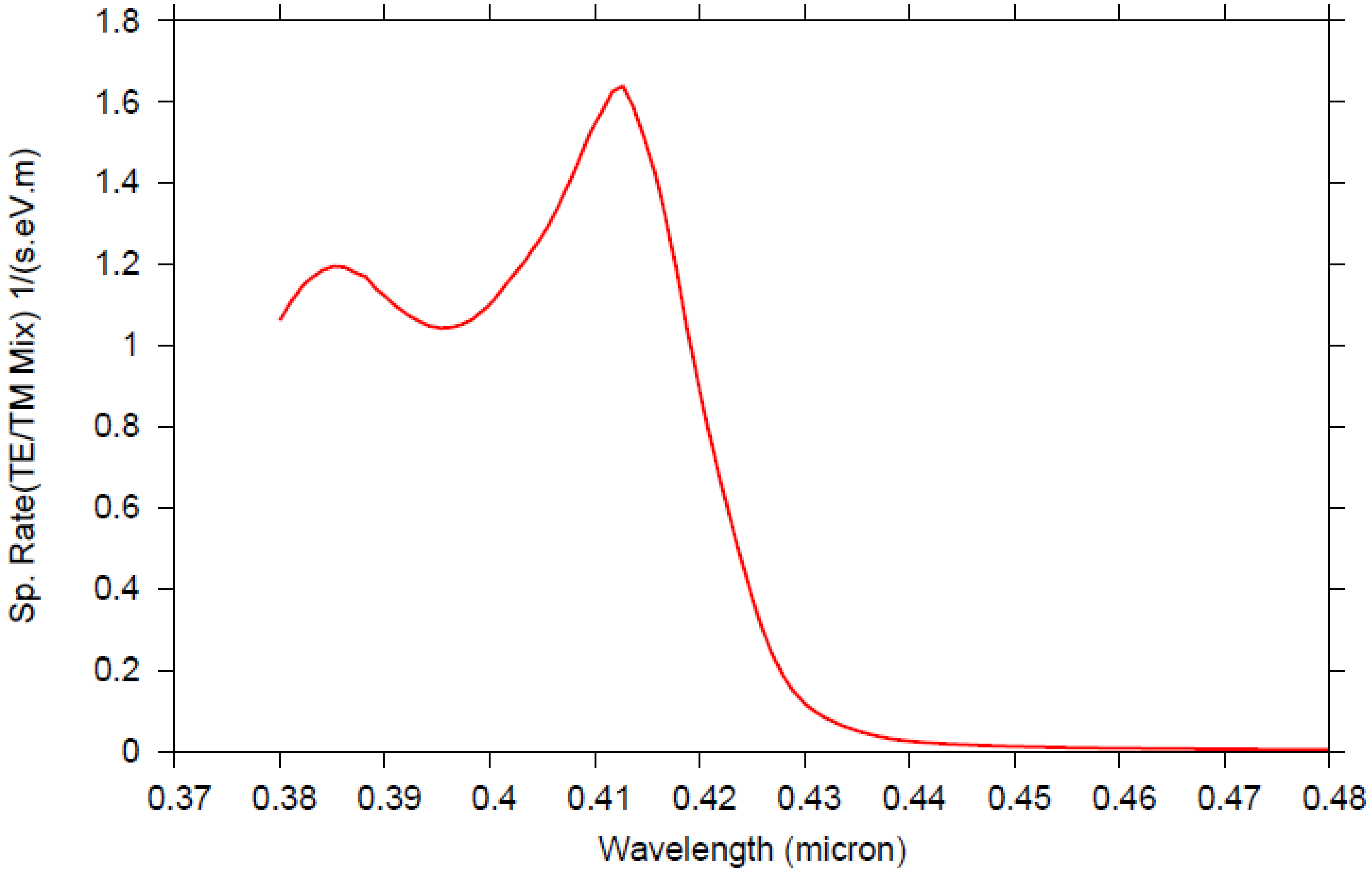


Different spectrum at the pit





Composite LED spectrum for the simulated area



Dislocation Model Summary

More sophisticated model of dislocations with ver. 2015 and later.

All advanced MQW models carried over to QW with arbitrary orientation.

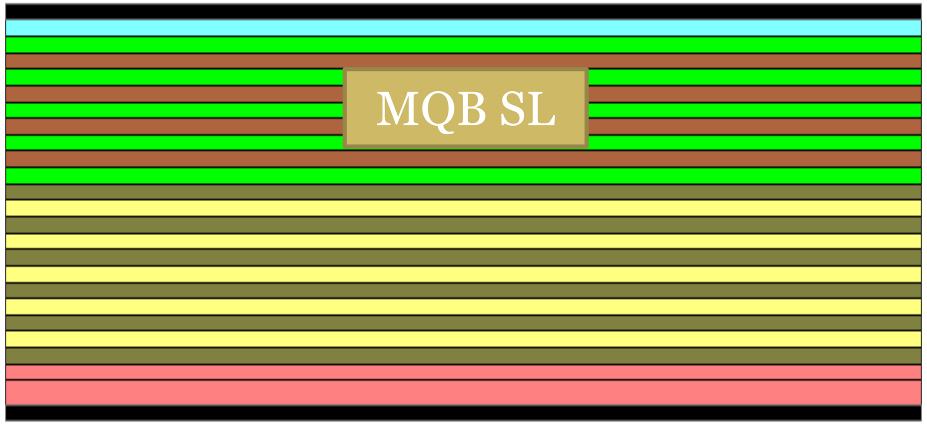
Very convenient to build V-pit using upgraded LayerBuilder.

Advanced Topics

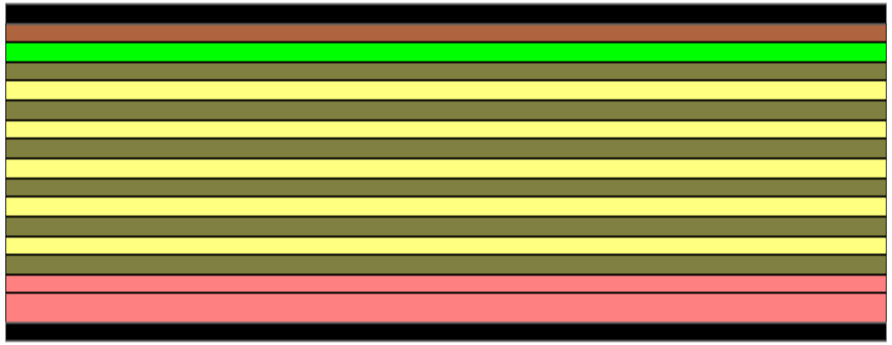
- Modeling dislocations and V-shaped pits
- **Multiple quantum barrier analysis**
- Hot Auger carrier non-local transport model

Structure

With SL



Without SL



MQB tunneling

Tunneling current through MQB SL is calculated by propagation matrix method. This model cuts the barrier potential into piece-wise constant segments.

For segment *j*, the wavefunction is

$$\psi(z) = A_j \exp[\mathrm{i}k_j(z - z_j)] + B_j \exp[-\mathrm{i}k_j(z - z_j)]$$

Boundary conditions relate segment *j* and *j+1*

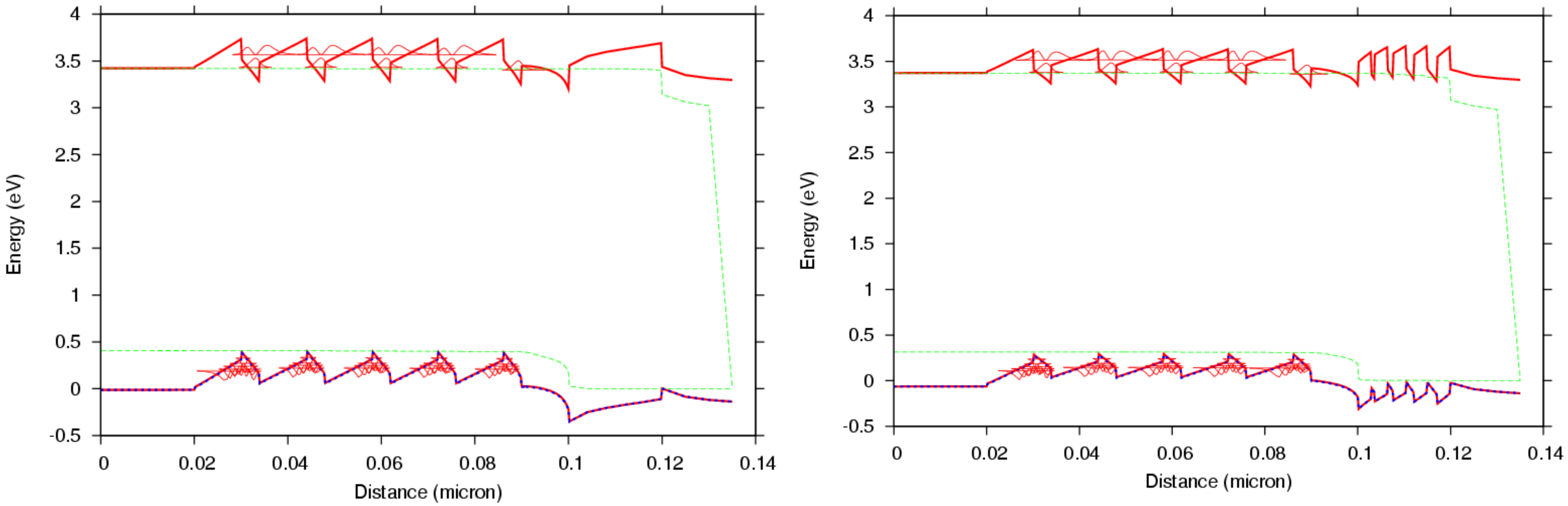
$$\begin{pmatrix} A_{j+1} \\ B_{j+1} \end{pmatrix} = T_{j,j+1} \begin{pmatrix} A_j \\ B_j \end{pmatrix}$$

Repeat for all segments, we get output at *N* with input at *0* segment

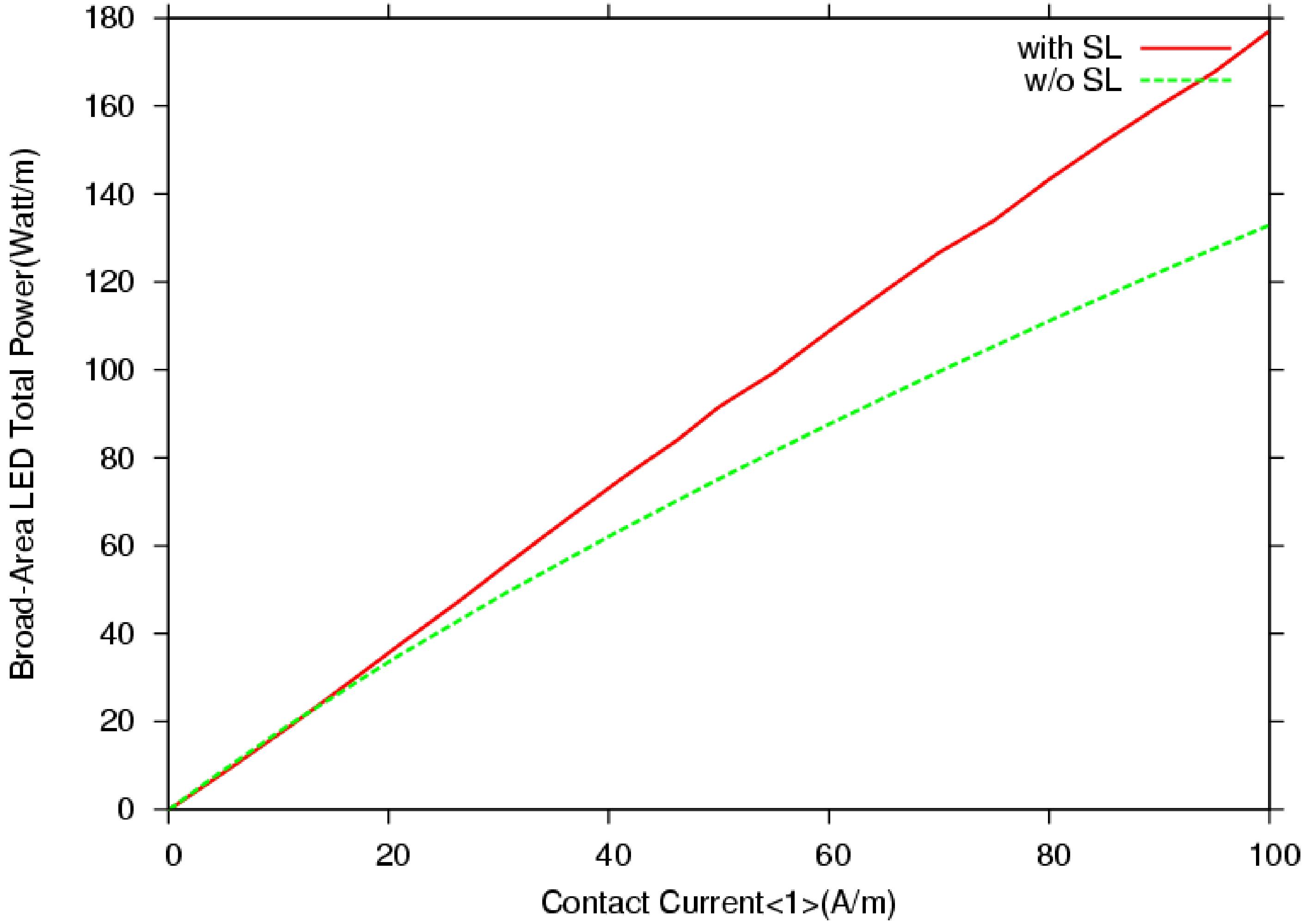
$$\begin{pmatrix} A_N \\ B_N \end{pmatrix} = T_{N-1,N} T_{N-2,N-1} \cdots T_{0,1} \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}$$

