

3D Simulation of Nanowire / Nanotube Light Emitting Diode

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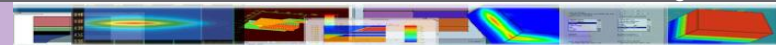
Physical models

- Self-consistent calculation combining quantum mechanical solution with drift-diffusion simulation.
- Polarization charges may be used for polar or semi-polar interfaces.
- Thermal model.
- Very mature GaN-based material data base incorporating latest understanding of IQE droop due to EBL doping, band-offset and polarization charges.
- FDTD extraction calculation.



Numerical Approach

- Basic device structure of a cross-section constructed using the user-friendly GUI LayerBuilder.
- Cross-section converted to a 3D format compatible with the new 3D GUI SemiCrafter.
- Symmetric polygons structures are formed using the `change_material` operation.
- As a preliminary demo, 15K mesh points used for a single tube with single quantum well.
- A typical I-V scan costs about 20 minutes on an i5 laptop with Windows 7 OS.

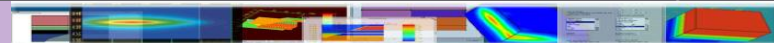
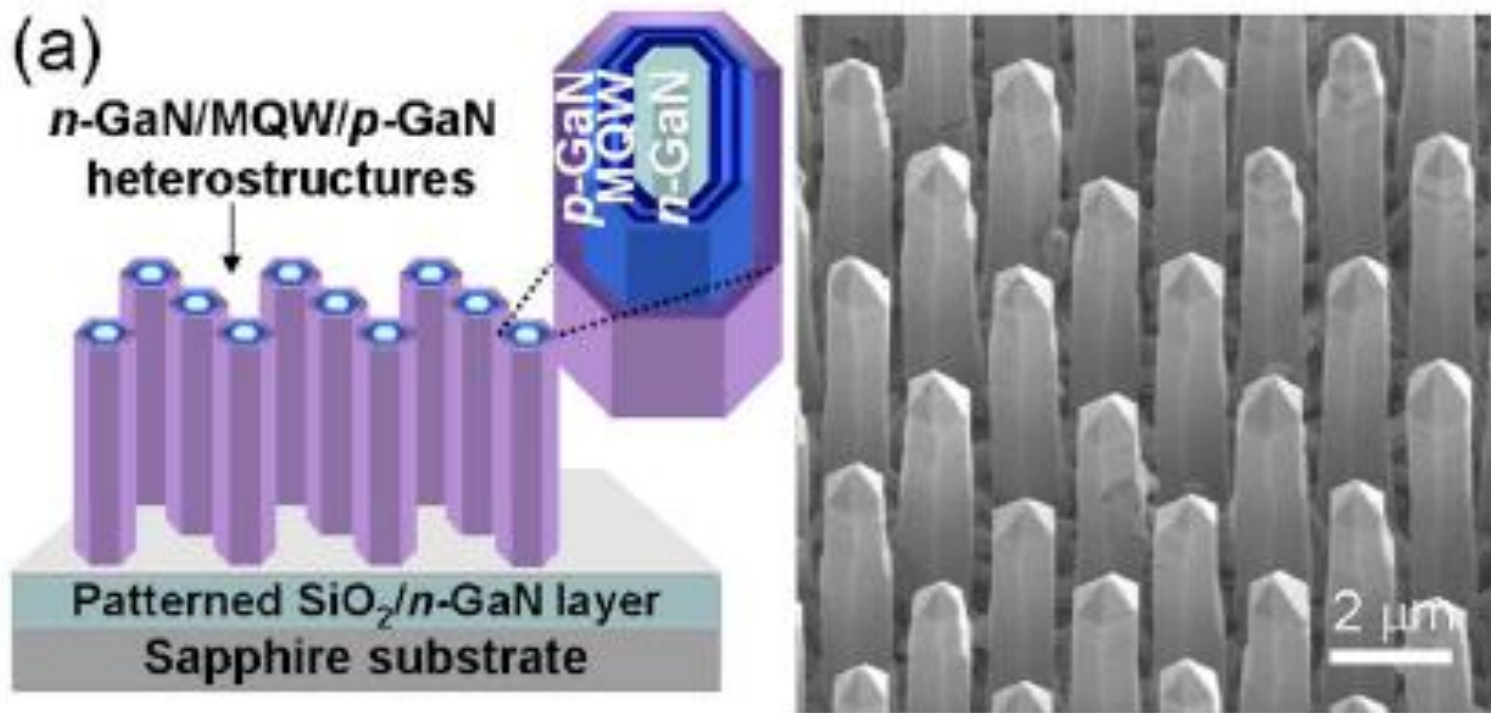


Reference structure:

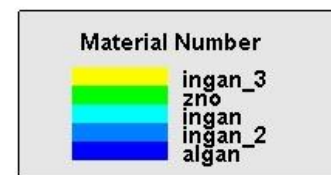
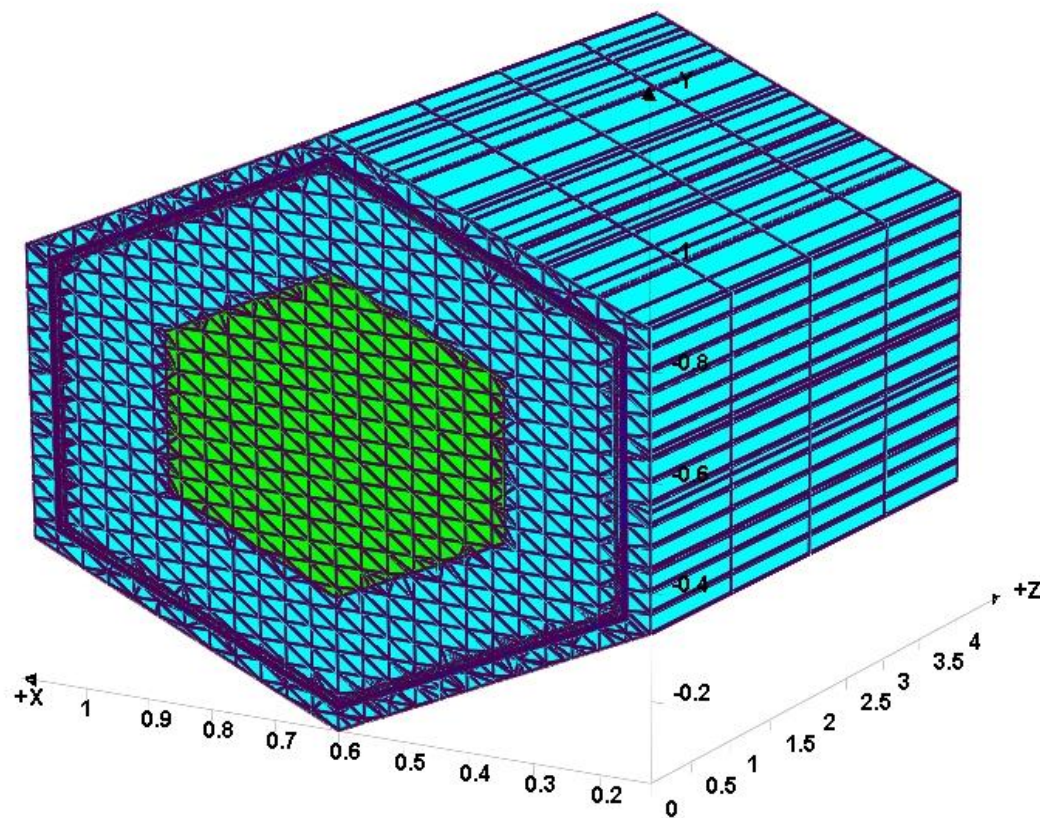
APPLIED PHYSICS LETTERS
94, 213101 2009

