Computer Aided Design of GaN Light-Emitting Diodes

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Contents

- Available tools and modules.
- Simulation of IQE droop .
- Design of superlattice.
- A typical 2D simulation of InGaN LED.
- Tunnel junction contact design.
- Full 3D Simulation.
- Summary.

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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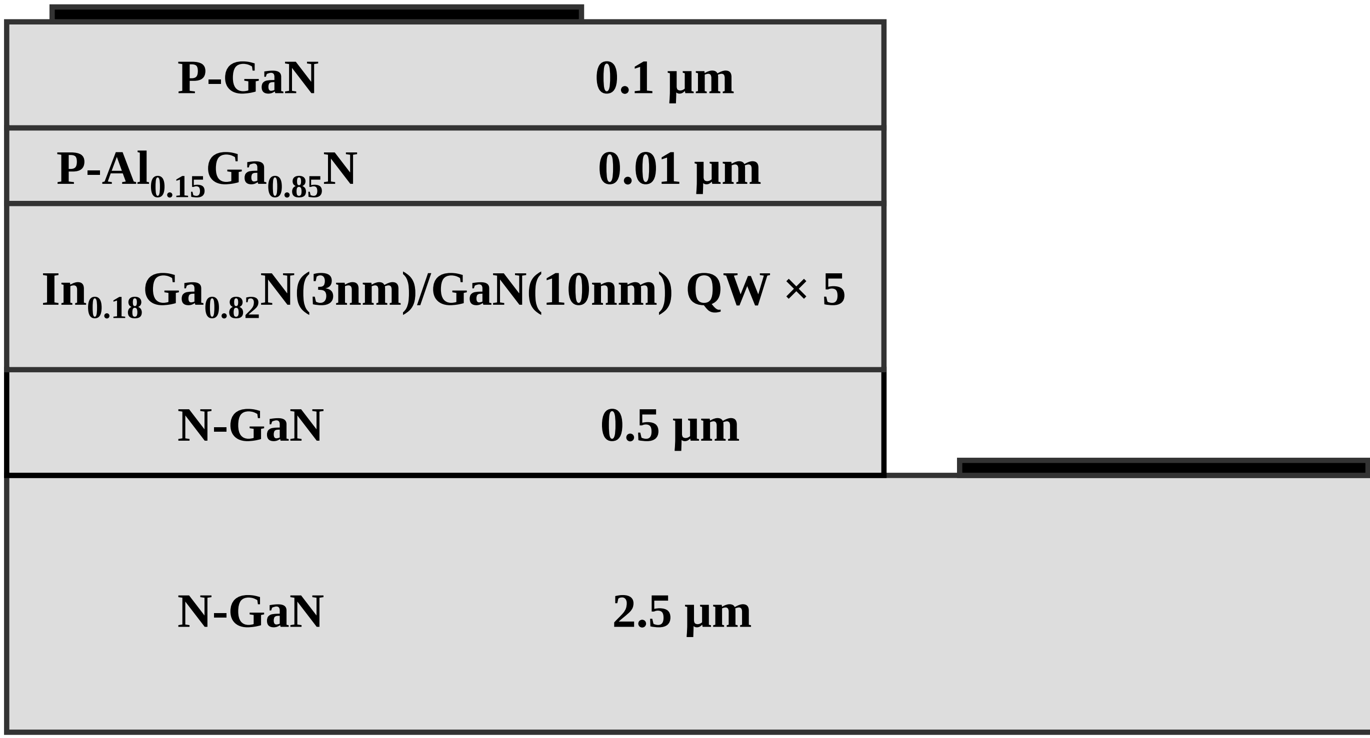
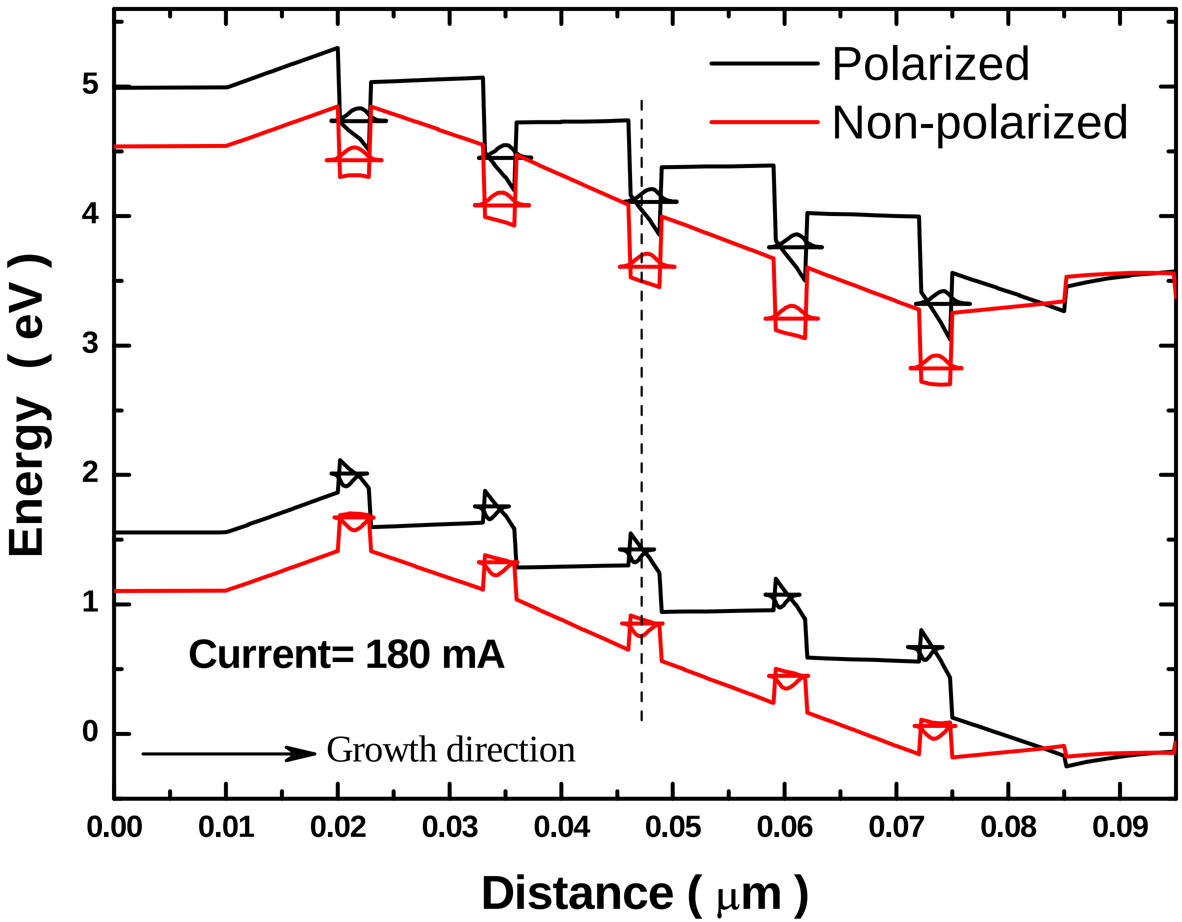
Structure



Size: 300 µm × 300 µm

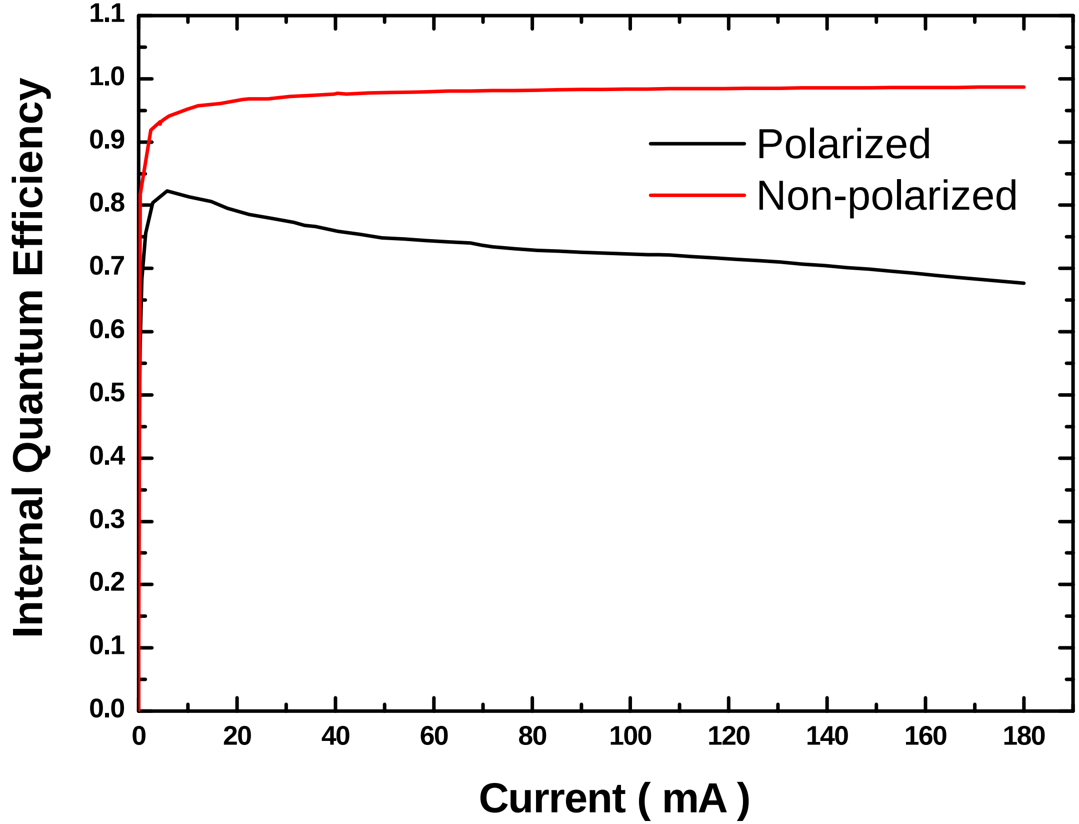
Lifetimes of carriers (τ) in the five QWs along the growth direction are assumed to be 30ns, 35ns, 40ns, 45ns and 50ns, respectively, because the quality of QWs improves (with less defects) with more QWs.
The polarization charge set on the QW interfaces is 50% of the theoretical value calculated based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