$$= \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}$$

Band diagram

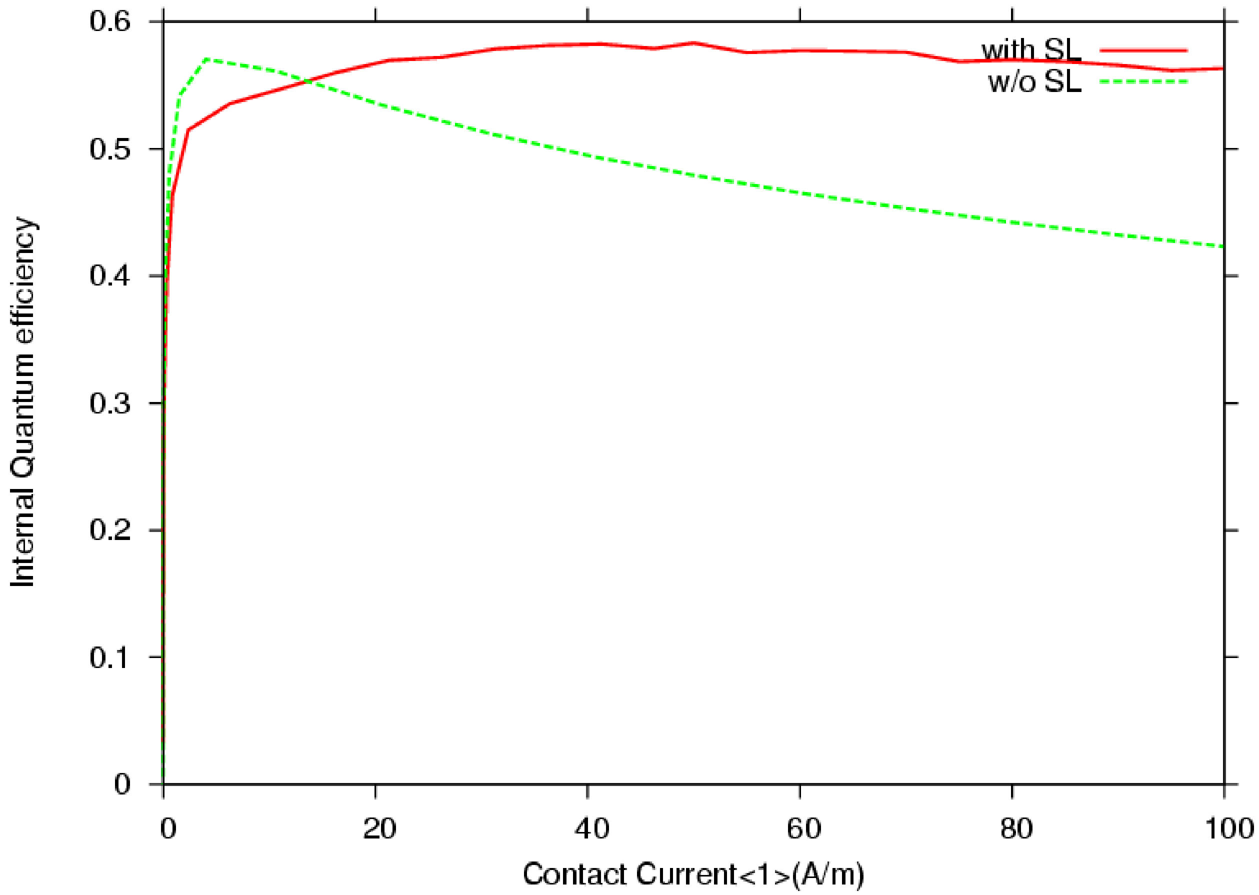


L-I



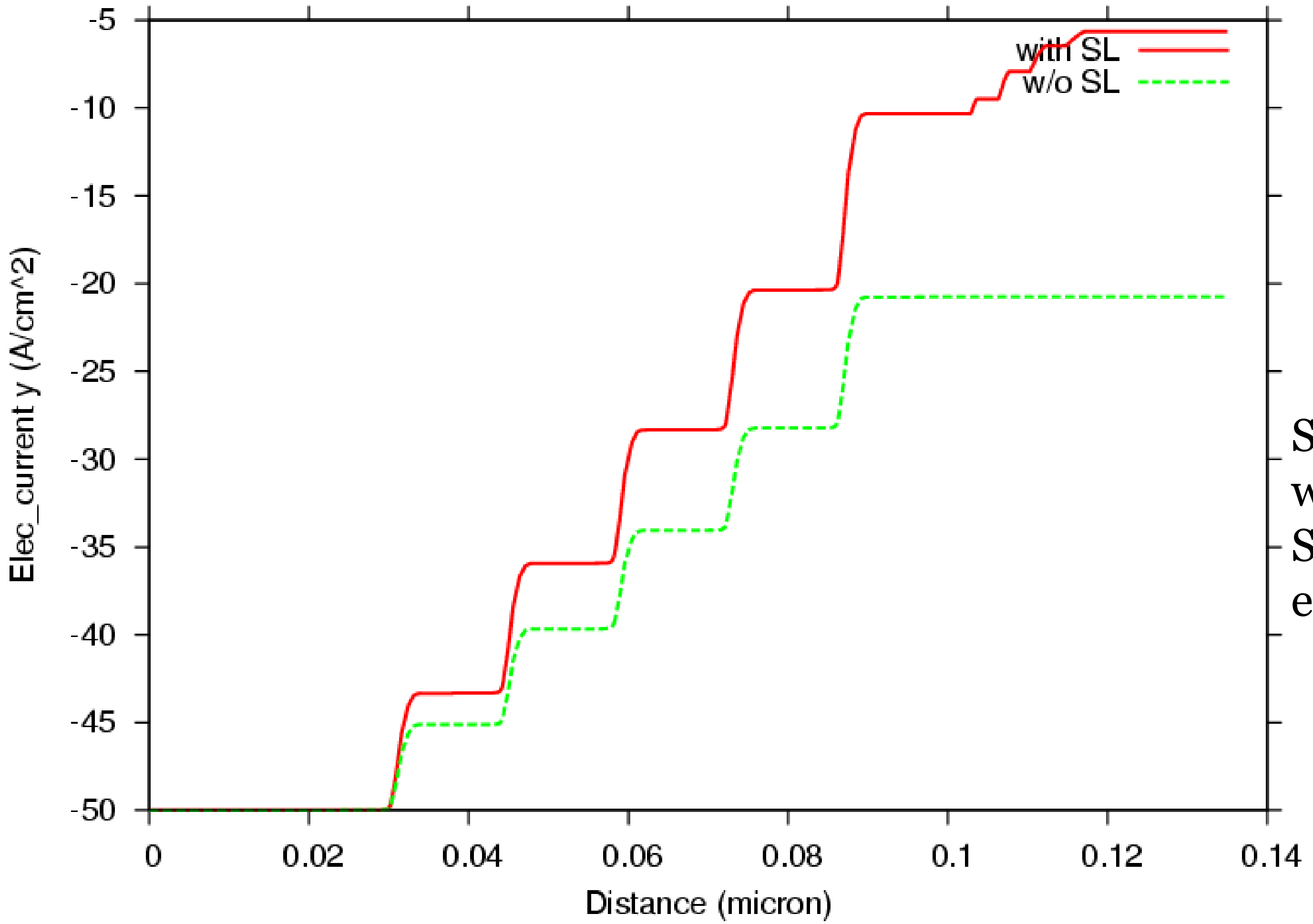
Higher power with SL

IQE



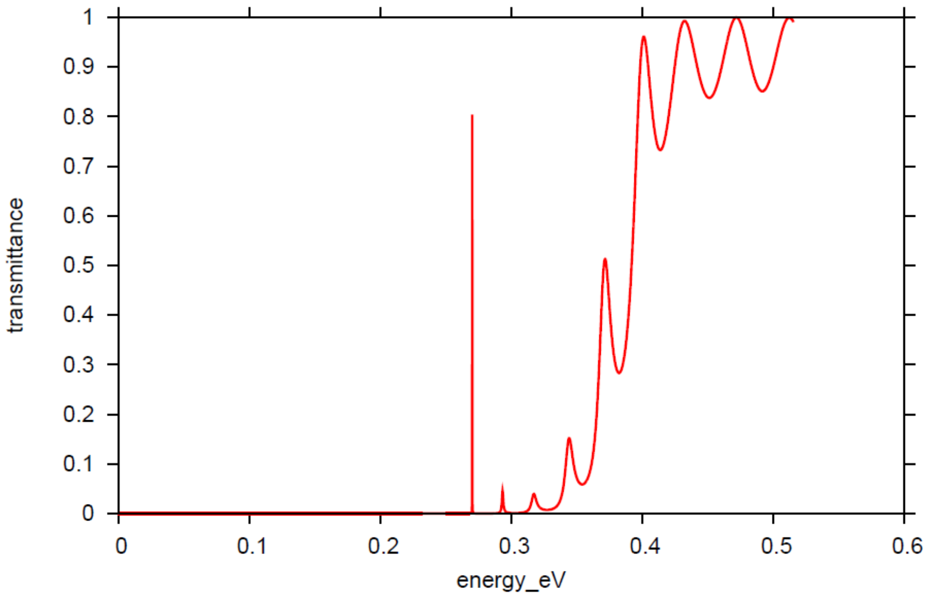
Smaller droop wish SL

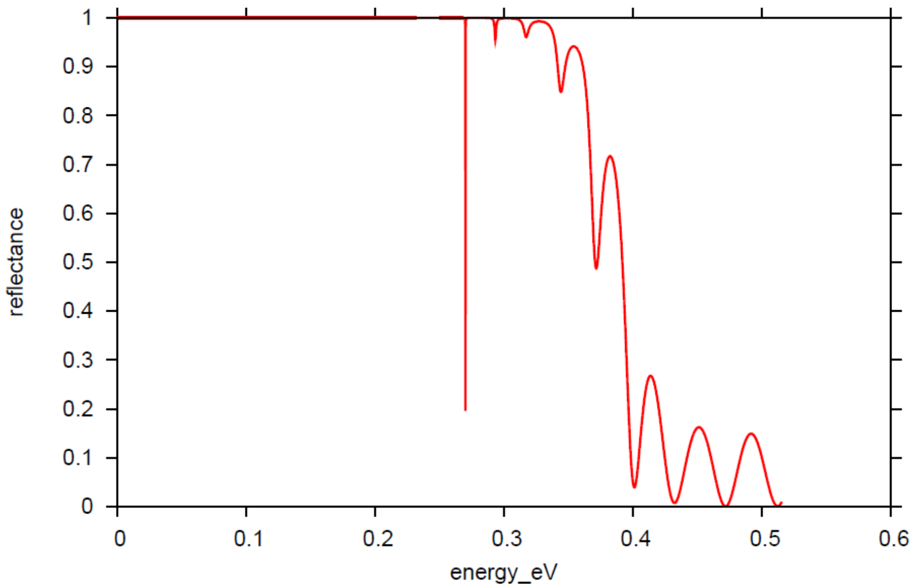
Electron leakage



Smaller electron leakage with SL.
SL is more effective in electron blocking

Tunneling Spectrum





Use of quantum tunneling for MQB leakage
Crosslight-Apsys Simulation

How to design & model Electron blocking layer In MQW GaN LED

- **Correct polarization charge model**
- **Accurate band offset**
- **Energy dependent quantum tunneling**

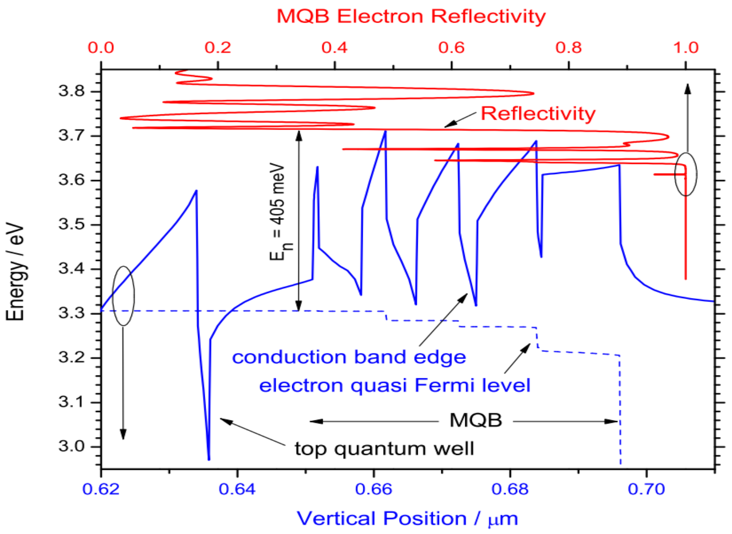


FIG. 4. Conduction band edge profile near the chirped MQB and MQB electron reflectivity spectrum simulated at 400 A/cm^2.