GaN/ In_{1-x}GaxN/GaN/ZnO nanoarchitecture light emitting diode microarrays

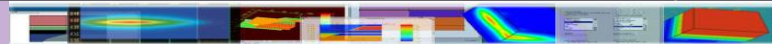
Chul-Ho Lee, Jinkyung Yoo, Young Joon Hong, Jeonghui Cho,
Yong-Jin Kim, Seong-Ran Jeon, Jong Hyeob Baek, and Gyu-Chul Yi



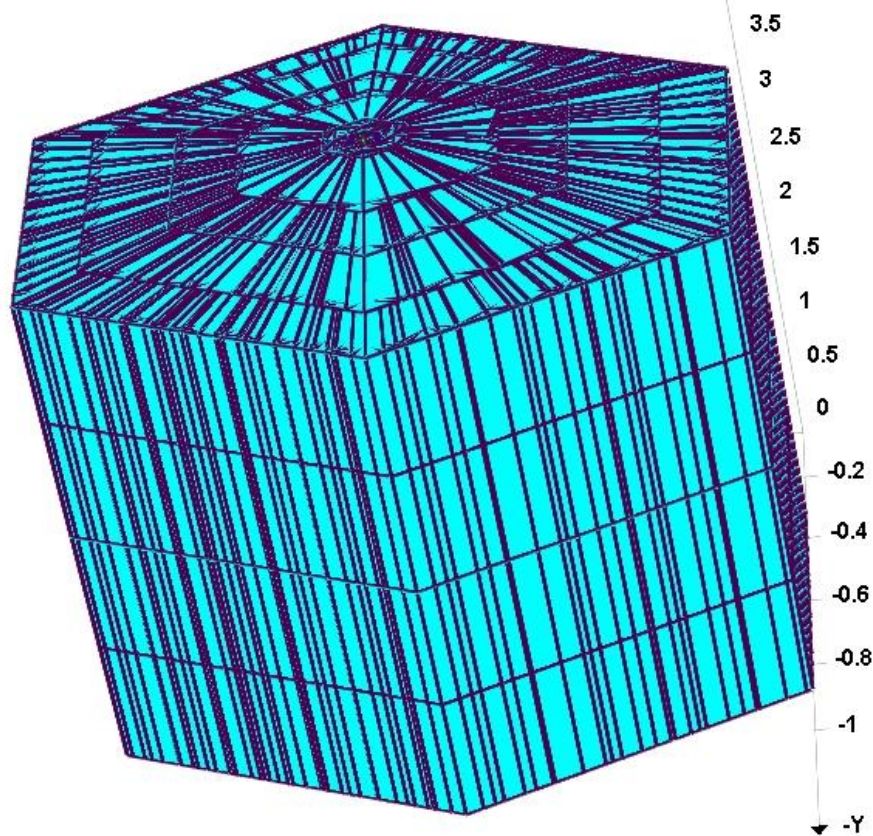
3D mesh; bottom view:



X=0.123686, Y=0.148695, Z=2.317



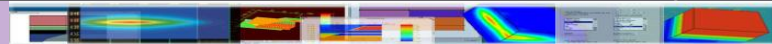
3D mesh; top view:



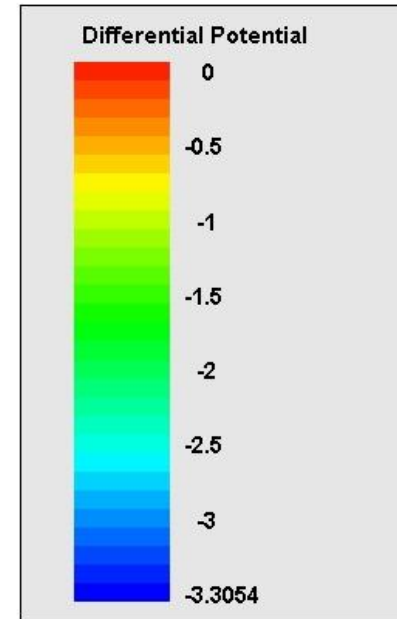
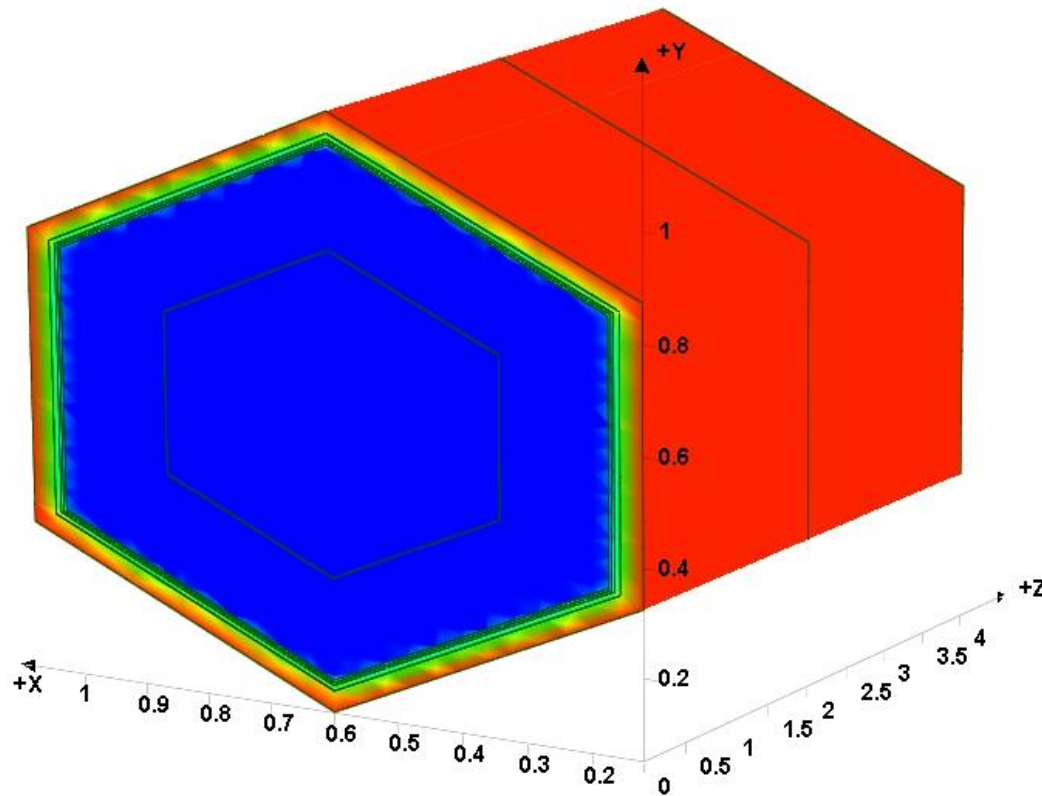
Material Number