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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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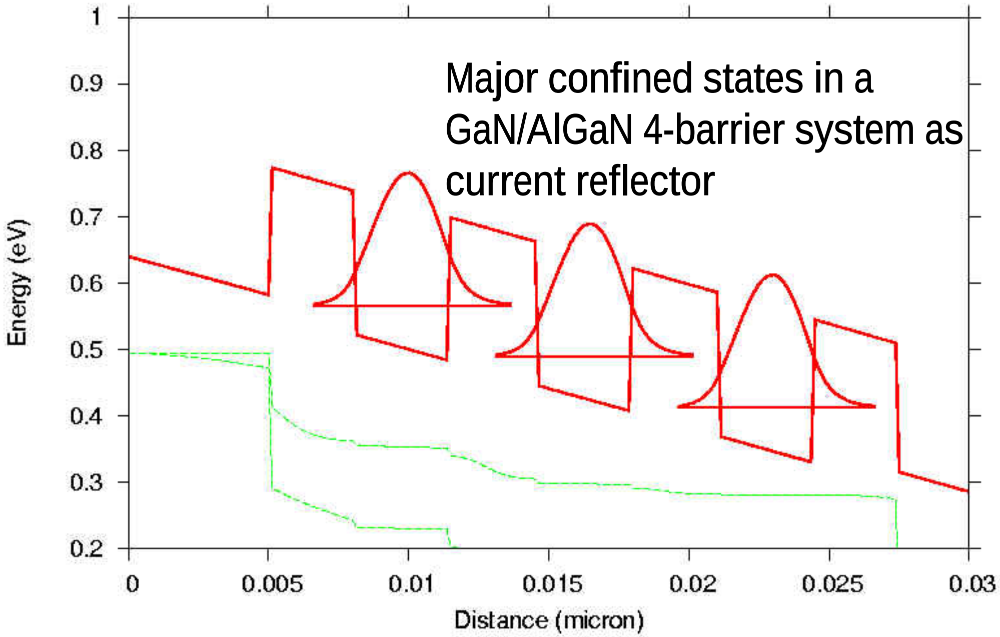
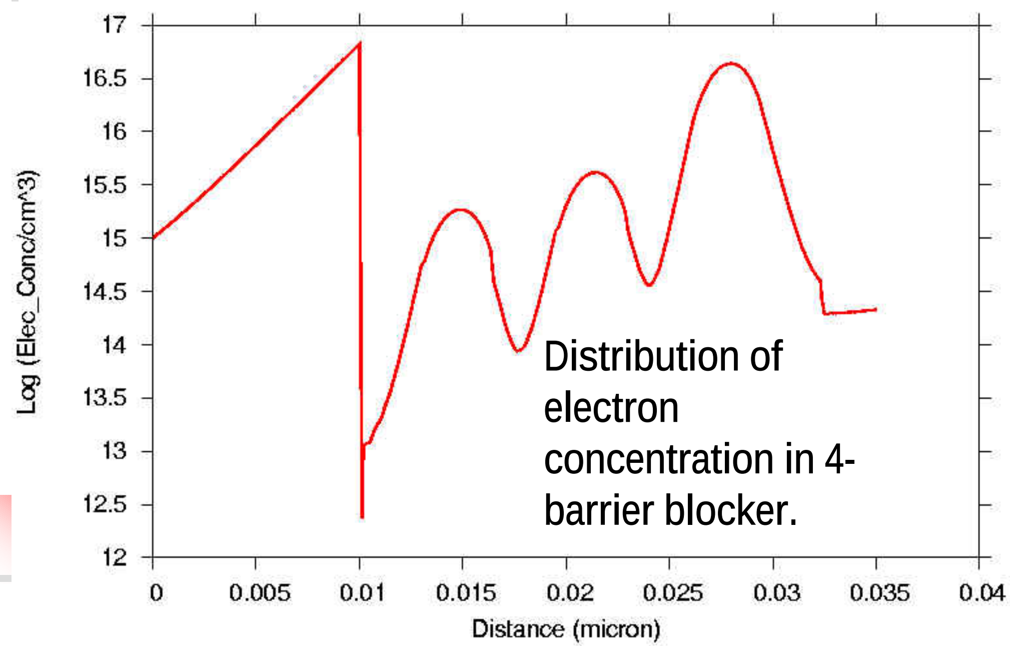
Use of superlattice





- 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.

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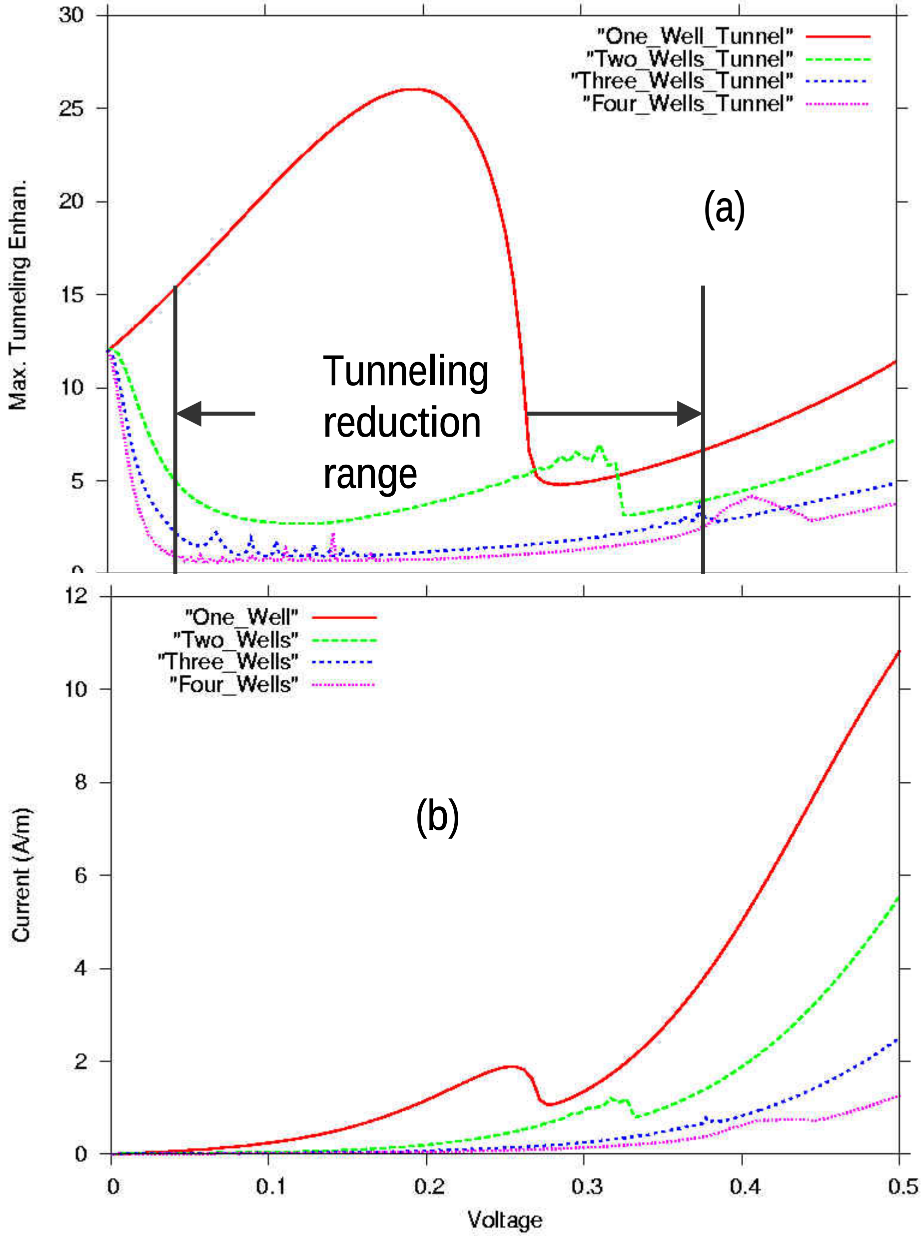
Formation of SL reflector