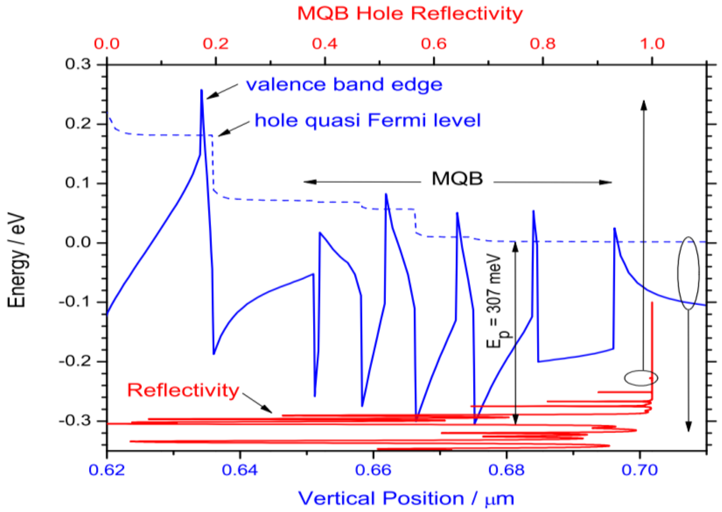


FIG. 5. Valence band edge profile near the chirped MQB and MQB hole reflectivity spectrum simulated at 400 A/cm^2.

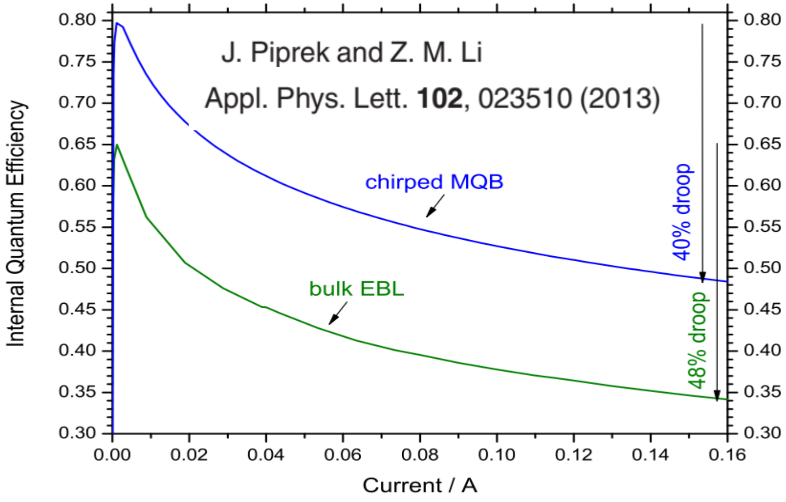


FIG. 2. Calculated internal quantum efficiency vs. current. The efficiency droop is measured relative to the peak efficiency. The maximum current density is 400 A/cm^2.

Conclusion on MQB

- MQB blocks electron leakage more efficiently by effectively increasing the potential barrier of electron.

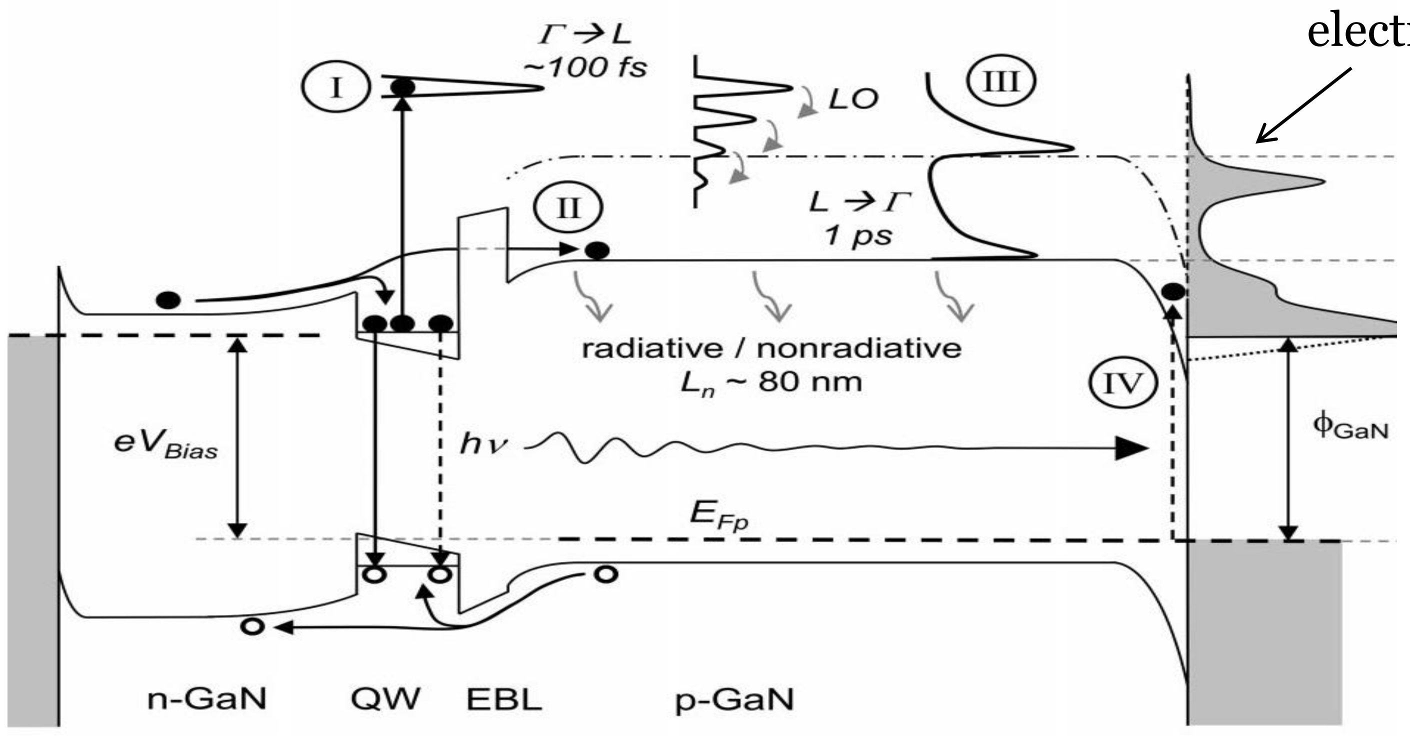
Advanced Topics

- Modeling dislocations and V-shaped pits
- Multiple quantum barrier analysis
- **Hot Auger carrier non-local transport model**

Introduction

Recent direct measurement of electron leakage triggered by QW Auger recombination. PRL 110, 177406 (2013)

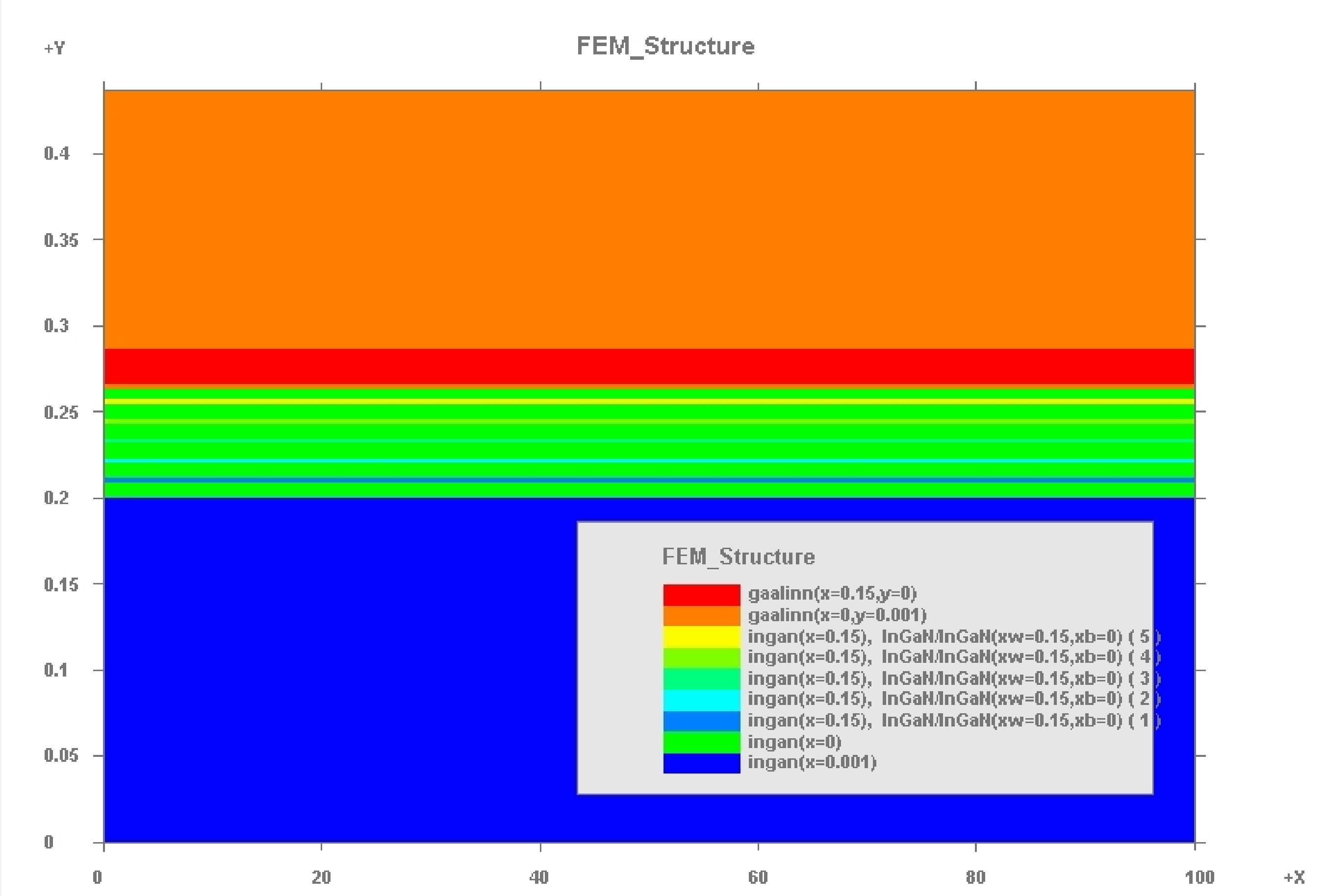
Hot Auger electrons



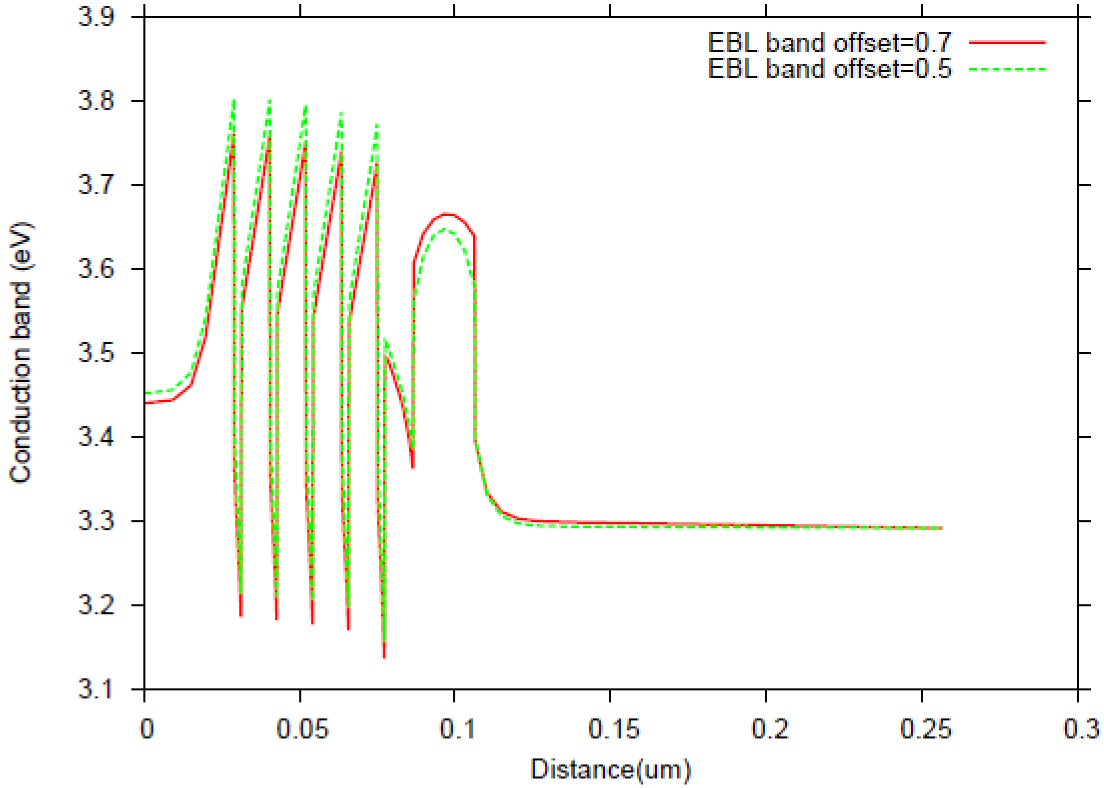
APSYS models related to efficiency droop

- Polarization charge induced well/barrier potential distortion.
- Cold carrier leakage over barriers and EBL, using default drift-diffusion and thermionic emission models.
- Hot-carrier induced non-local transport. Quantum well escape or capture, and barrier-to-barrier fly-over. Sequential or collective non-local hot carrier transport.
- Collective non-local hot Auger carrier leakage from above well to p-contact via thermionic emission (Auger-thermionic model).
- Collective non-local direct escape of confined carriers from well to p-contact with Auger recombination rate (Auger-direct model).
- Collective non-local emission of above-barrier hot carriers to p-contact with Auger rate (Auger-indirect model).