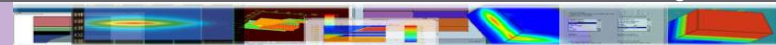
X=0.0960945, Y=-0.764768, Z=4.4



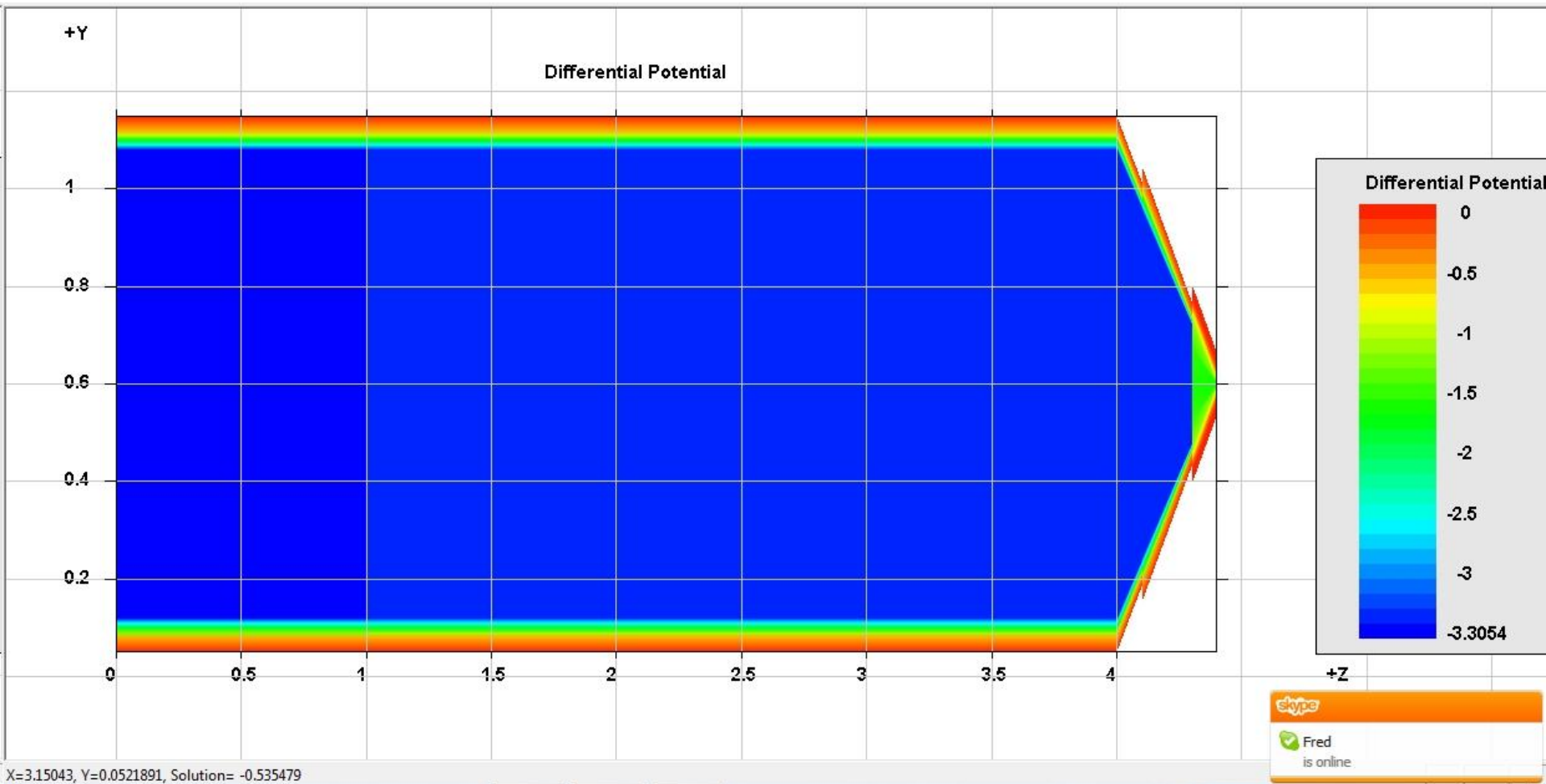
Nanowire /nanotube 3D potential distribution