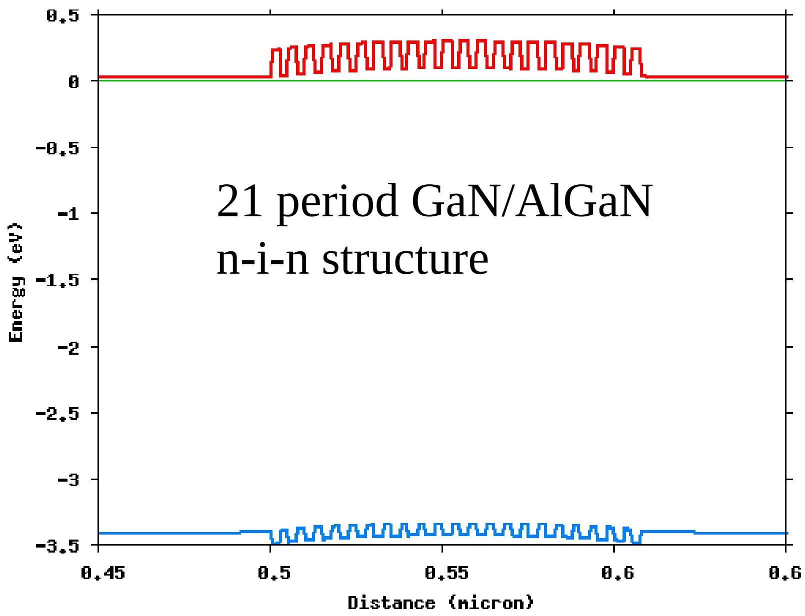


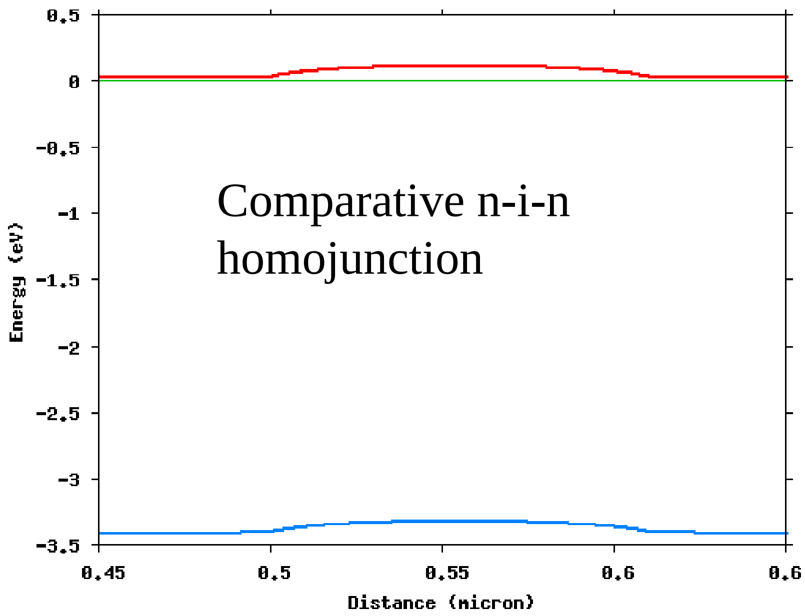
(a) Maximum tunneling enhancement factor (quantum correction to drift-diffusion) as a function bias showing a large bias range with reduction in tunneling current due to quantum interference effects, as superlattice (SL) size increases to larger than three wells.

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

➔ Conclusion: superlattice is effective in leakage current blocking.

Simple test structures for mini-band model





Remark: tunneling region defined from n to n regions. Al fraction is 16 percent for the barriers and well/barrier width is 2.5nm. Polarization charge ignored for simplicity.

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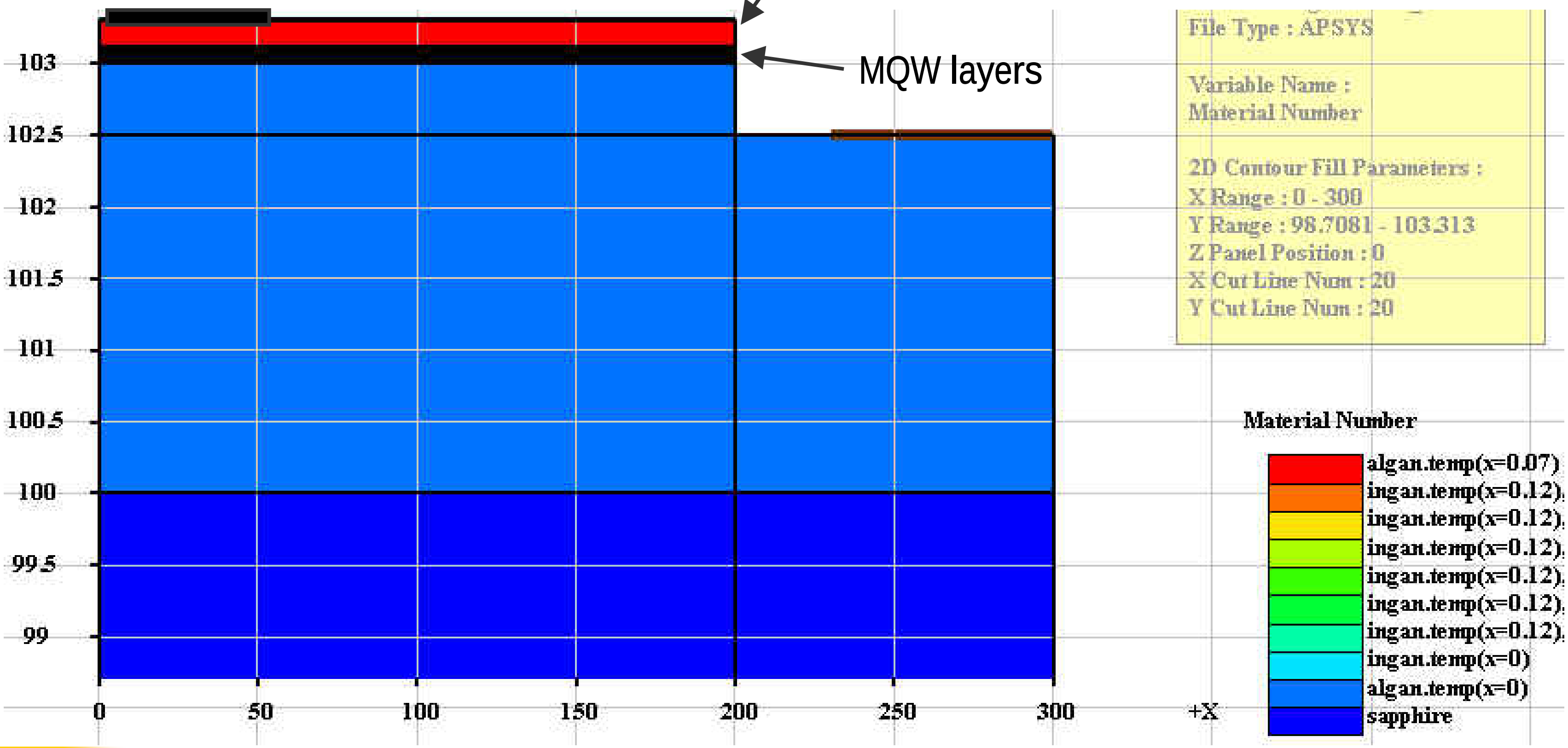
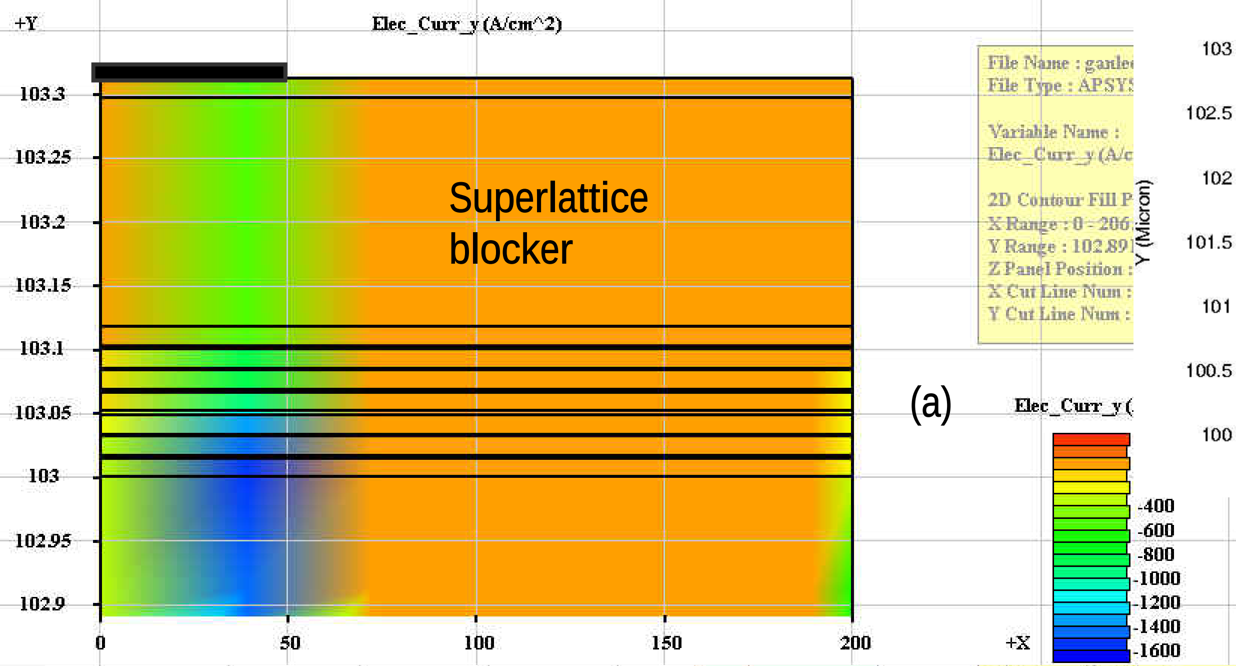
A Common InGaN LED

AlGaN/GaN SL modeled as effective medium with anisotropic mobility and thermal conductivity.