Demo example: InGaN/GaN MQW LED with EBL

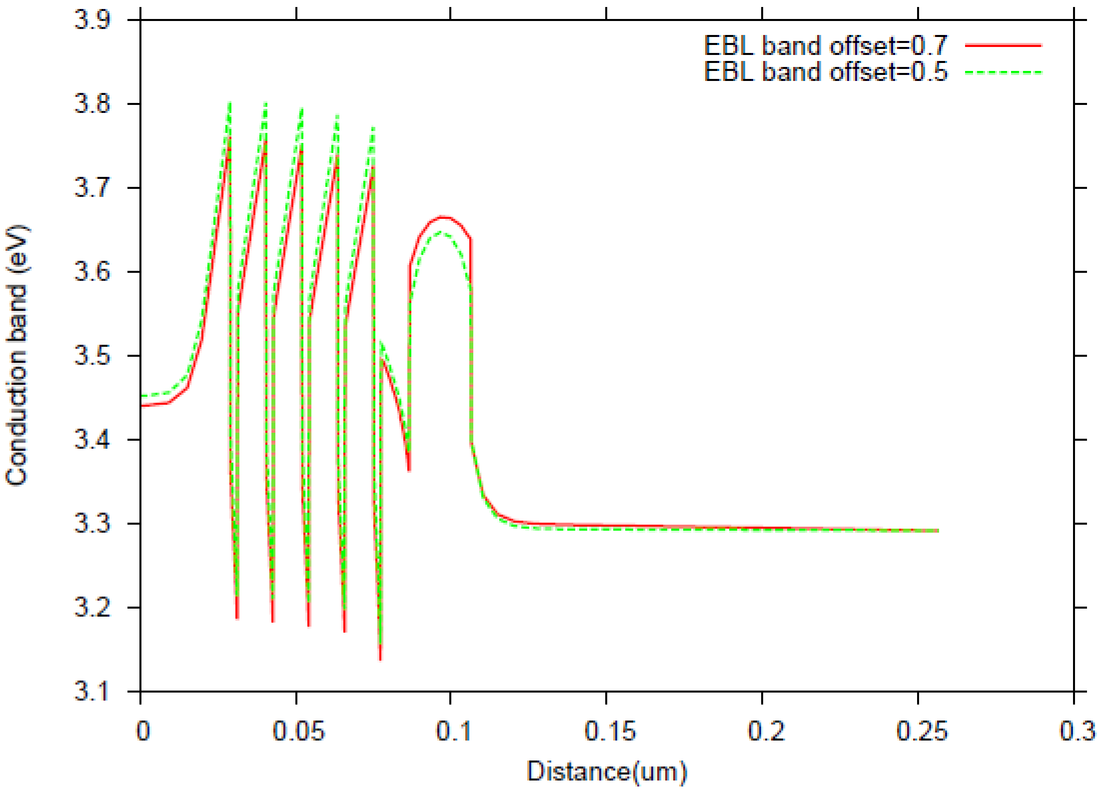


Conduction band for different EBL band offsets



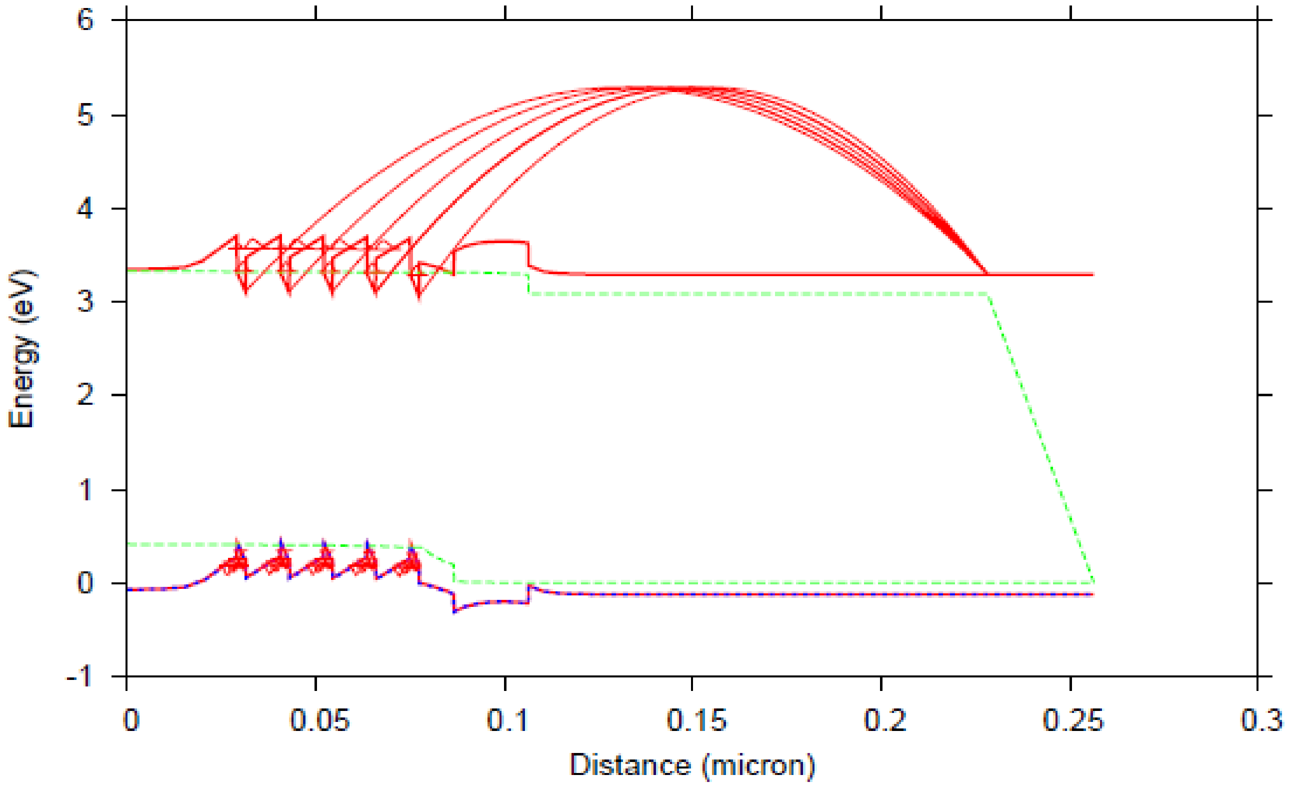
Comparison of conduction band showing polarization charge induced potential distortion for different EBL band offsets

Conduction band for different EBL band offsets



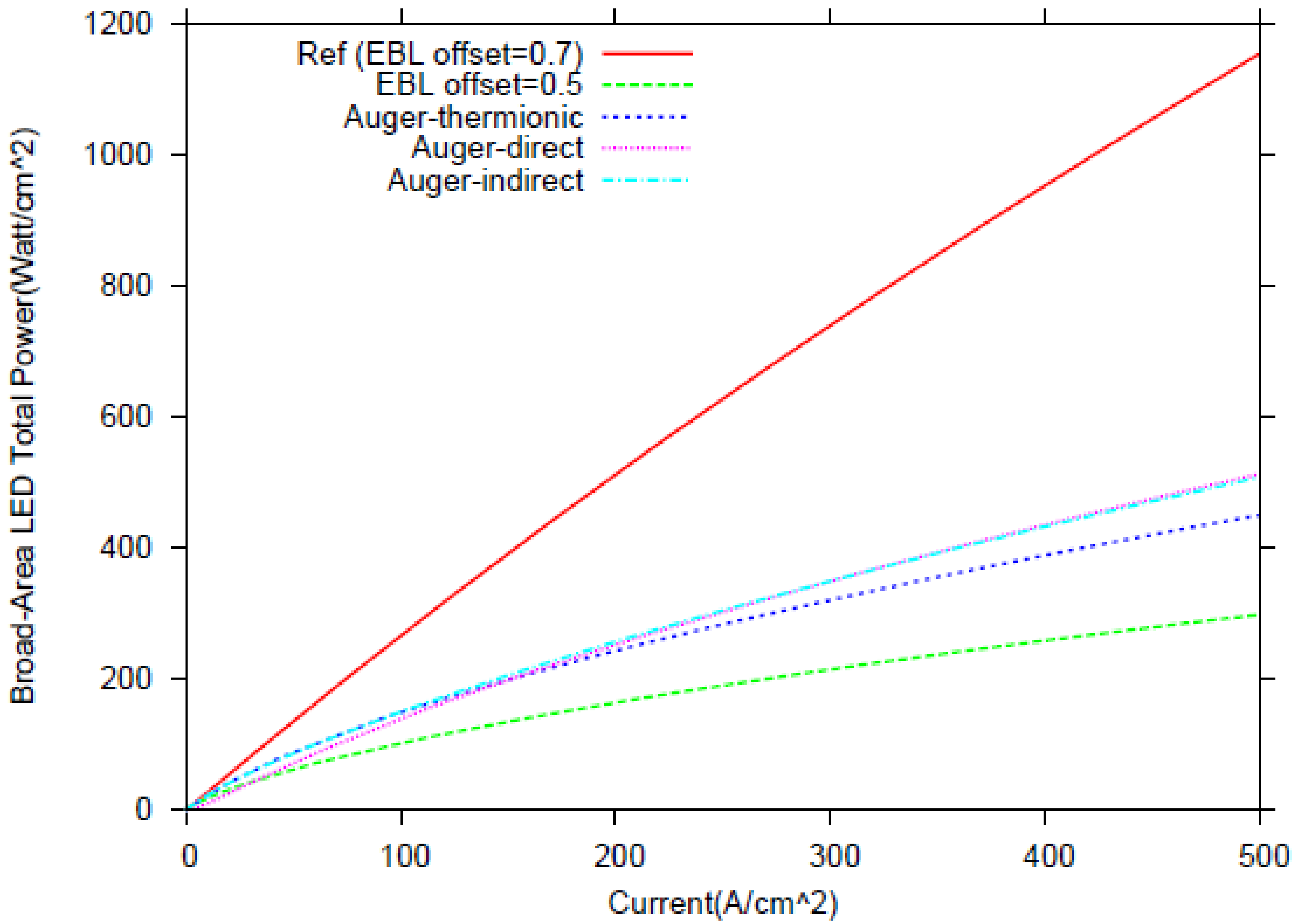
Comparison of conduction band showing polarization charge induced potential distortion for different EBL band offsets

Hot carrier non-local transport

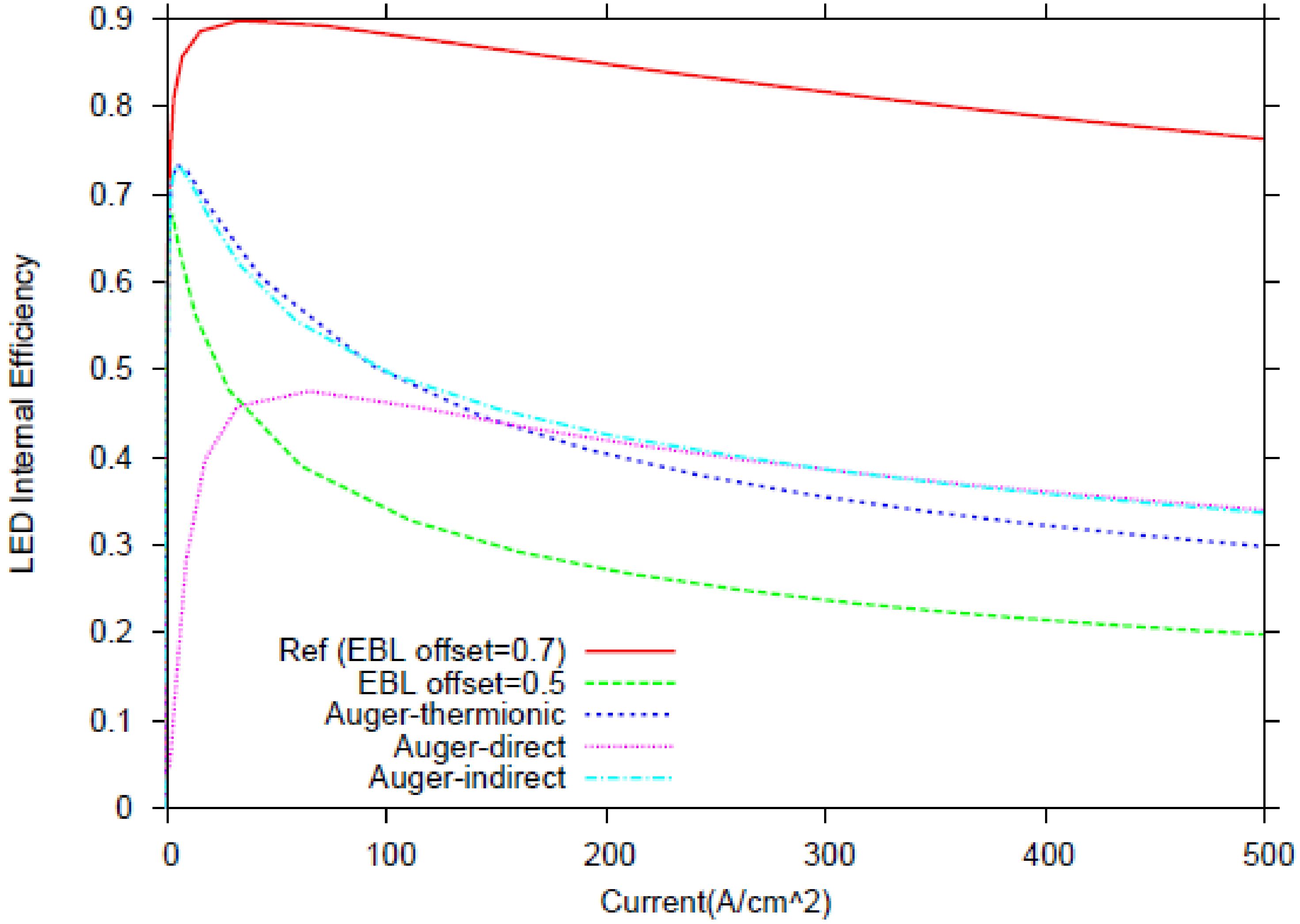


Band diagram indicating collective hot carrier non-local transport mesh connections through the MQW system. Superimposed on default drift-diffusion/thermionic solution.