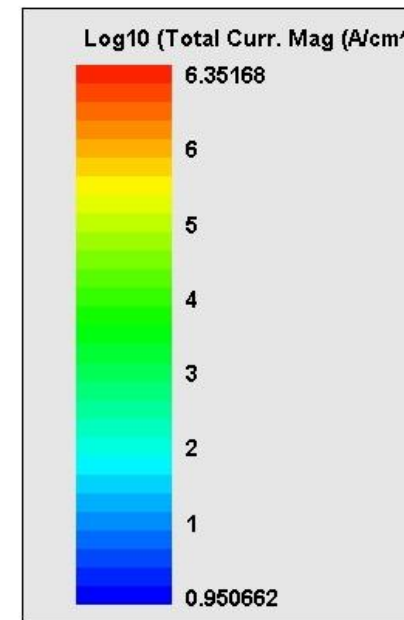
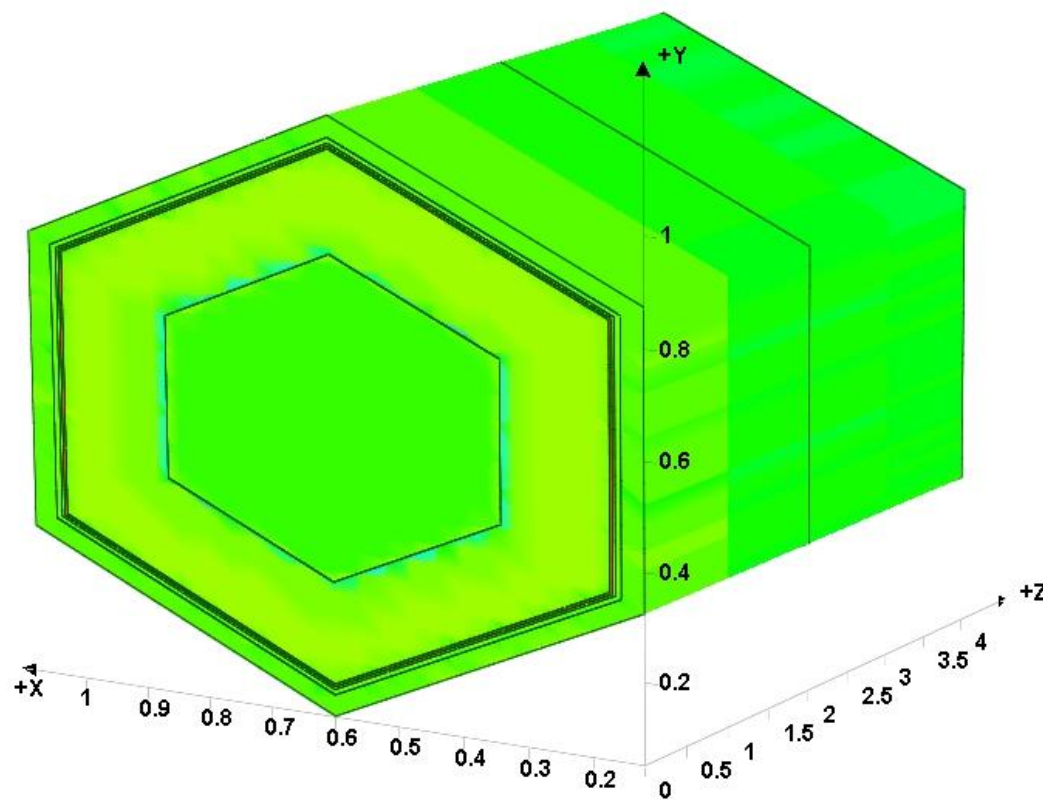
X=-0.163577, Y=0.200309, Z=-1.34502e-006



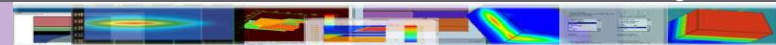
Potential distribution: y-z plane



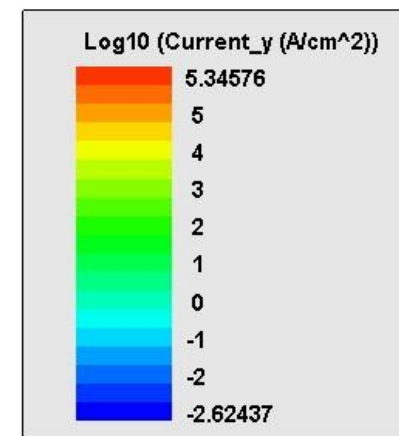
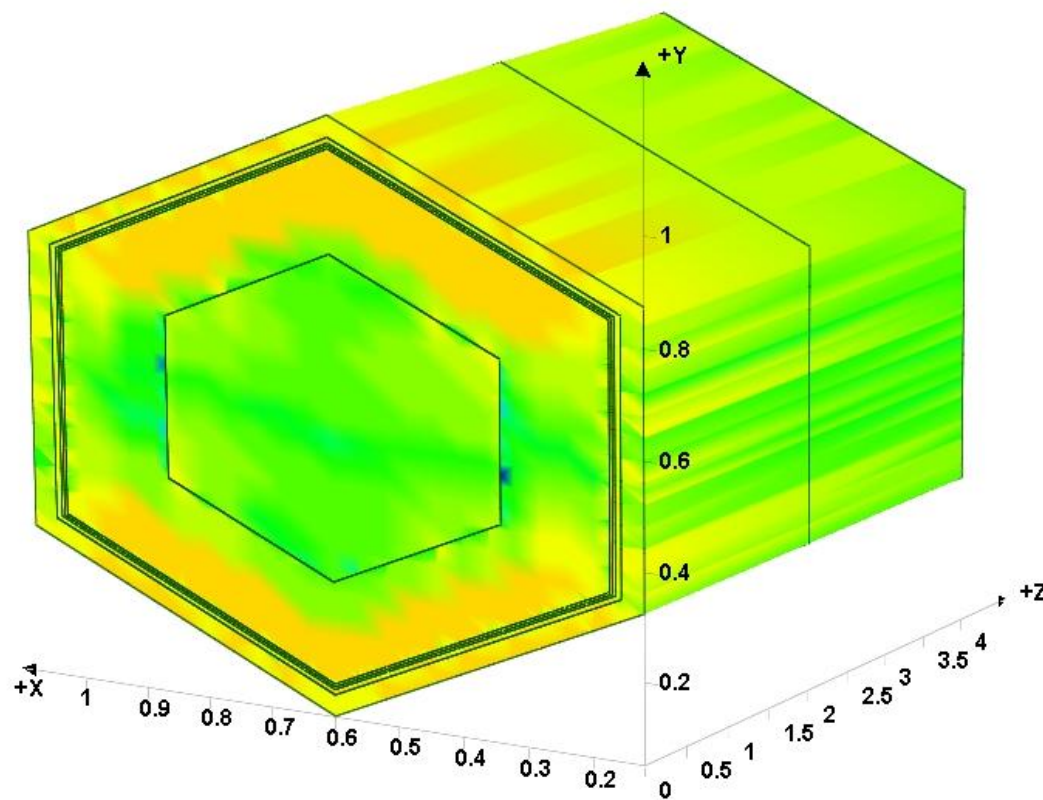
Nanowire current flow distribution