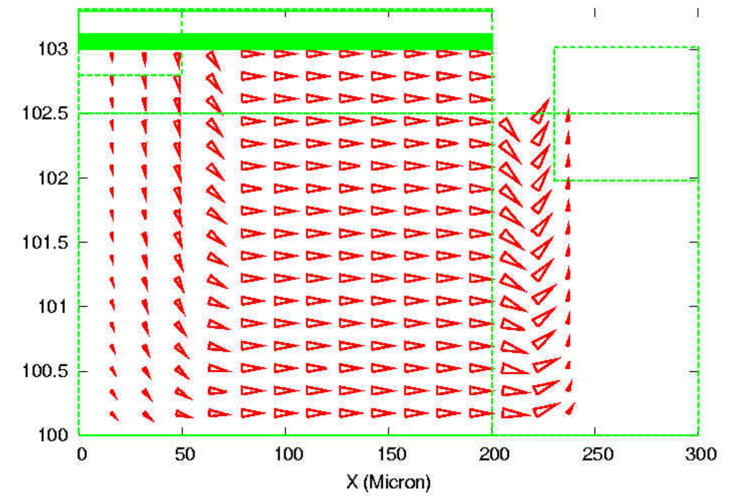
MQW layers

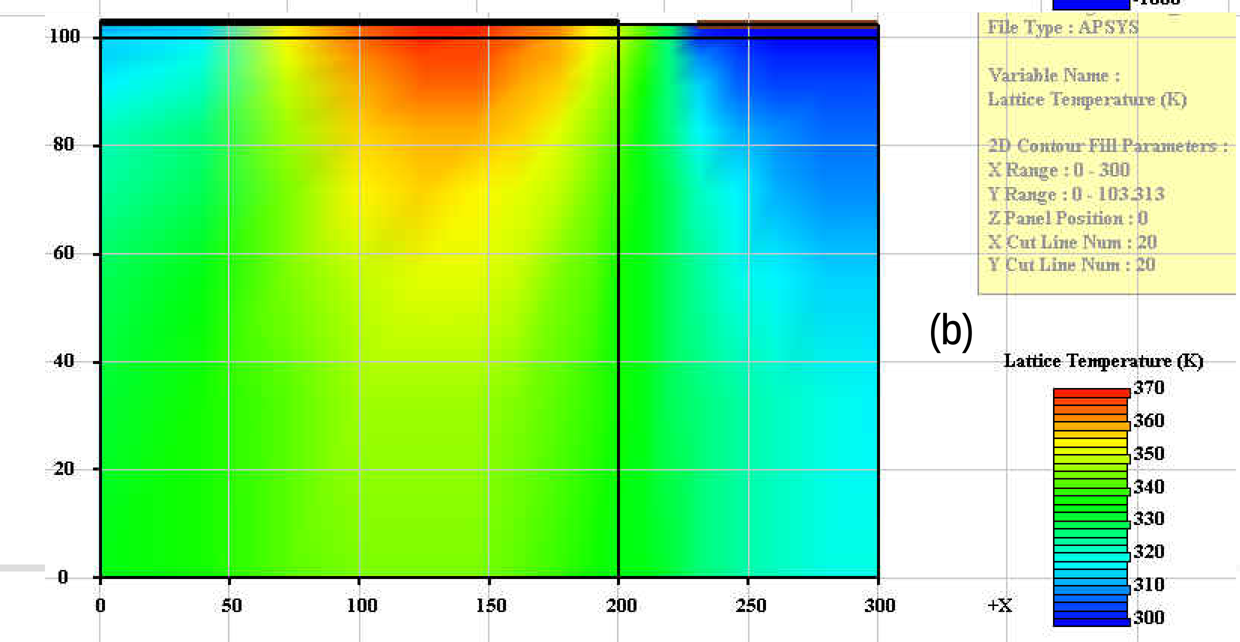


Current crowding and self-heating



(a)



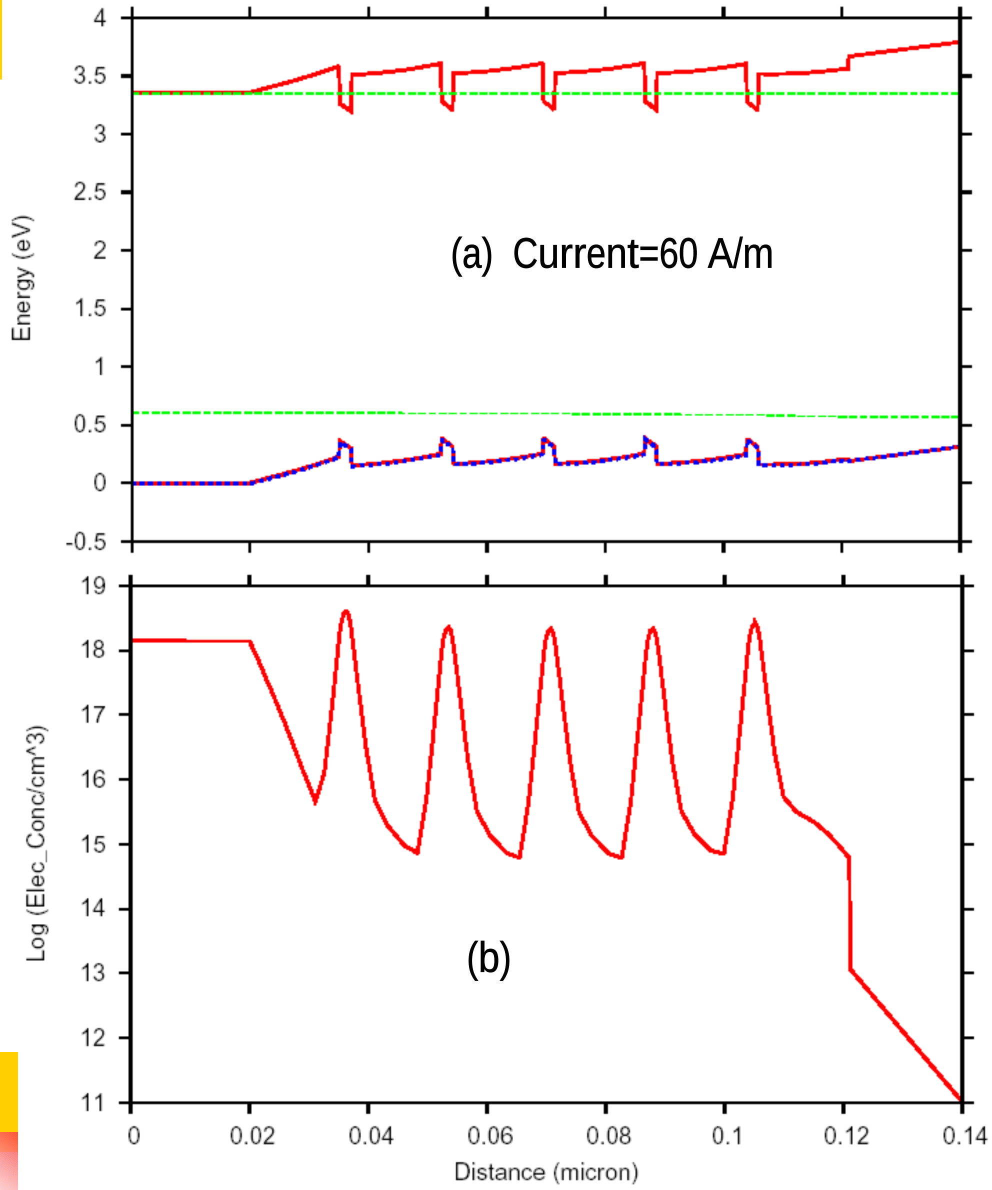


(b)

(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.

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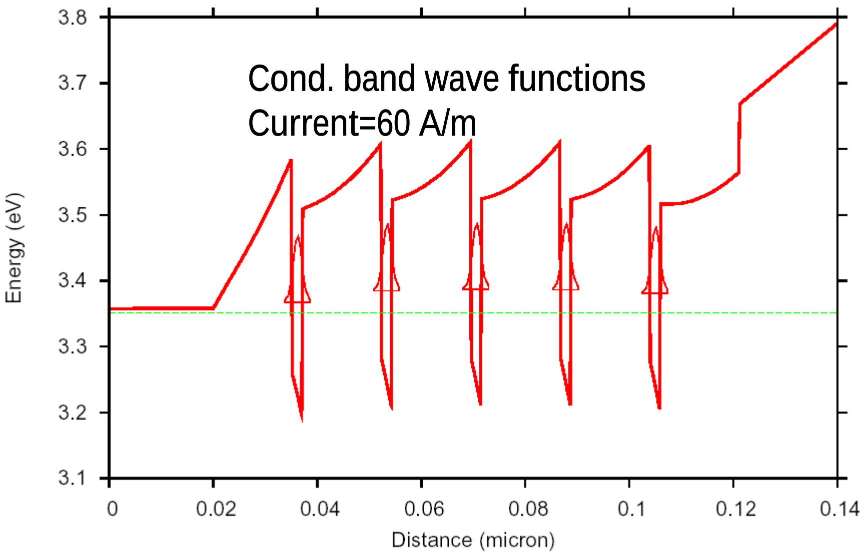
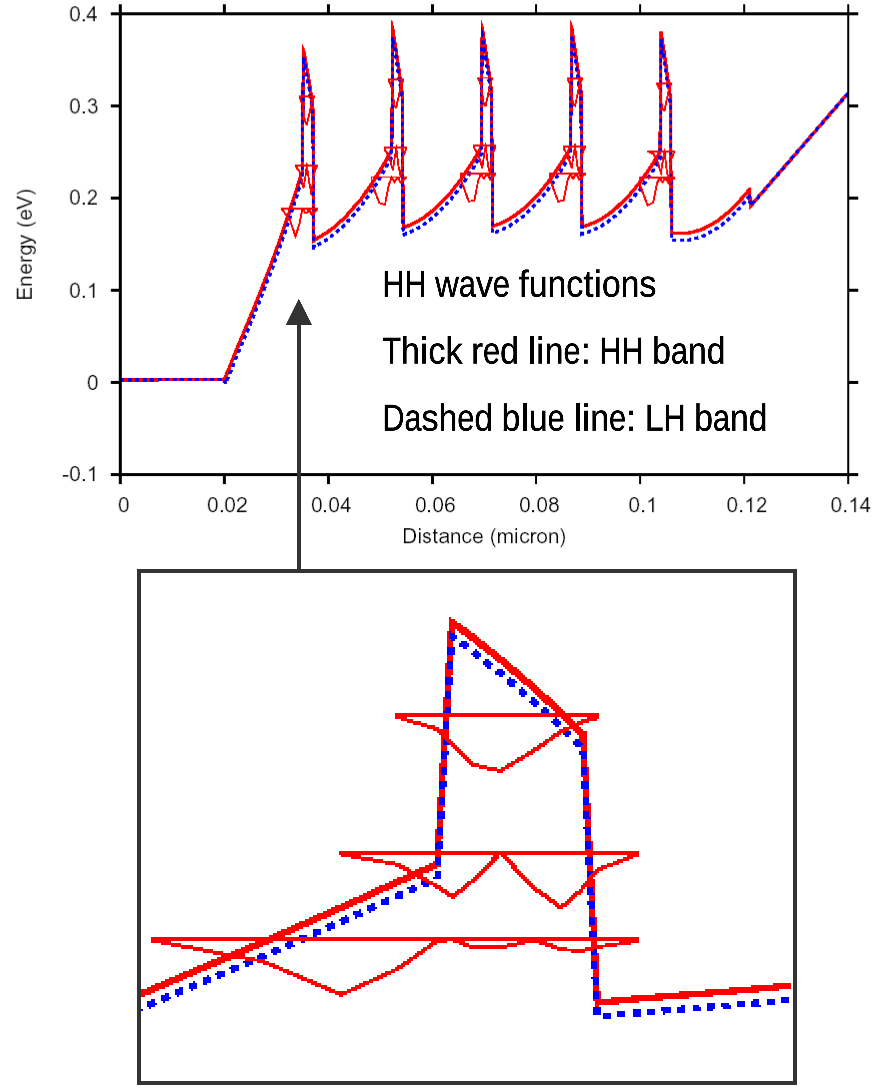
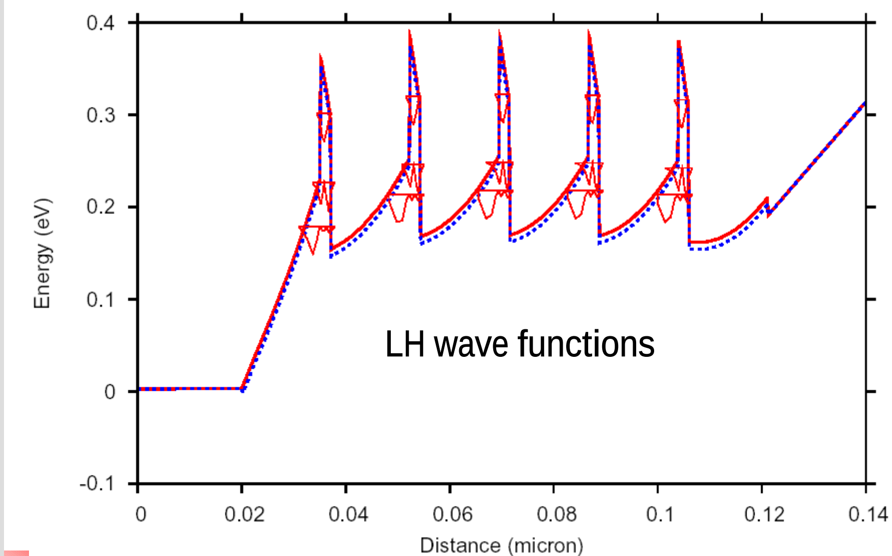
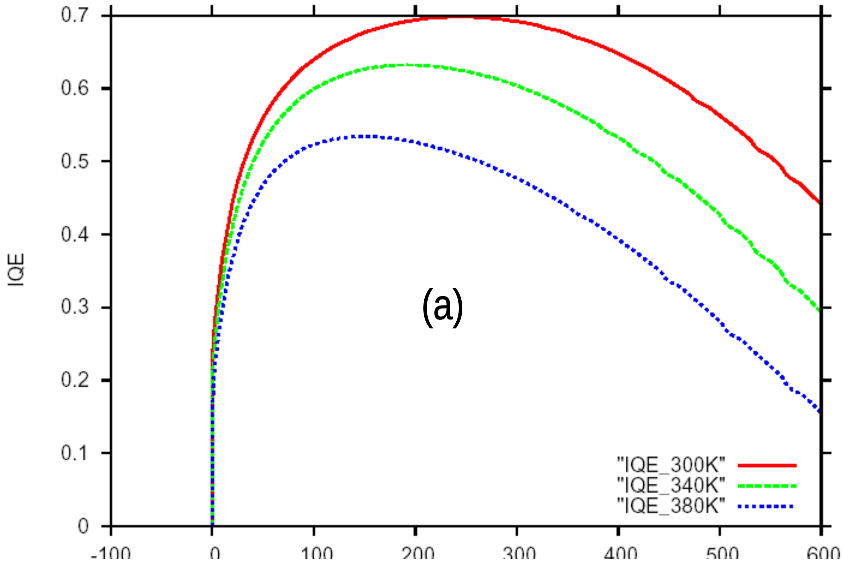
A close look at wave functions