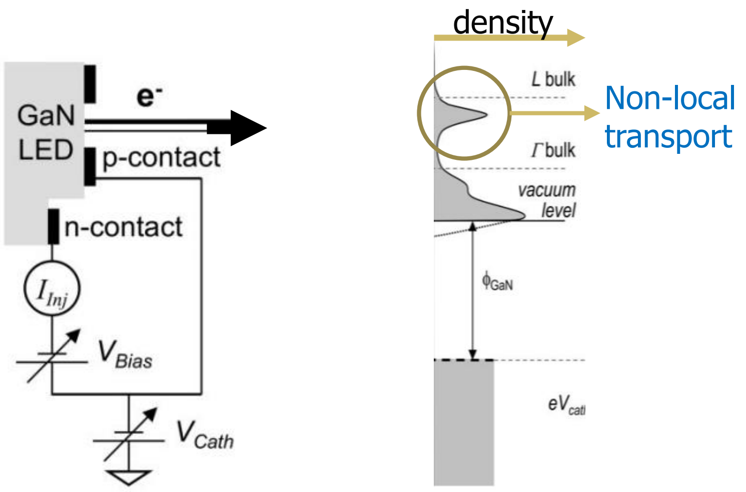
Comparison of LED emission power



Comparison of LED IQE



Non-local transport within DD framework



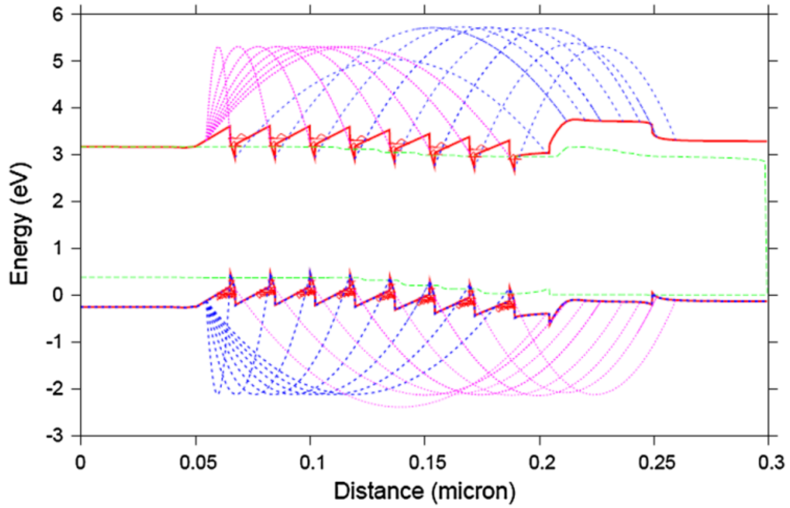
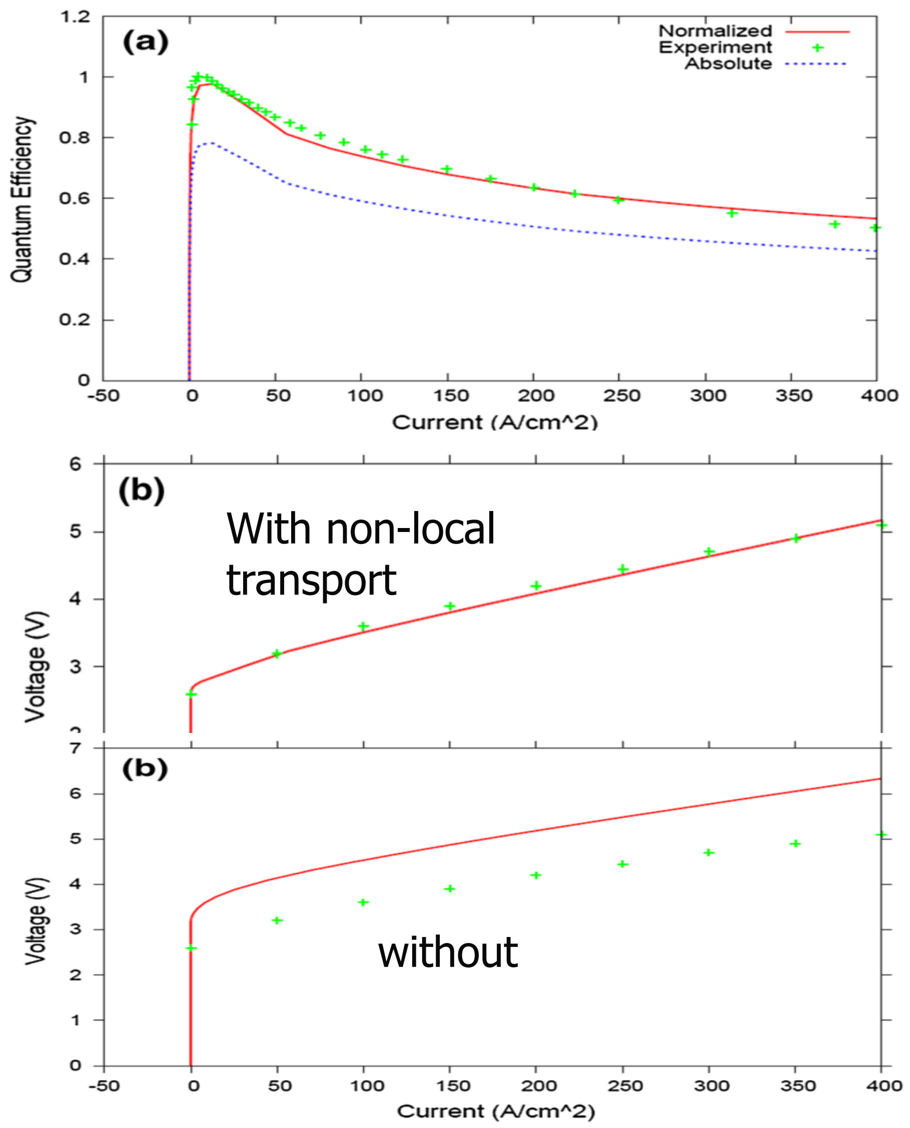


Fig. 5 Band diagram from simulation using direct Auger non-local transport model. Indicated are non-local paths for the collective transport model



J Comput Electron (2015) 14:409–415
DOI 10.1007/s10825-015-0693-1

Non-local transport in numerical simulation of GaN LED
Z. M. Simon Li[1]

Conclusion on non-local transport

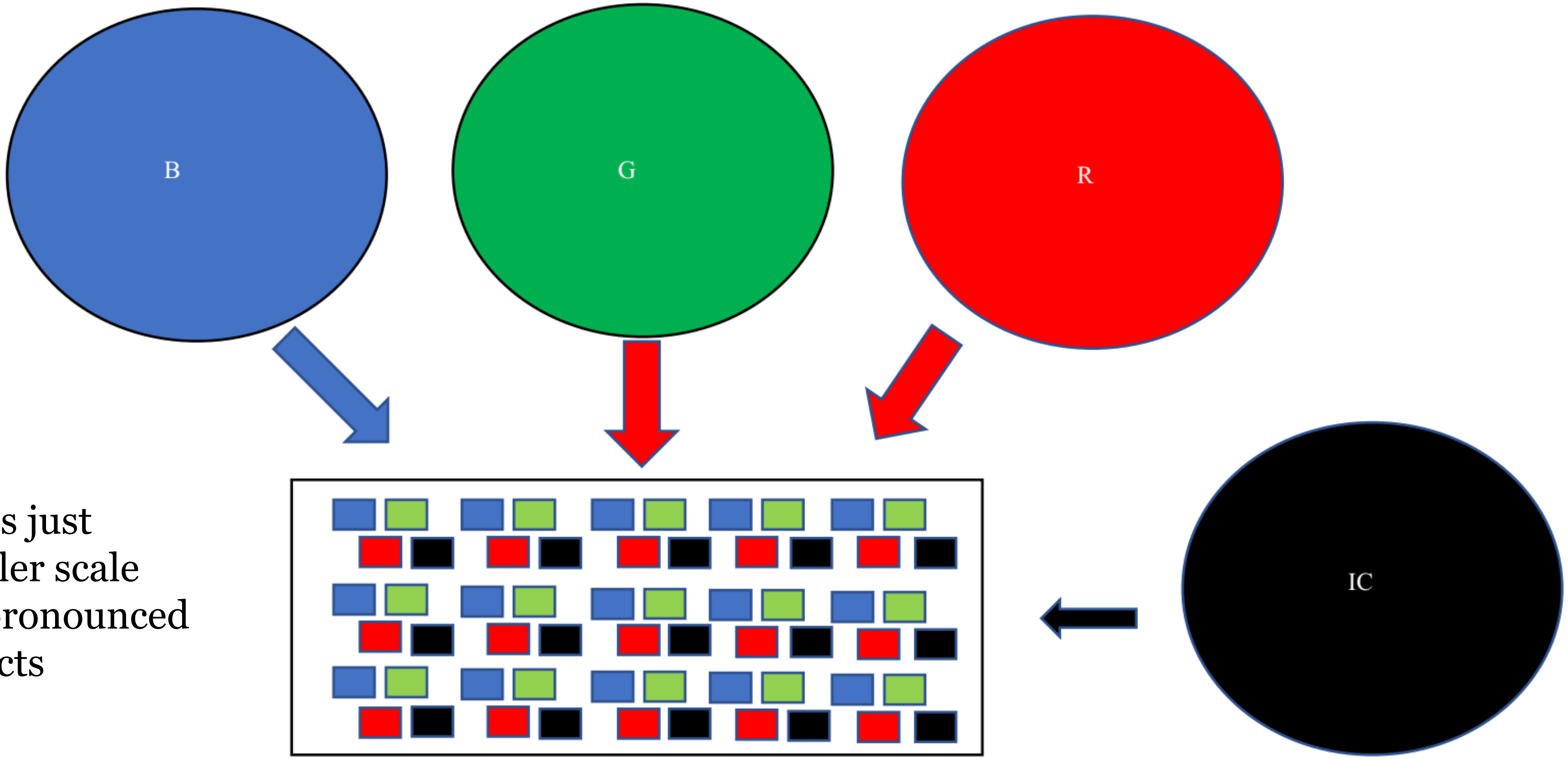
- GaN IQE droop can be explained by many models including electron leakage, Piezo charge induced carrier non-confinements, and Auger non-radiative recombination.

- The higher than theory value of turn-on voltage of GaN LED can only be explained by non-local carrier transport as powered by hot carrier generated by Auger recombination. The effective of hot Auger carrier helps to reduce the turn voltage and thus improves the EQE.

Contents

- Crosslight introduction: quantum simulation
- GaN LED simulation capabilities
- Advanced topics in GaN LED simulation
- Surface effects and micro-LED
- Summary

Mass Transfer of Micro-LED Dies & IC chips



Micro-LED is just
LED in smaller scale
With more pronounced
Surface defects

More than simple scaling

- Regular scale LED (~ 500 um) is optimized with lateral leakage in mind and little vertical surface effects.

- Needs to redesign LED MQW to consider vertical injection and side wall recombination.