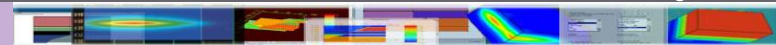
X=-0.194588, Y=0.189131, Z=-1.34263e-006



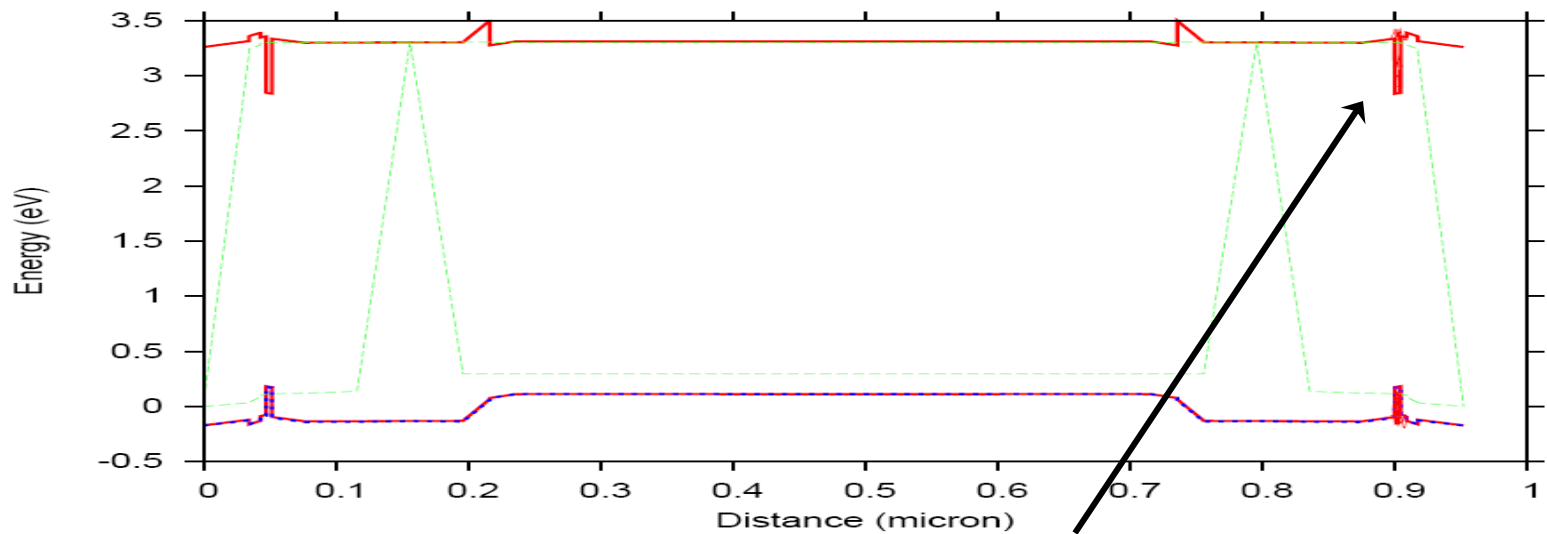
Nanotube current y-comp. distribution



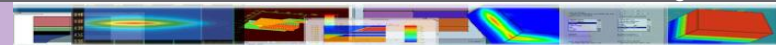
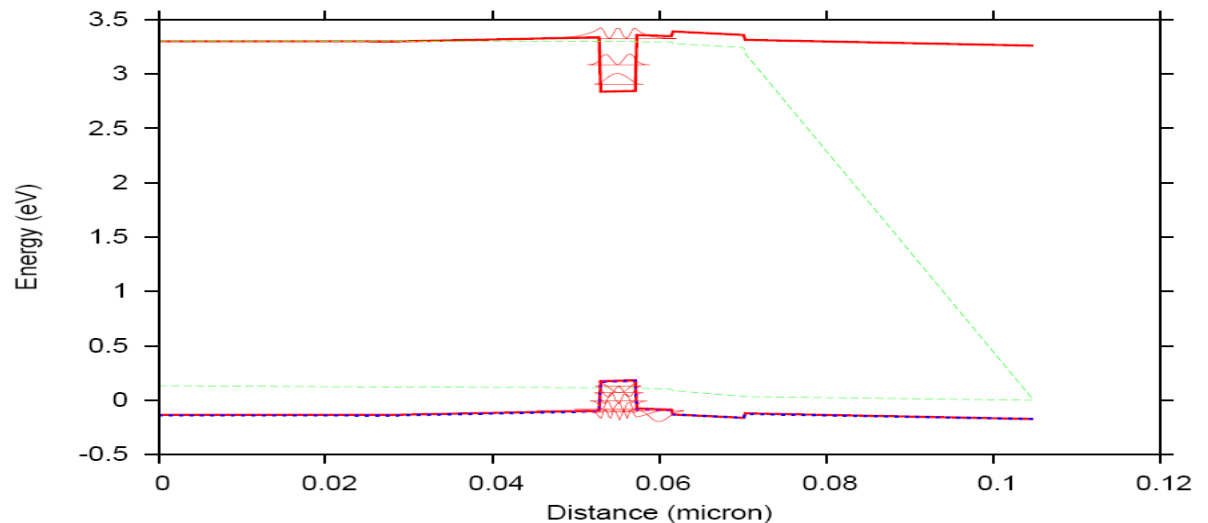
X=-0.201233, Y=0.187499, Z=-1.34212e-006