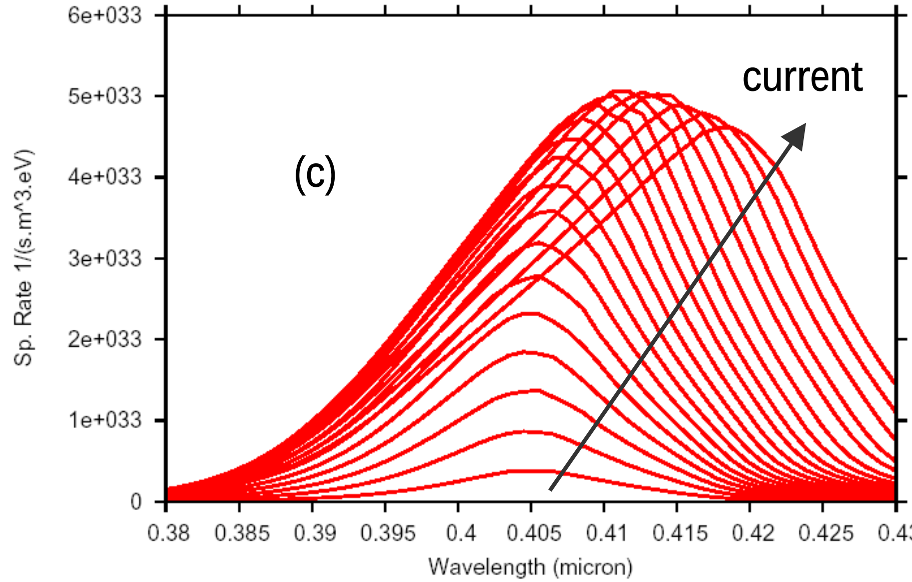


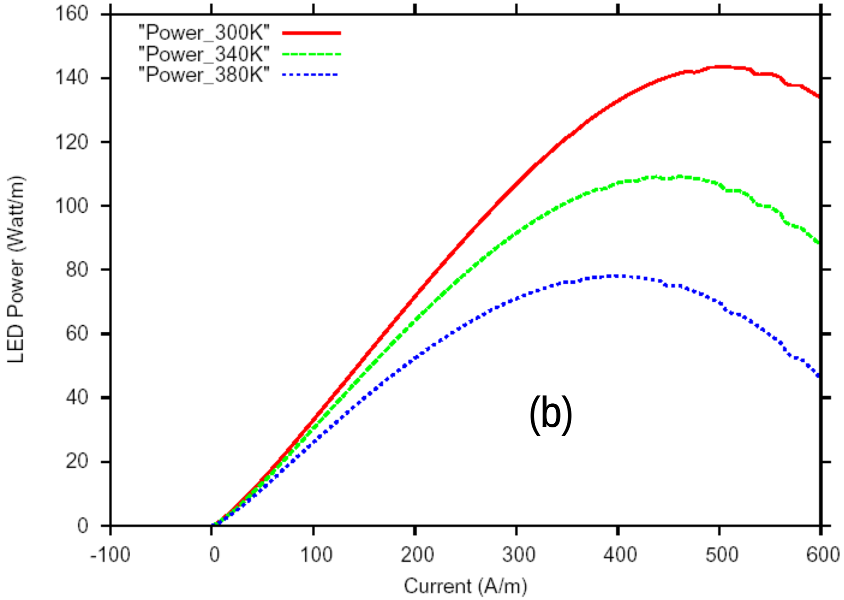




Performance





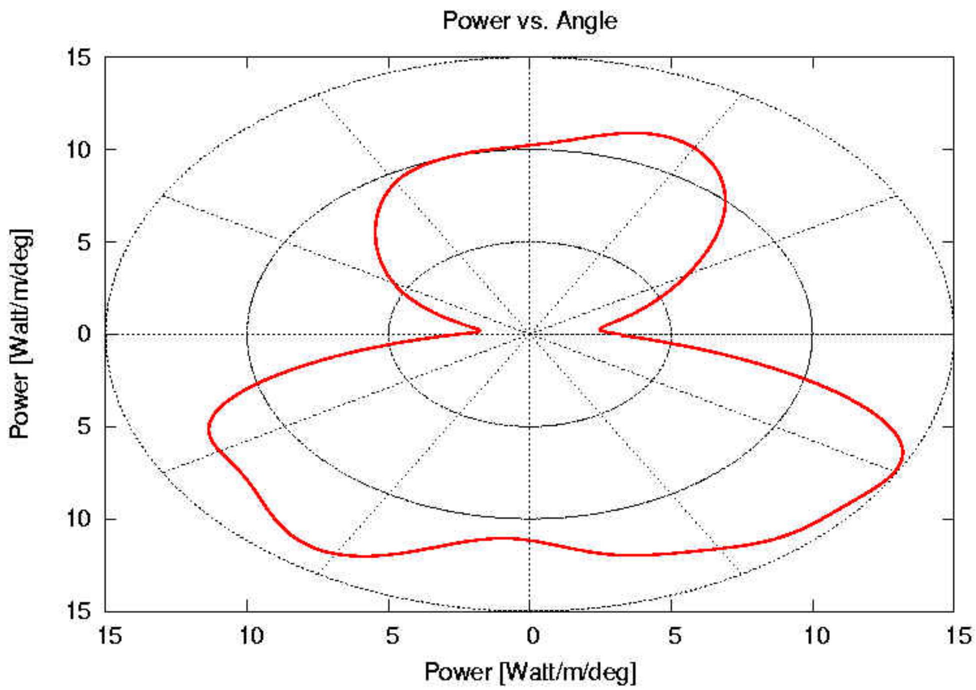


(a) IQE showing decrease at high injection condition due to thermal reduction of spontaneous emission rate.

(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.