- Fortunately, TCAD capability of Crosslight built up over the years can still be applied in micro-LED design

Micro-LED Case Study Using Crosslight

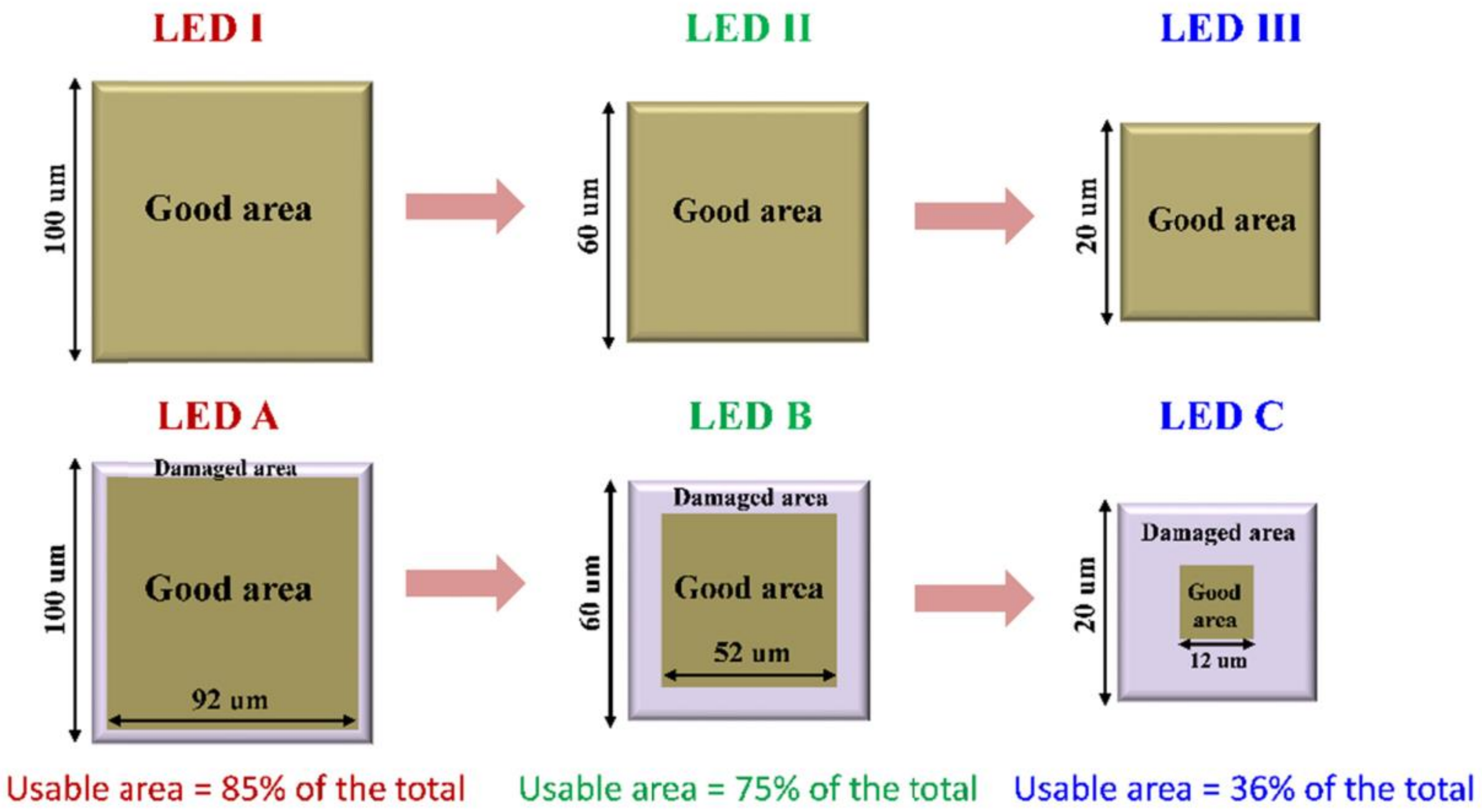


Fig. 1. Schematic structures for LEDs I, II and III without sidewall damages and LEDs A, B, C with sidewall damages. The usable area ratios for LEDs A, B and C are 85%, 75% and 36%, respectively.

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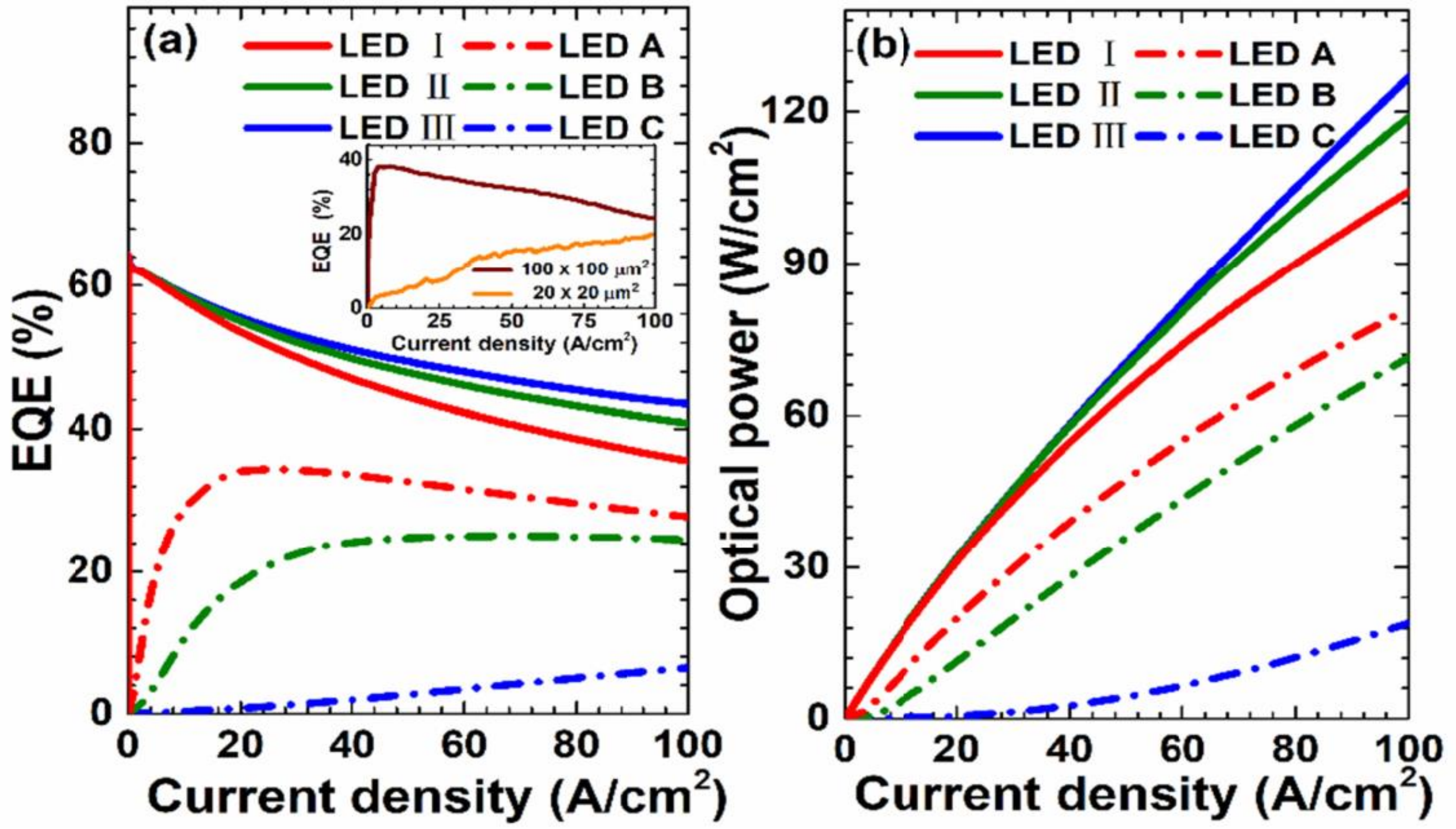


Fig. 2. (a) EQE, and (b) optical power density in terms of the injection current density for LEDs I, II, III, A, B and C, respectively. Inset figure shows the measured EQE in terms of the injection current density for the 100 × 100 μm^2 μLEDs and 20 × 20 μm^2 μLEDs, respectively. The experimental data are extracted from [19].

Remark: there is a limit how one can scale down in a common sense defect model

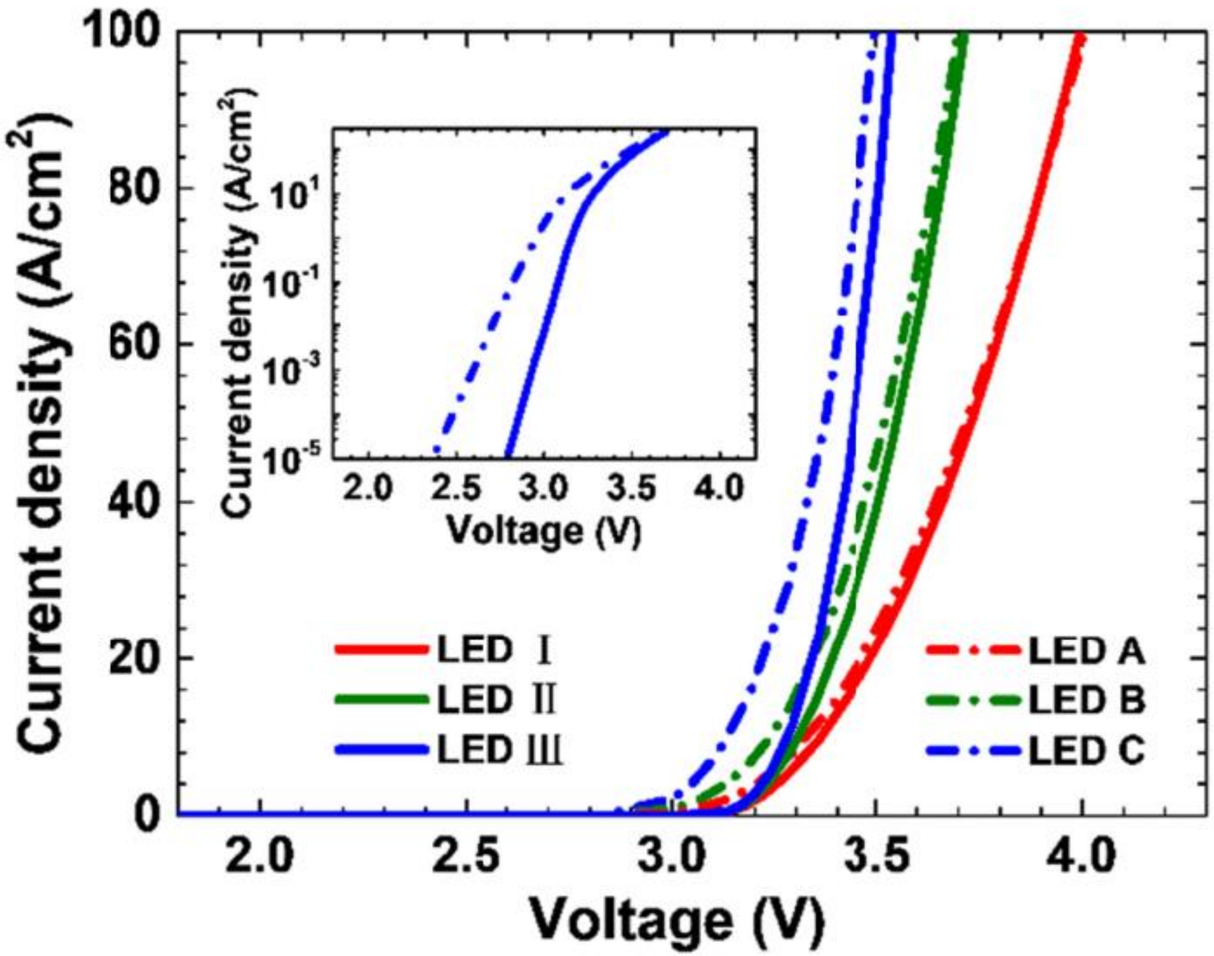


Fig. 3. Numerically calculated current density-voltage characteristics for LEDs I, II, III, A, B and C, respectively. Inset figure shows the current-voltage characteristics in semi-log scale for LEDs III and C.