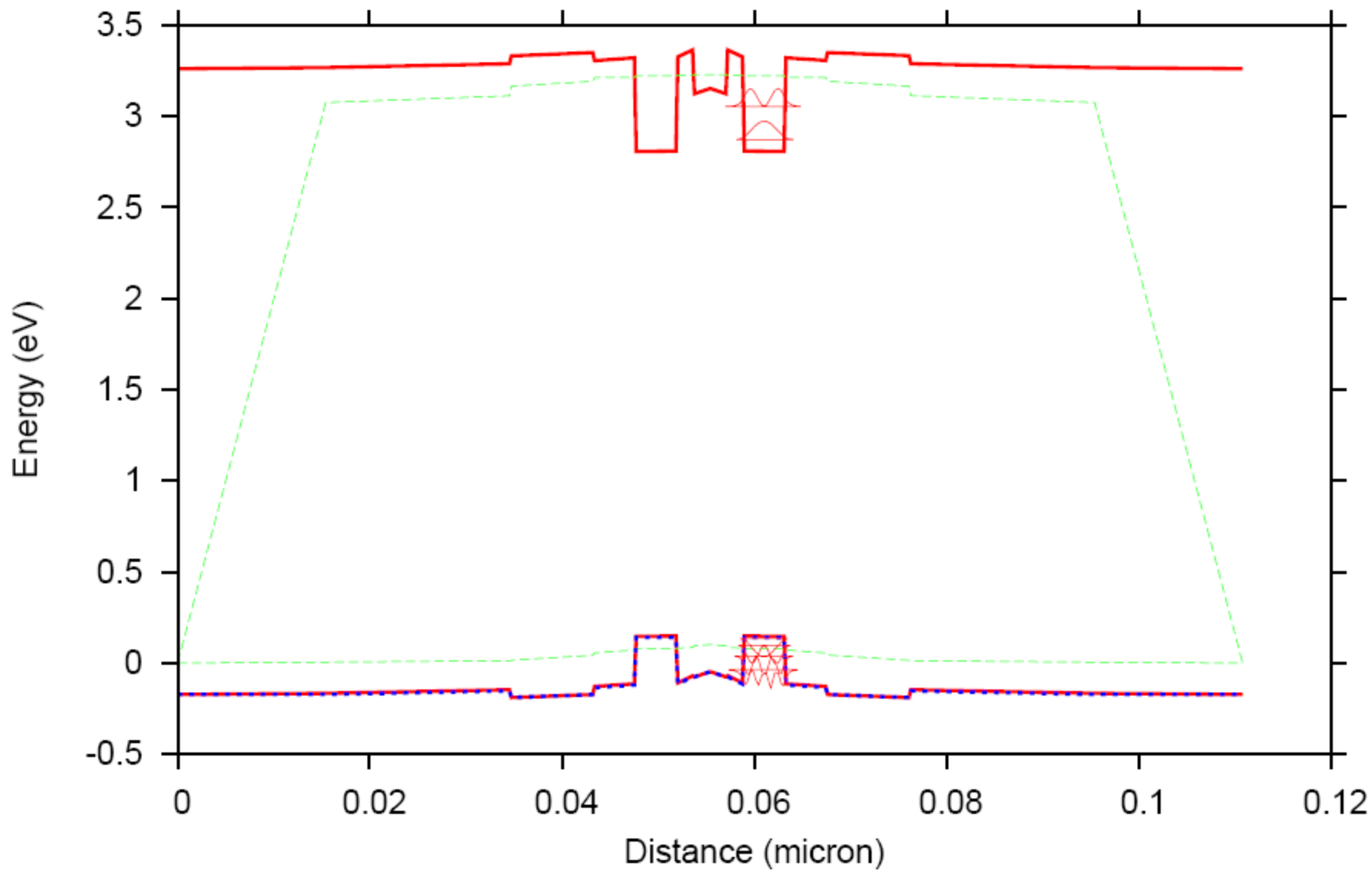
Nanotube band structure



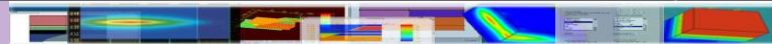
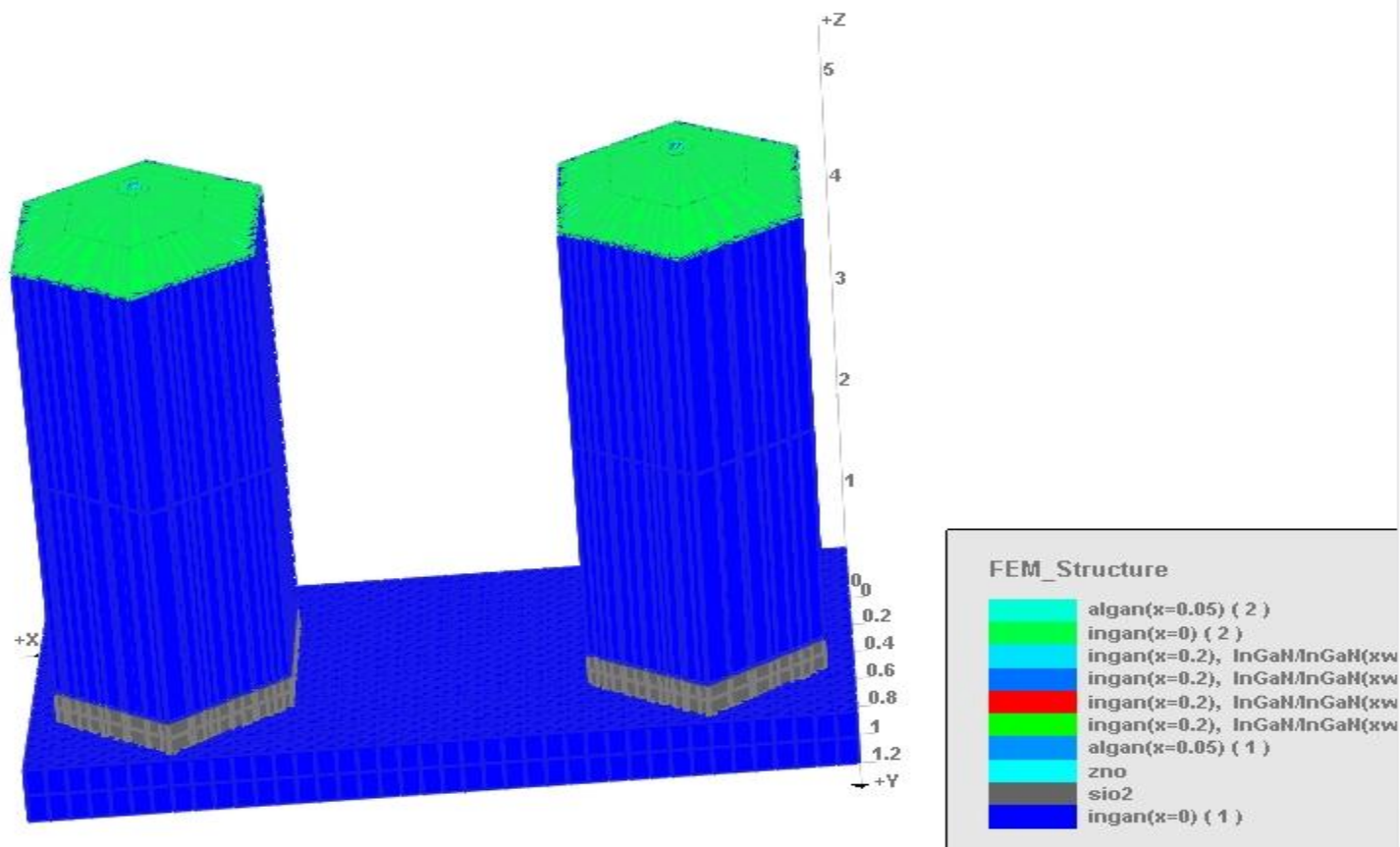
Cross-section
made across the
wire with single
quantum well of
InGaN/GaN