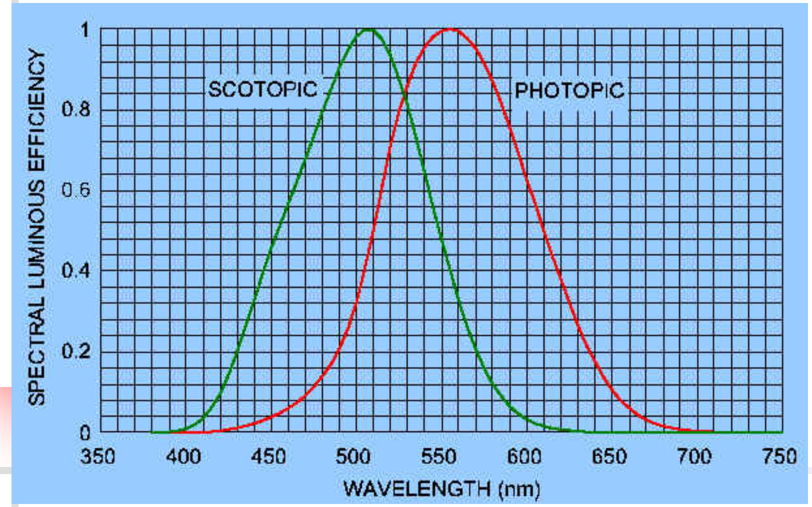
Power vs. angle from ray-tracing



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)

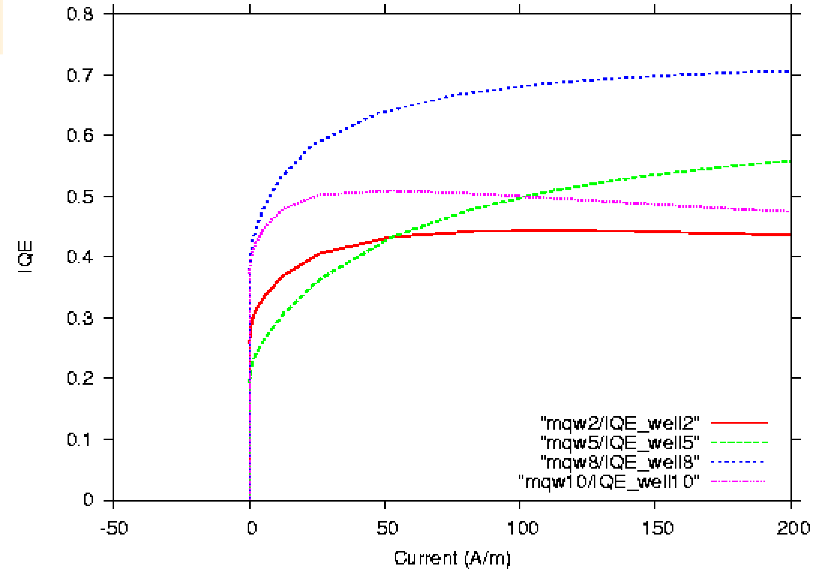
Factor of ½ above ensures integral over 4pi stereo-radian equals the total light source power.

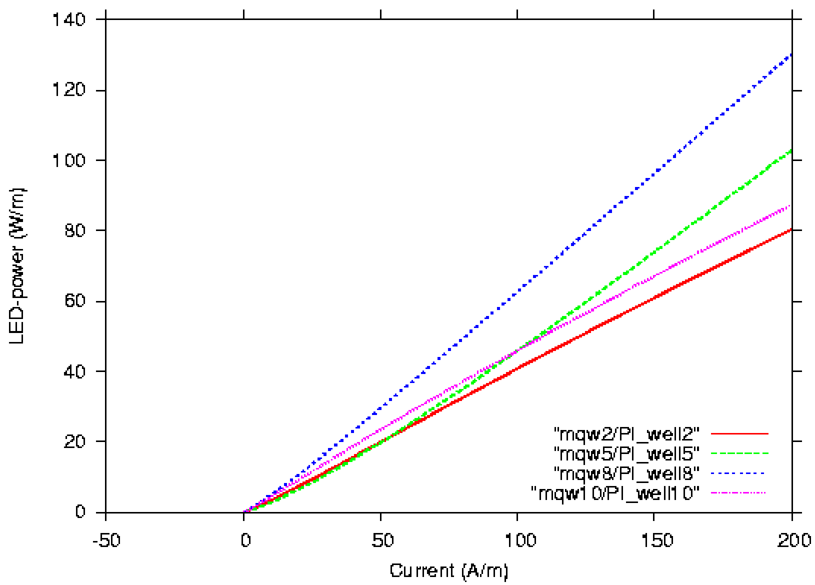


Photopic=day time eye sensitivity adapted data

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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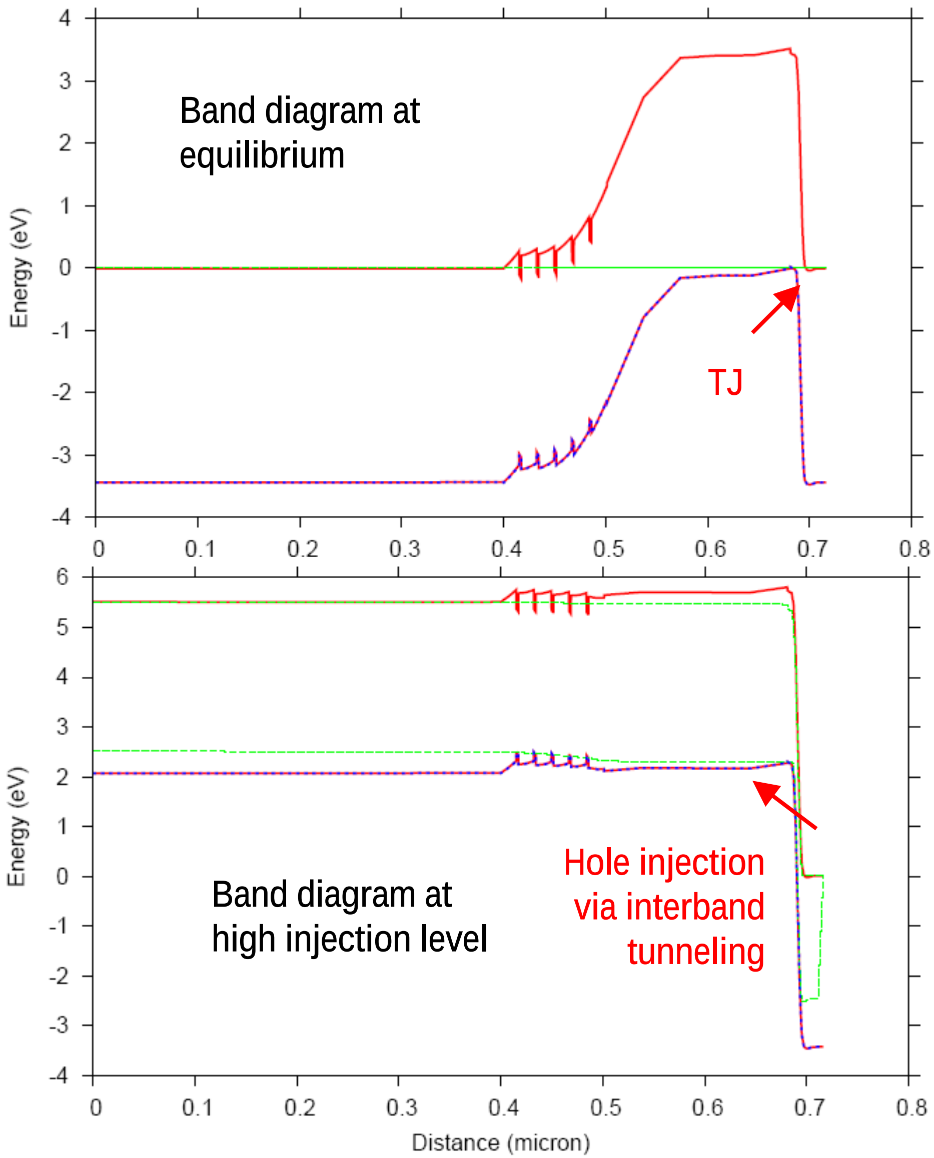
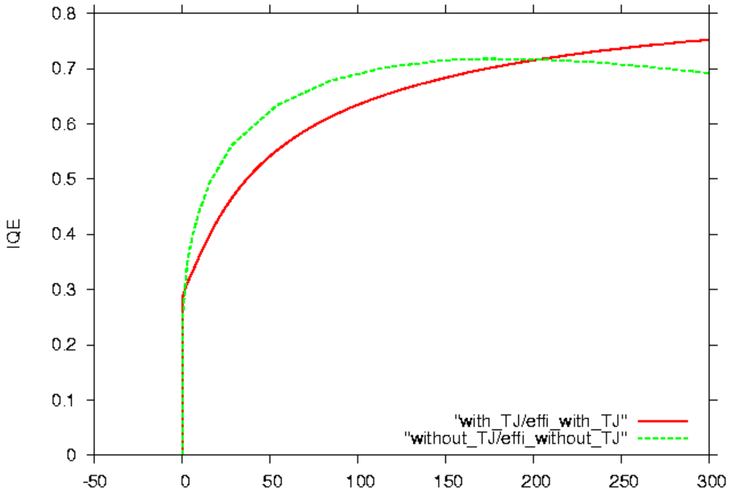
Tunnel junction contact design