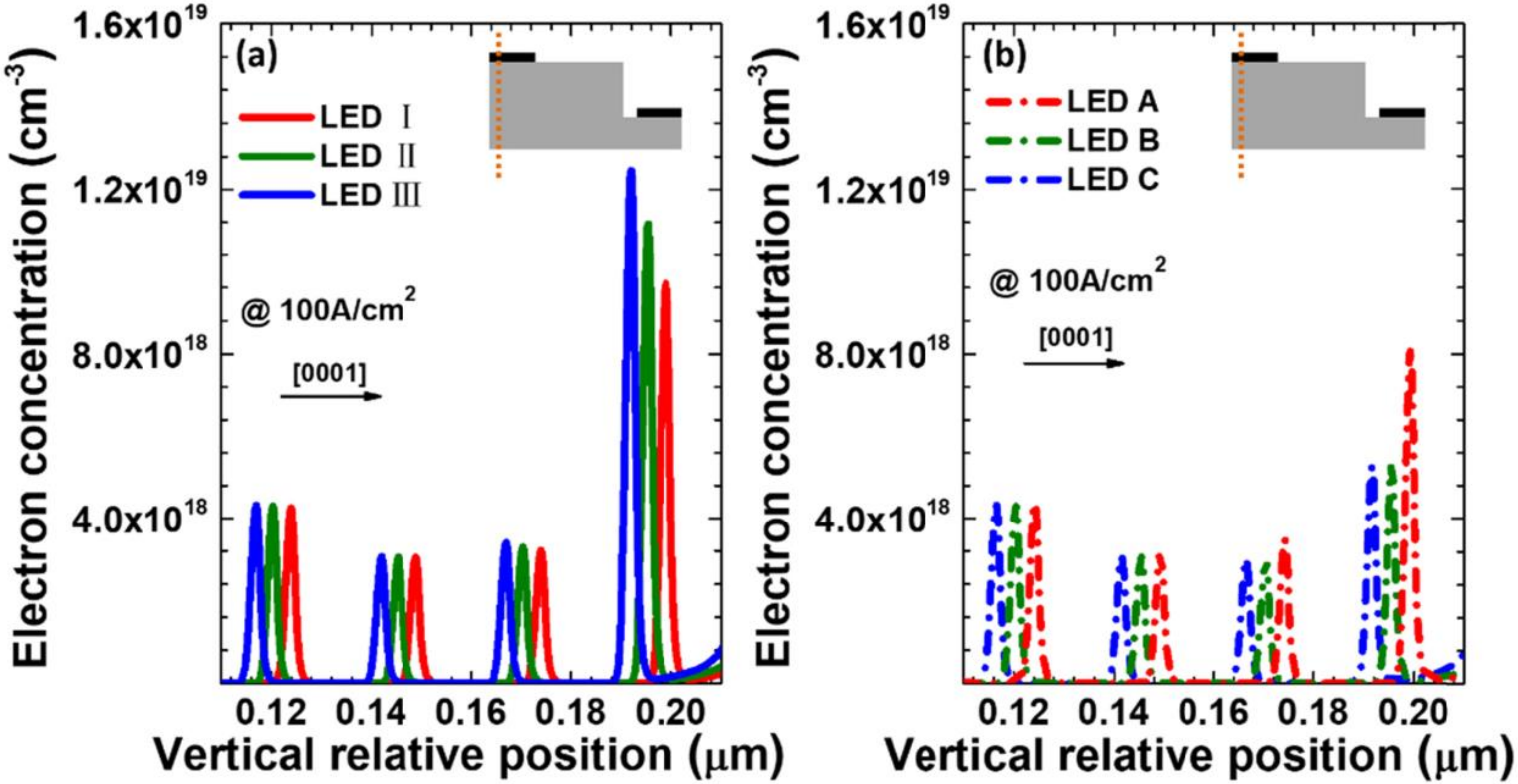


Fig. 4. Numerically calculated electron concentration profiles in the MQW region for (a) LEDs I, II and III (b) LEDs A, B and C, respectively. Data are calculated when the injection current is 100 A/cm^2. Inset figure shows the position along which the electron concentration profiles are captured.

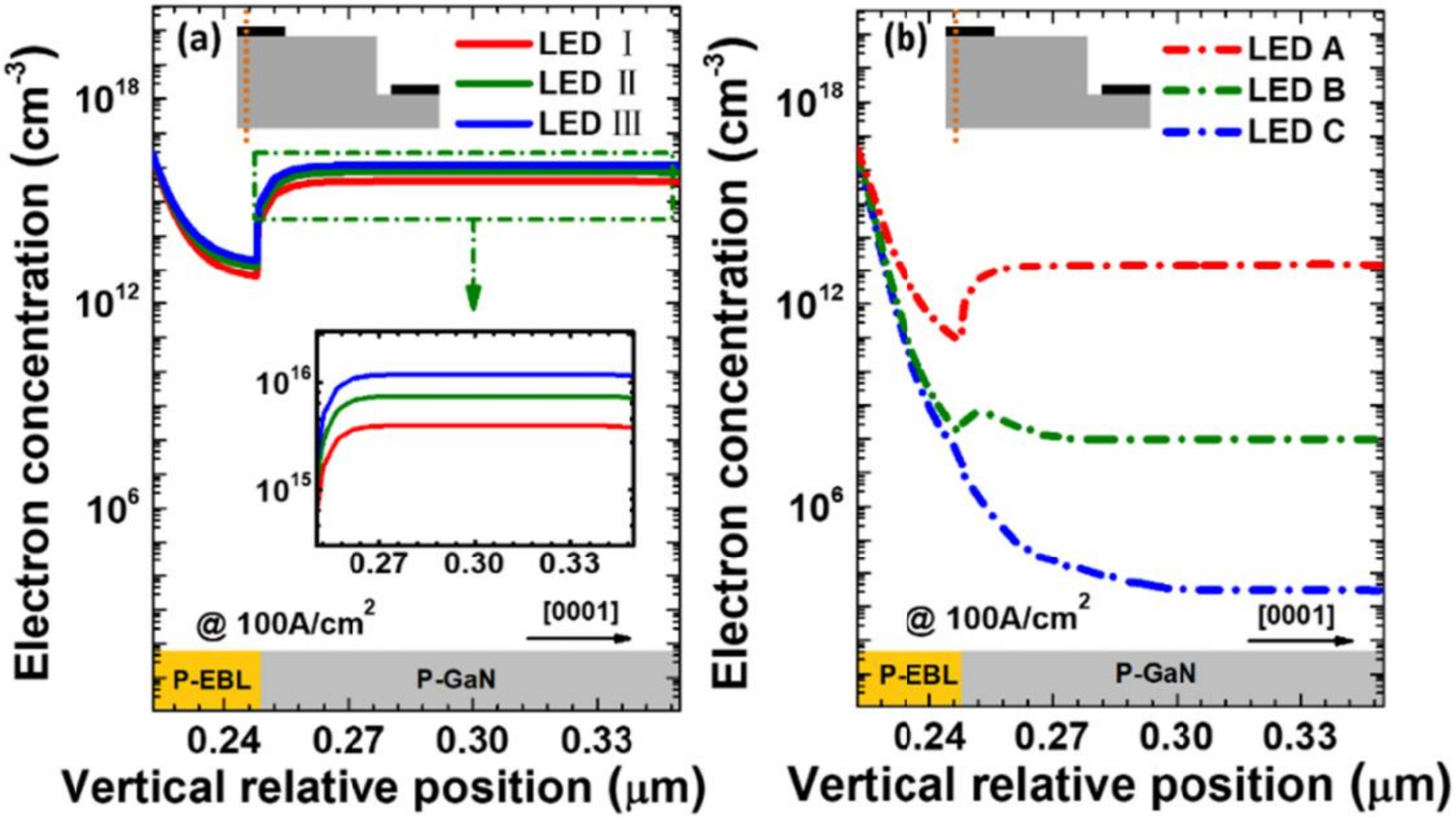


Fig. 5. Numerically calculated electron concentration profiles in the p-EBL and p-GaN layer for (a) LEDs I, II and III, (b) LEDs A, B and C, respectively. Data are calculated when the injection current is 100 A/cm^2. Inset figure shows the zoom-in electron concentration profiles in the p-GaN layer. Inset figure shows the position along which the electron concentration profiles are captured.

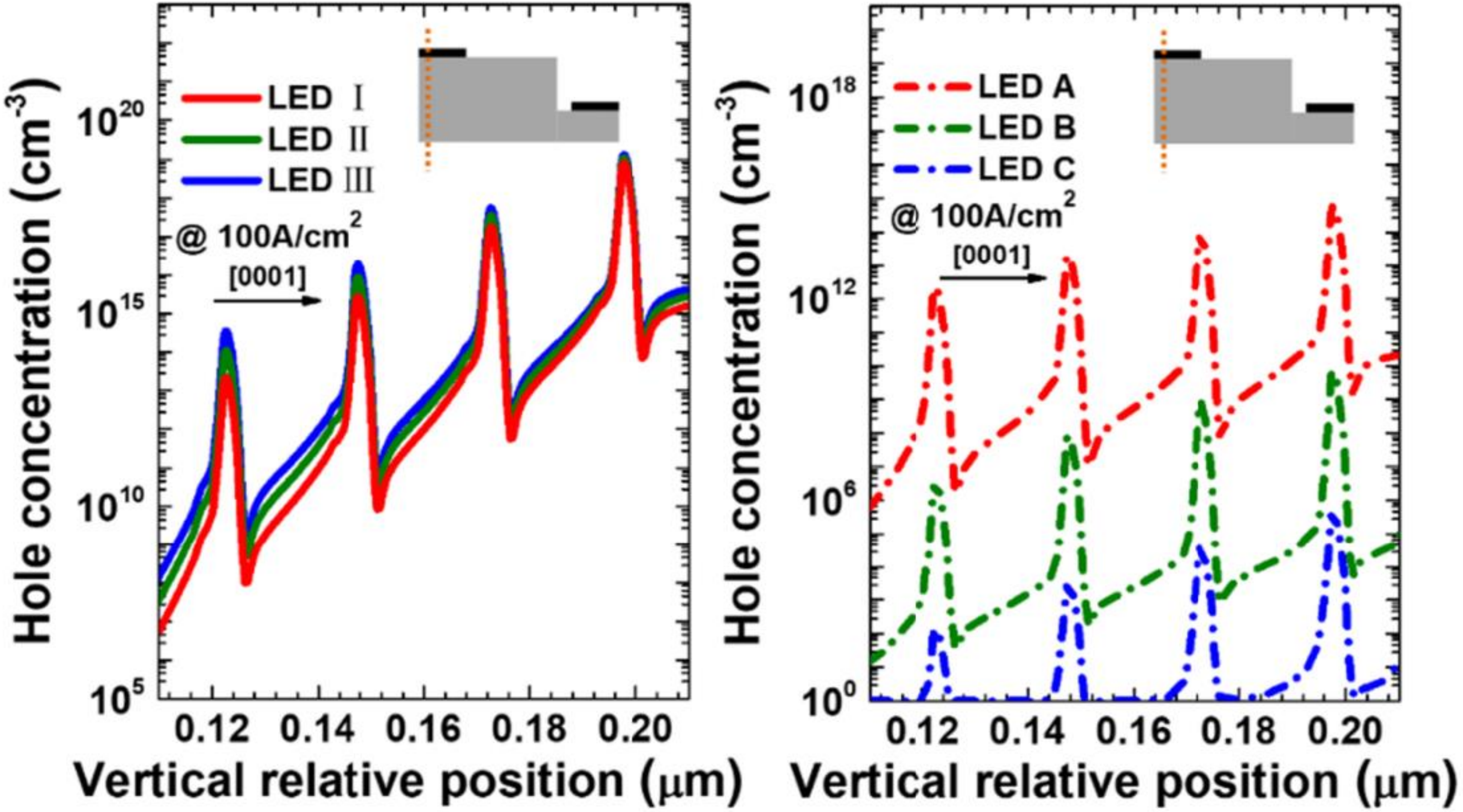


Fig. 6. Numerically calculated hole concentration profiles in the MQW region for (a) LEDs I, II and III, (b) LEDs A, B and C, respectively. Data are calculated when the injection current is 100 A/cm^2. Inset figure shows the position along which the hole concentration profiles are captured.

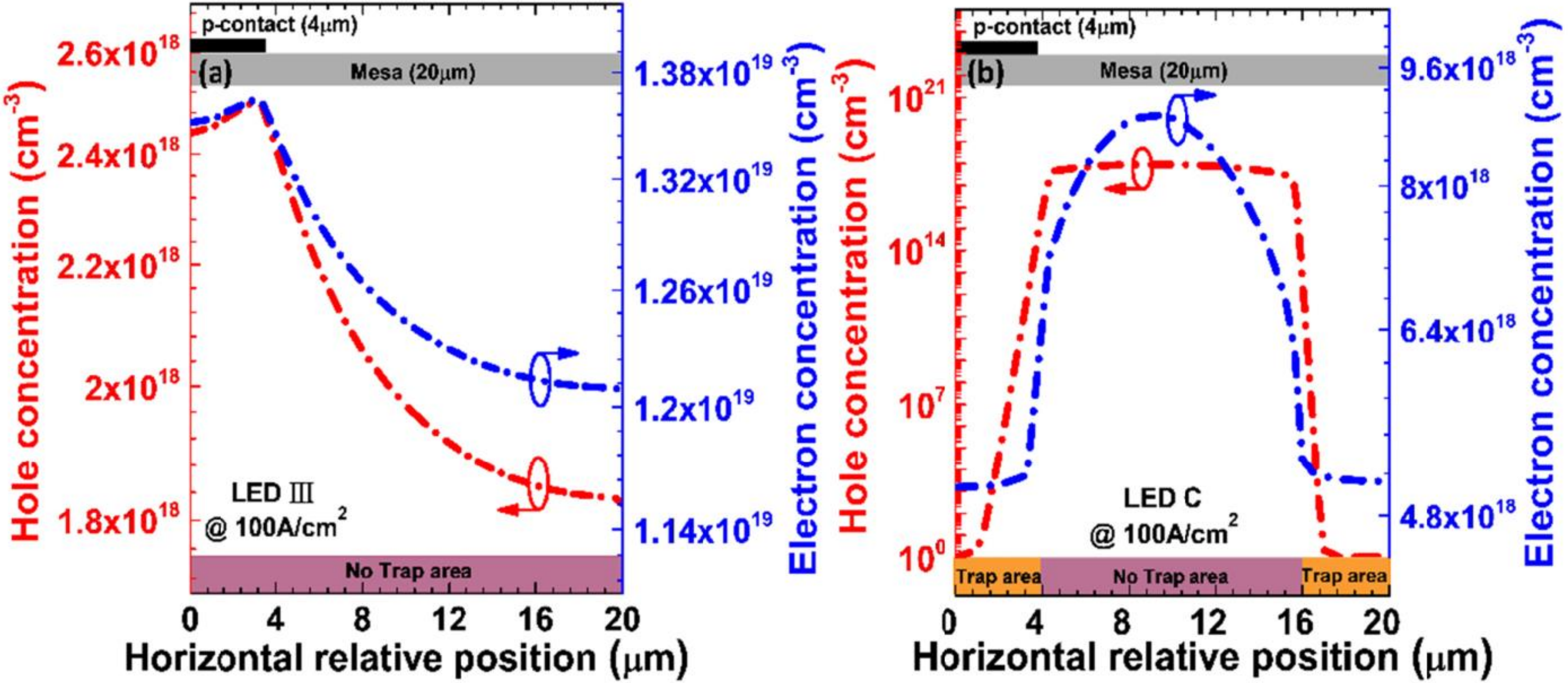


Fig. 7. Numerically calculated carrier concentration profiles in the first quantum well near the p-region for (a) LED III, and (b) LED C, respectively. Data are calculated when the injection current is 100 A/cm^2.