Nanowire band structure at the tip

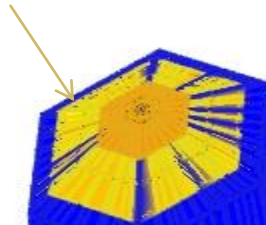


Multiple nanowires in same 3D simulation

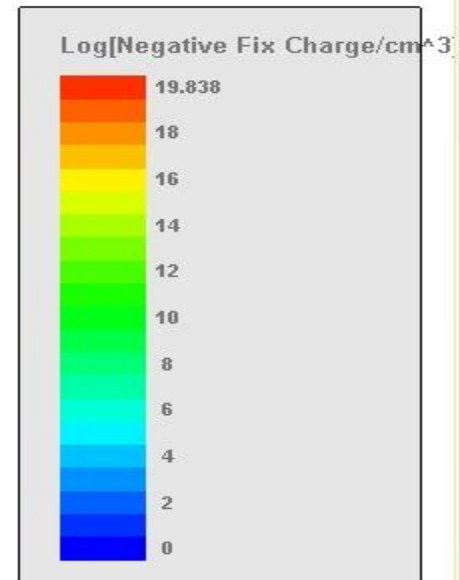
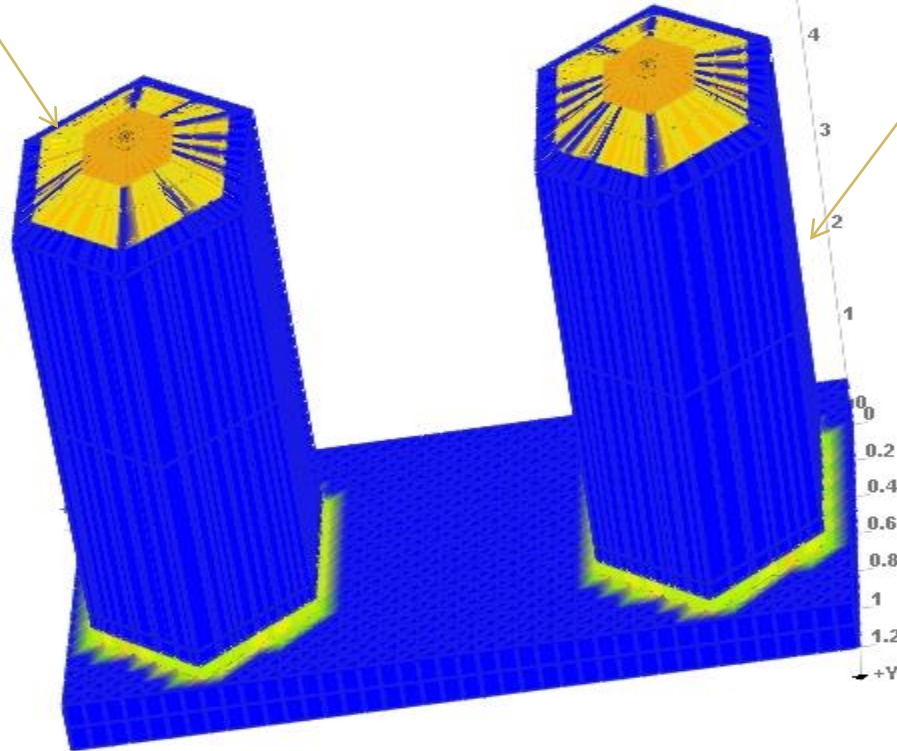
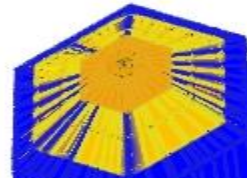


Nanotube crystal orientation models.

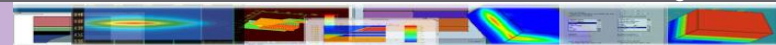
MQW of (1 1 -2 1)