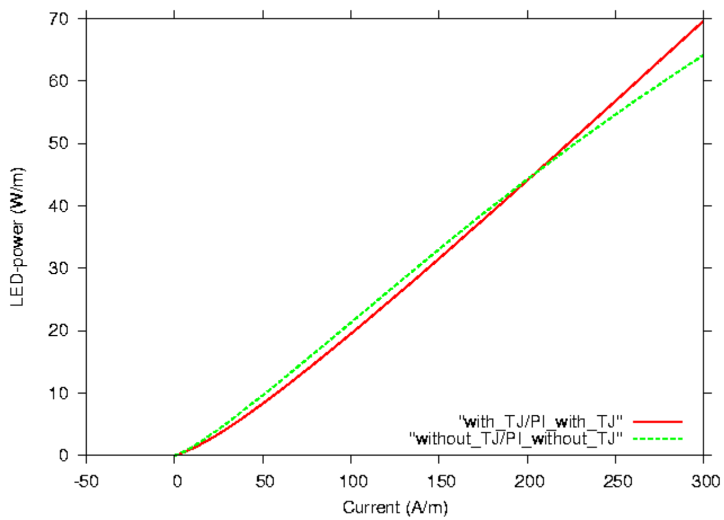


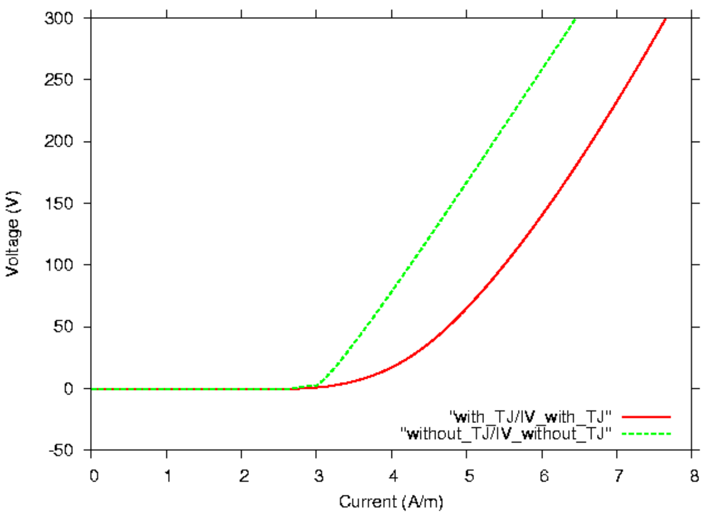
p-GaN's conductivity is low and thus carrier crowding is a limiting factor in GaN LEDs. Tunnel junction (TJ) can be used to supply holes efficiently to the p-type region by electron tunneling effects. S.R. Jeon et al., "Lateral current spreading in GaN-based light-emitting diodes utilizingtunnel contact 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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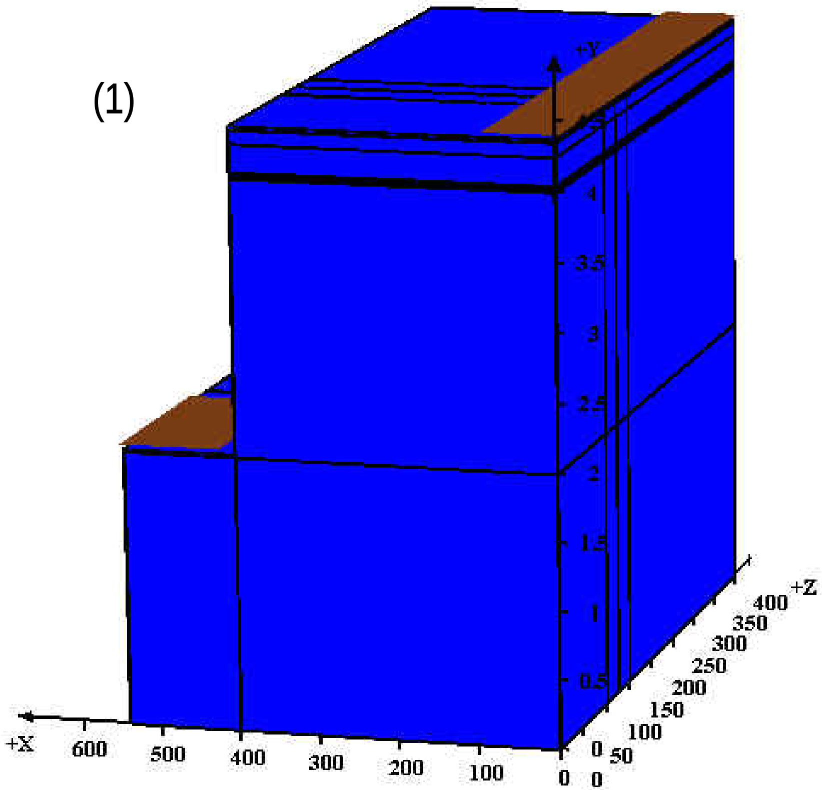
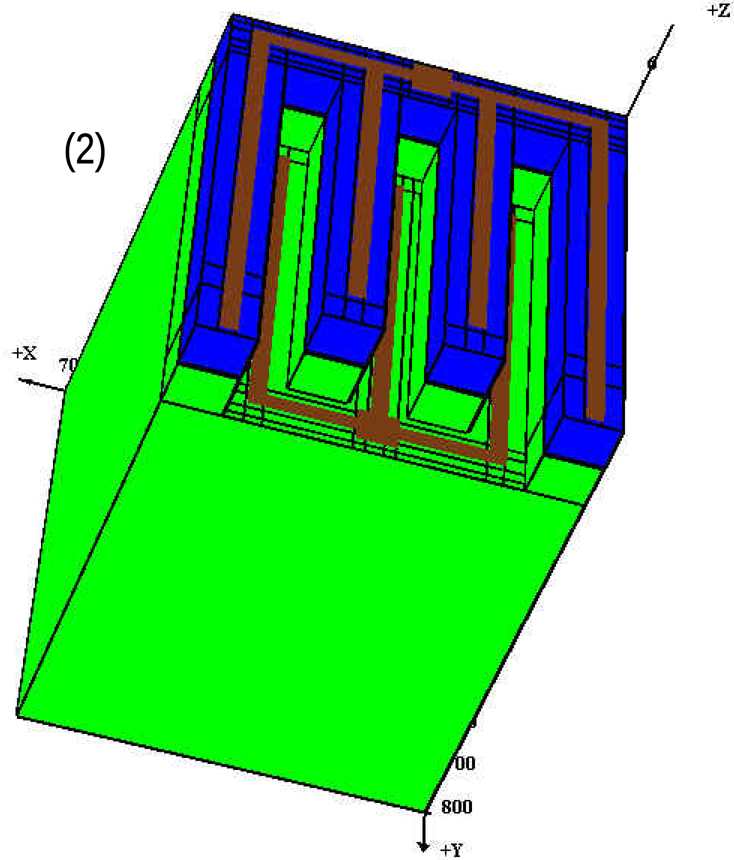
Two 3D configurations

(1)



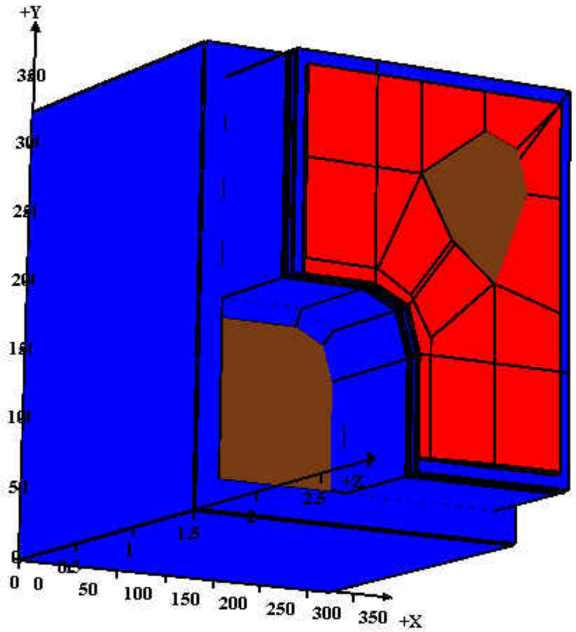
(2)



(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

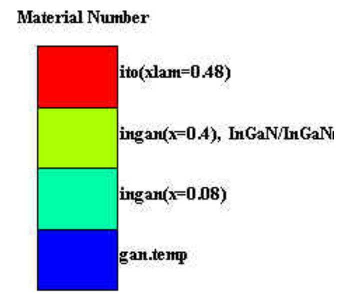


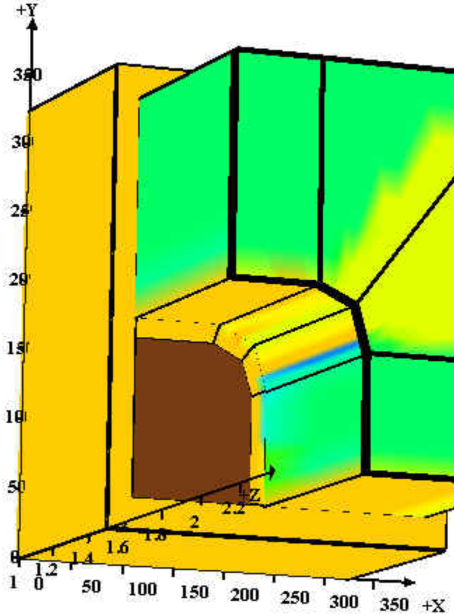
File Name : rotstd_0007
File Type : APSYS

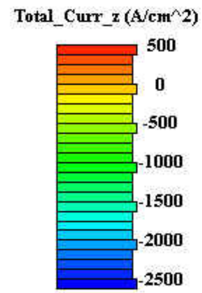
Variable Name :
Material Number

3D Cube Contour Parameters :
X Range : 0 - 325
Y Range : 0 - 325
Z Range : 0 - 2.081

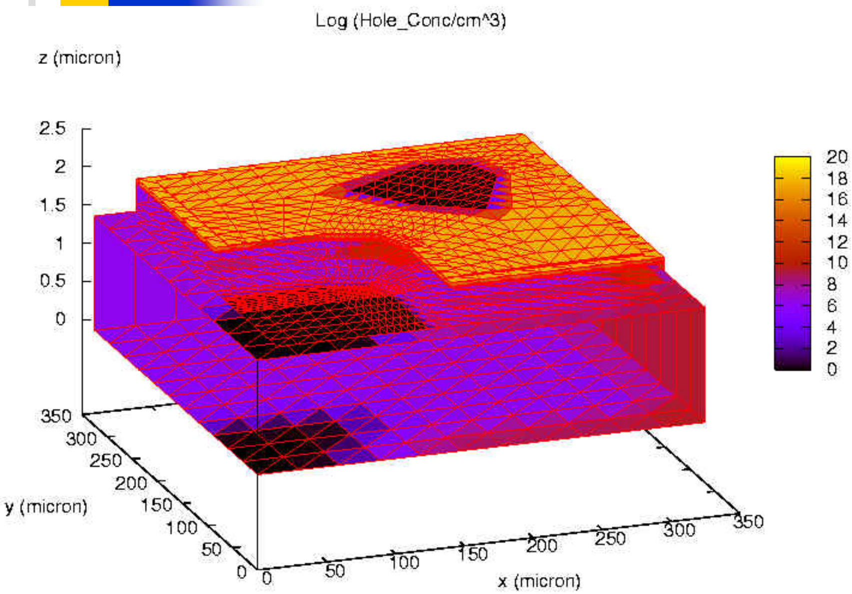
X Cut Line Num : 20
Y Cut Line Num : 20
Z Cut Line Num : 20