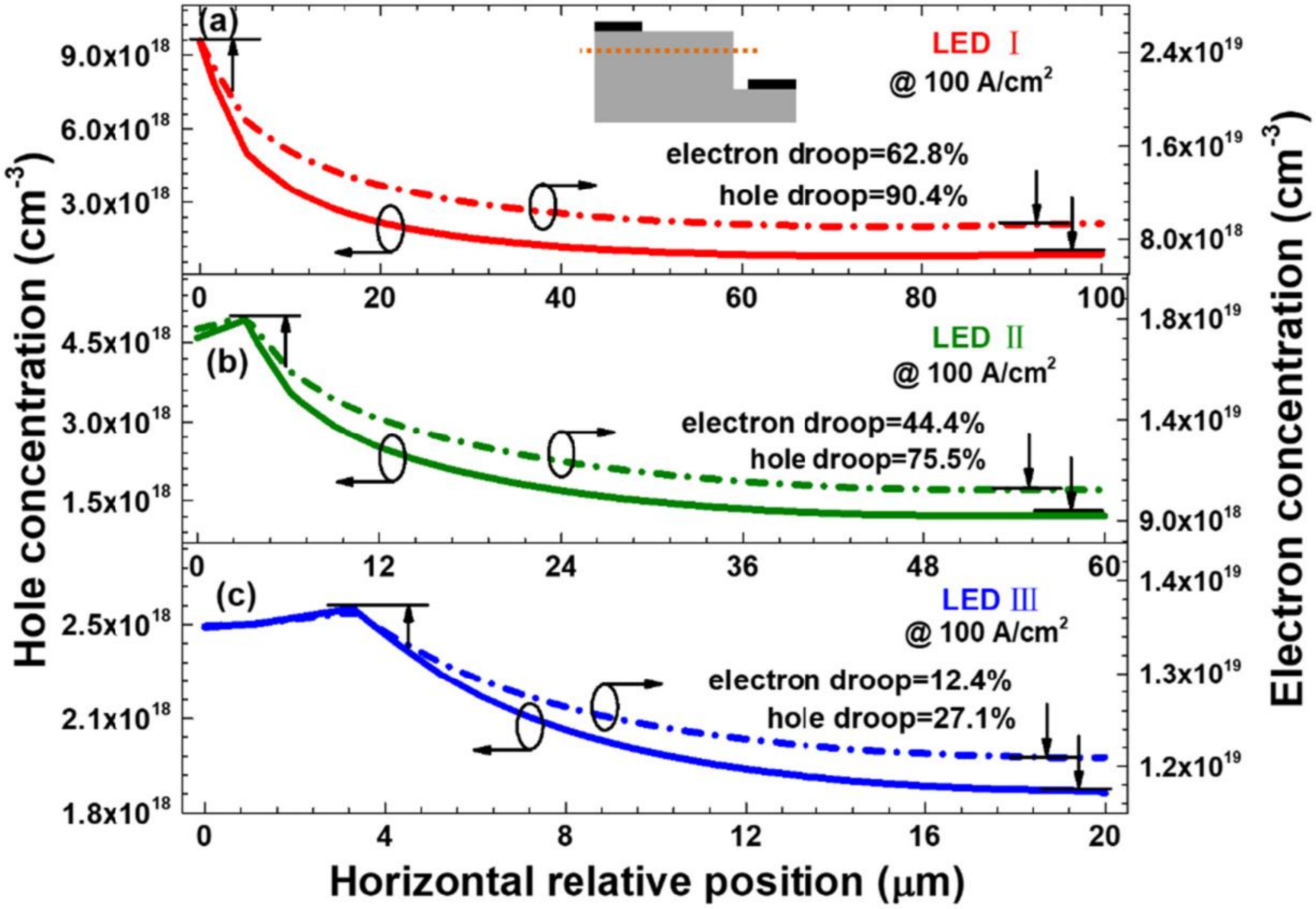


Fig. 8. Numerically calculated carrier concentration profiles in the first quantum well near the p-region for LEDs I, II and III, respectively. Data are calculated when the injection current is 100 A/cm^2. Inset in Fig. 8(a) shows the position along which the carrier concentration profiles are captured for LEDs I, II and III.

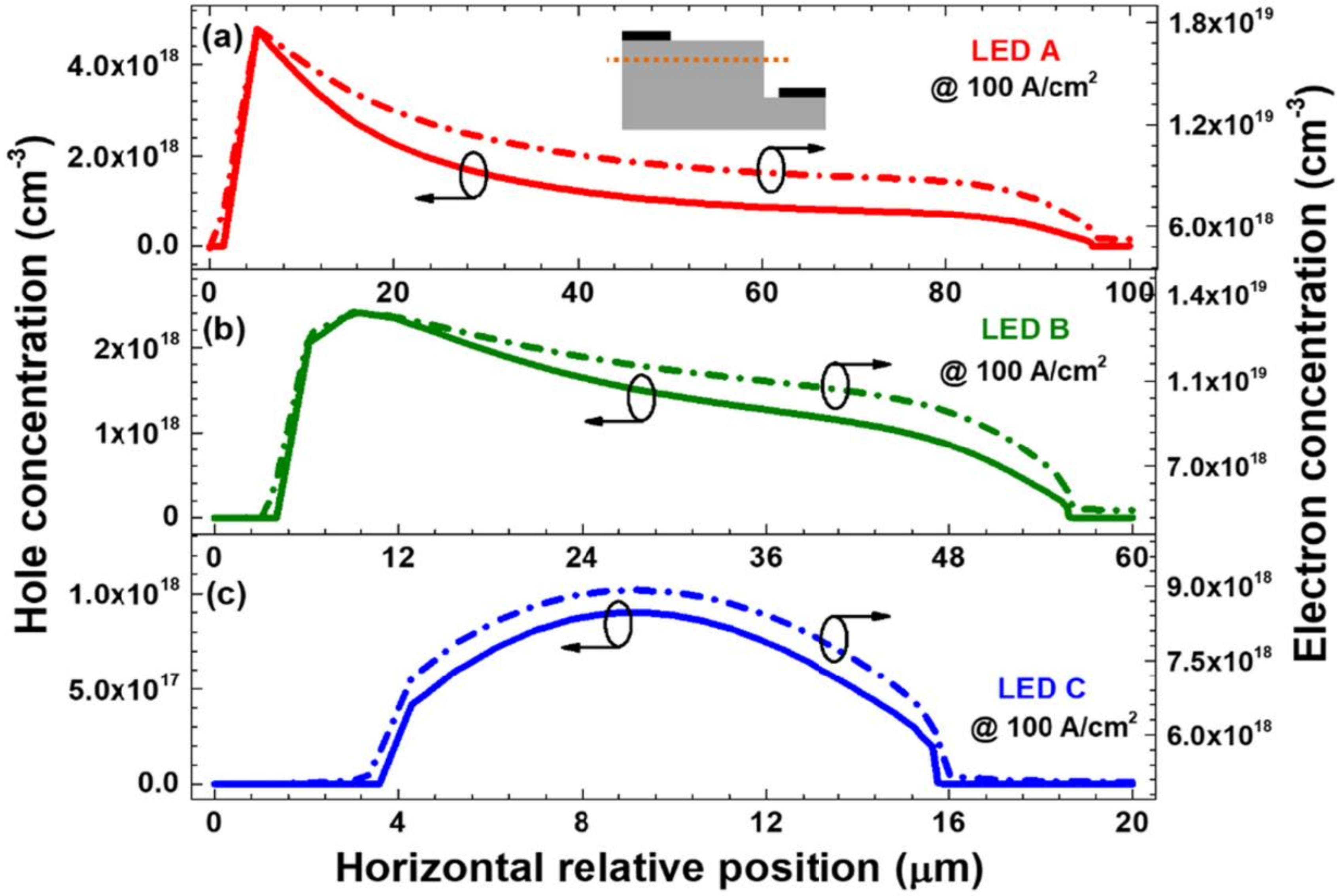
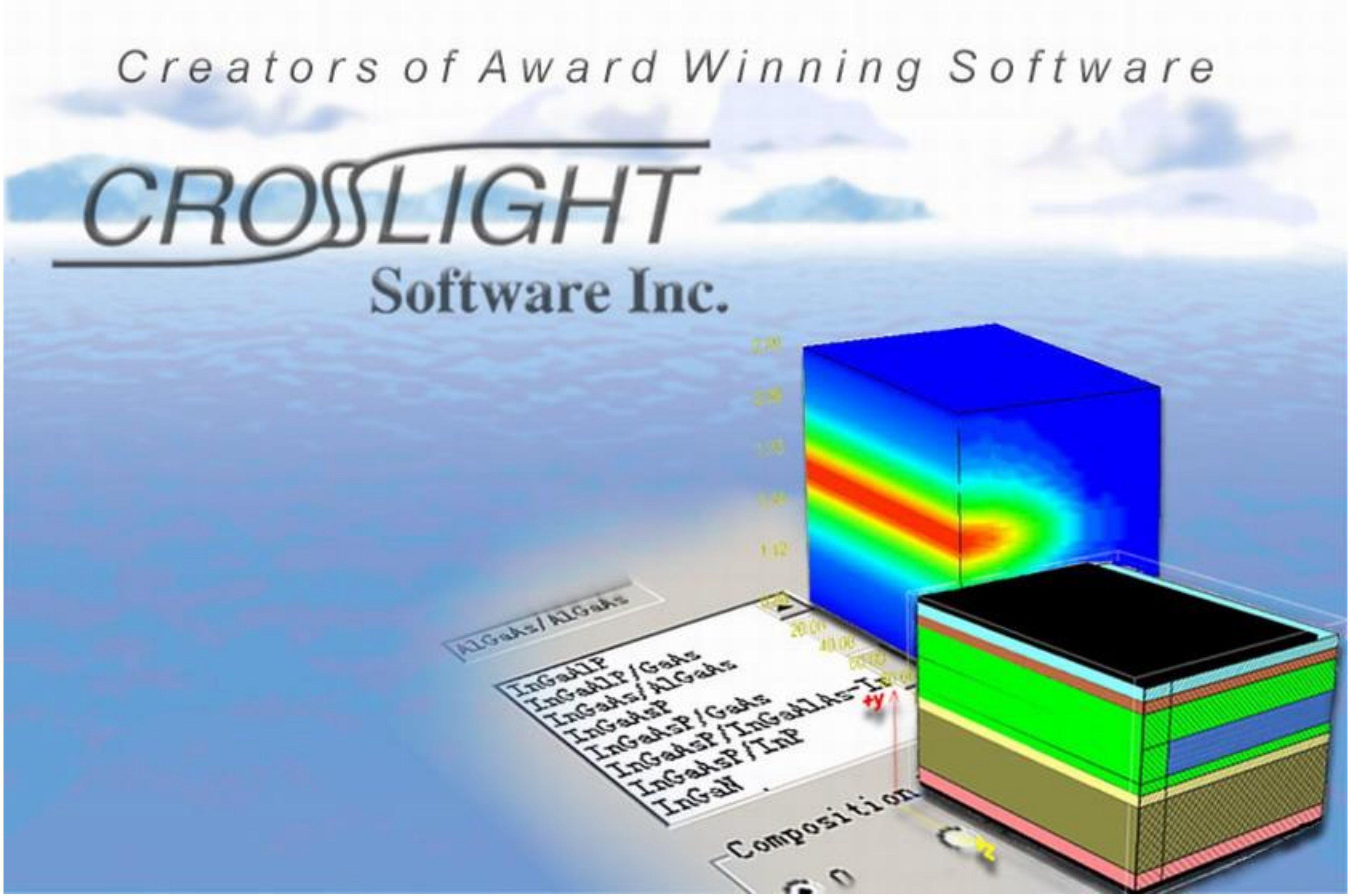


Fig. 9. Numerically calculated carrier concentration profiles in the first quantum well near the p-region for LEDs A, B and C, respectively. Data are calculated when the injection current is 100 A/cm^2. Inset in Fig. 9(a) shows the position along which the carrier concentration profiles are captured for LEDs A, B and C.

Simulation Conclusions

- Smaller uLED improves vertical injection
- Smaller uLED causes waste of QE due to finite-sized sidewall defects
- Research and simulation shall handle the trade off injection and defects
- If defects can not be completely eliminated, we shall seek for more efficiency-friendly types of defects

Thanks for your attention!


Creators of Award Winning Software
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AlGaAs/AlGaAs
InGaAlP
InGaAlP/GaAs
InGaAs/AlGaAs
InGaAsP
InGaAsP/GaAs
InGaAsP/InP
InGaN
Composition