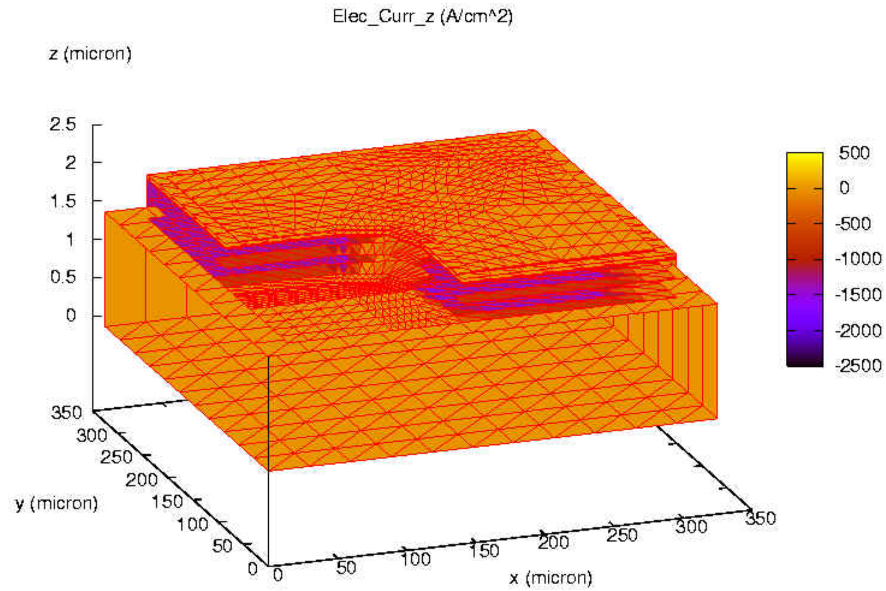


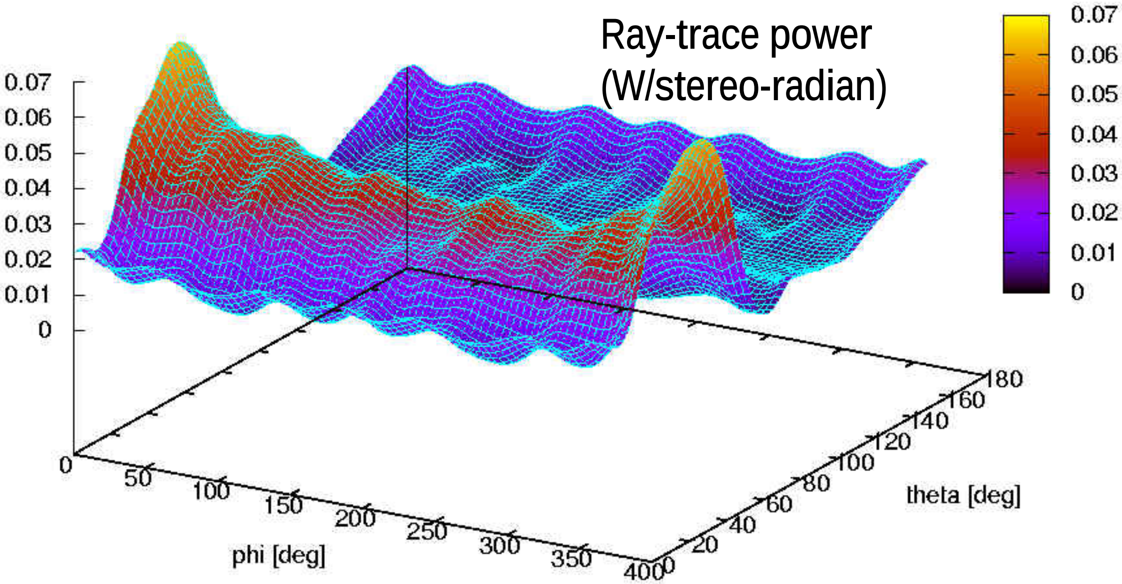


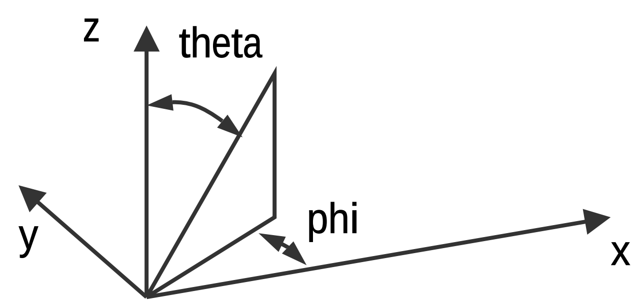


More 3D results









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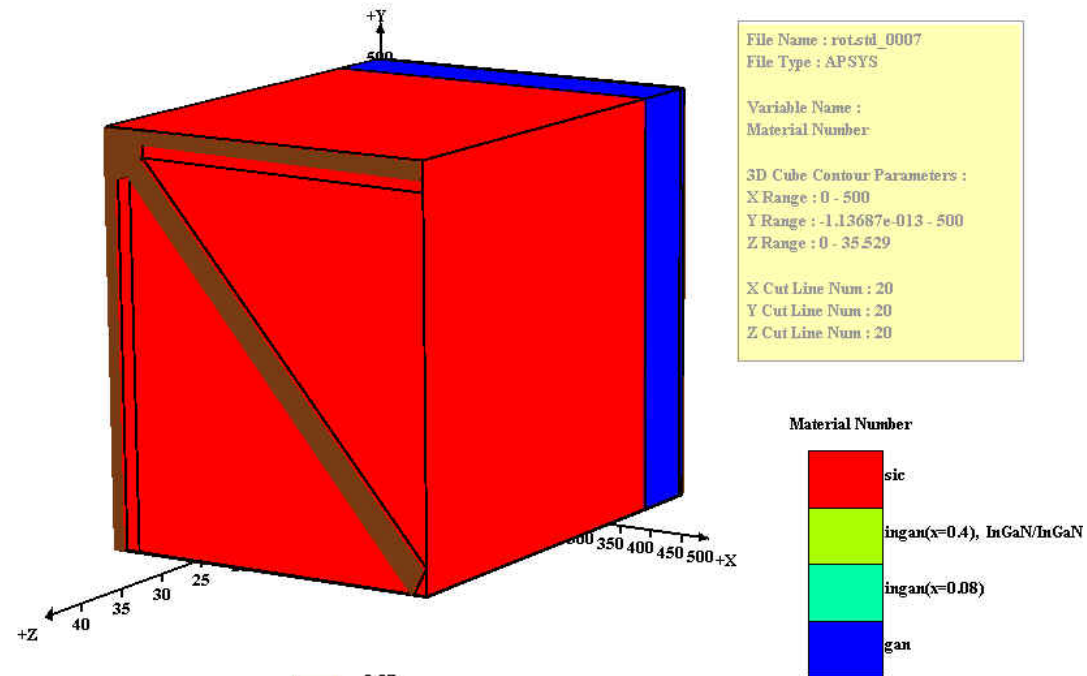
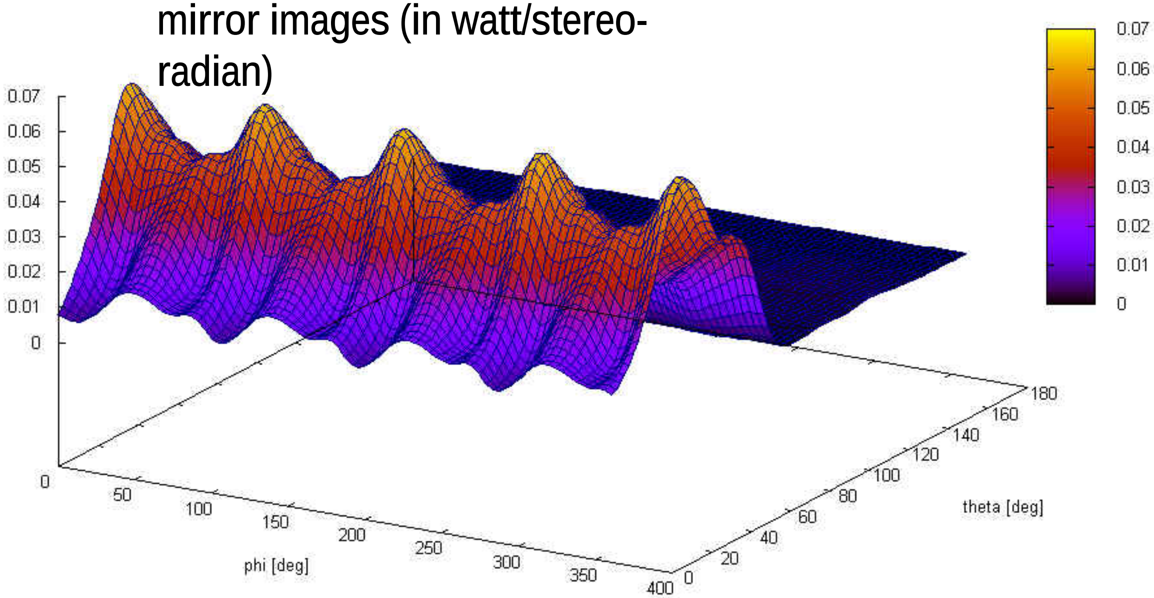
3D mirror boundaries

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.

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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.