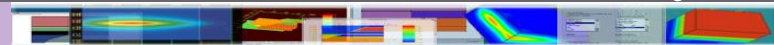
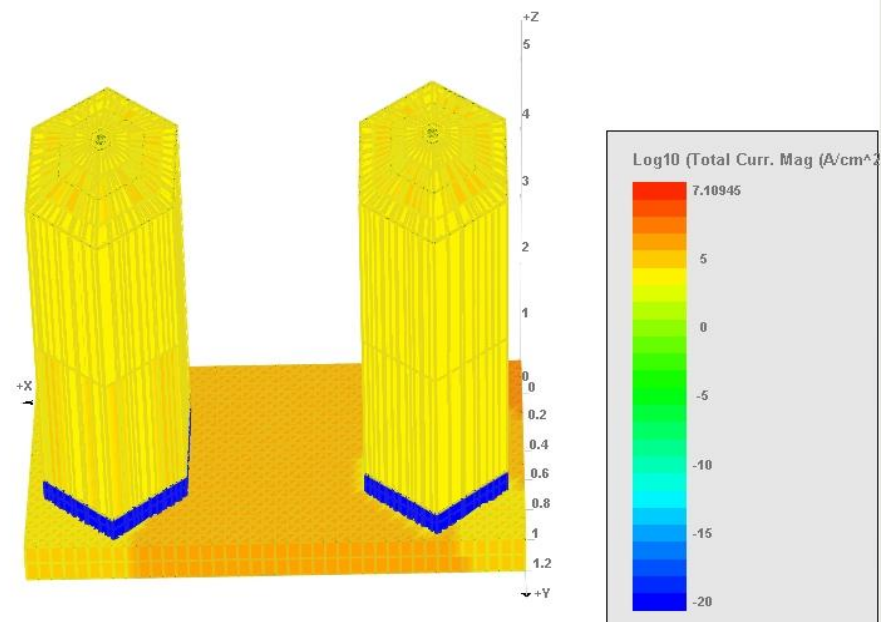
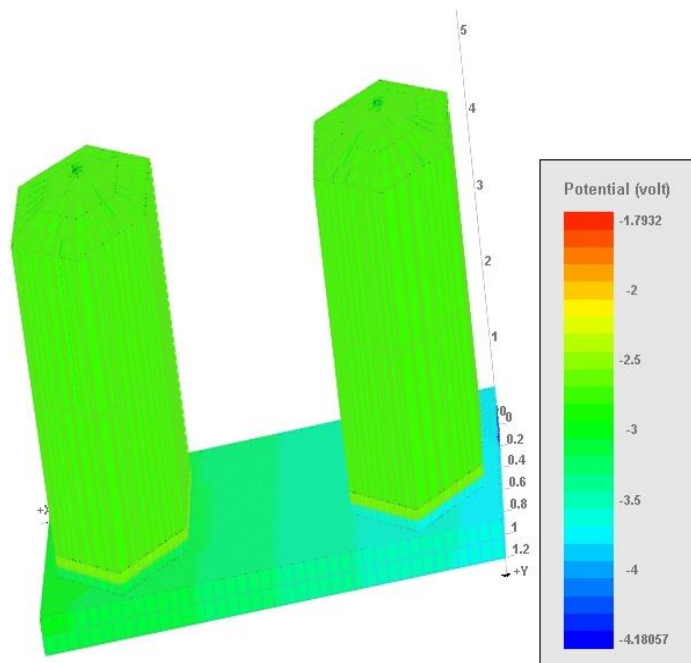
MQW of (1 0 -1 0)
m-plane



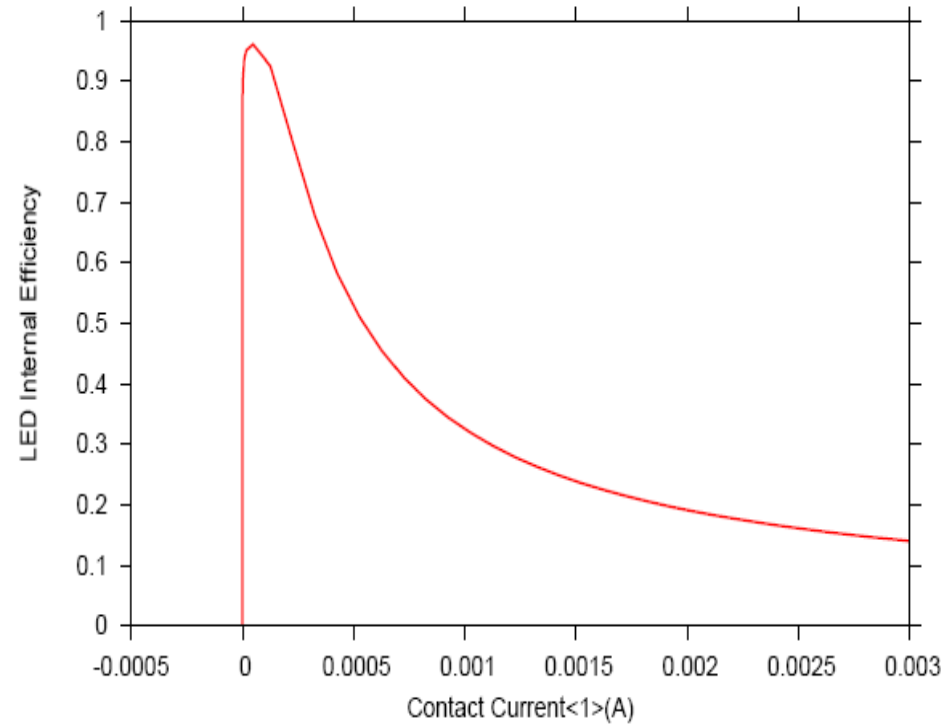
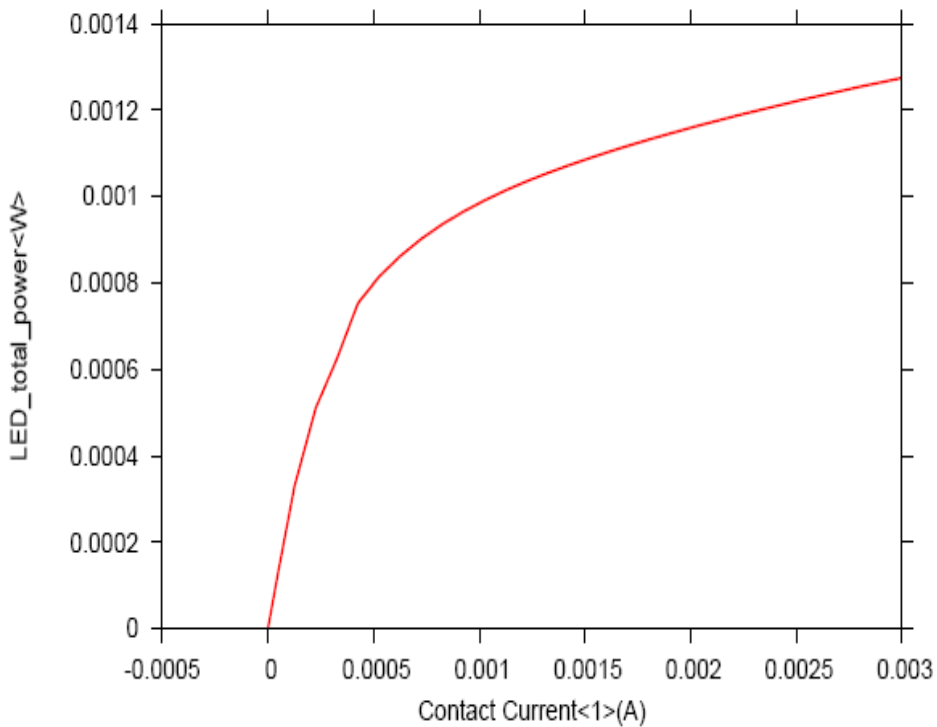
Polarization charge appears at bottom
and on the tip of the nanowire



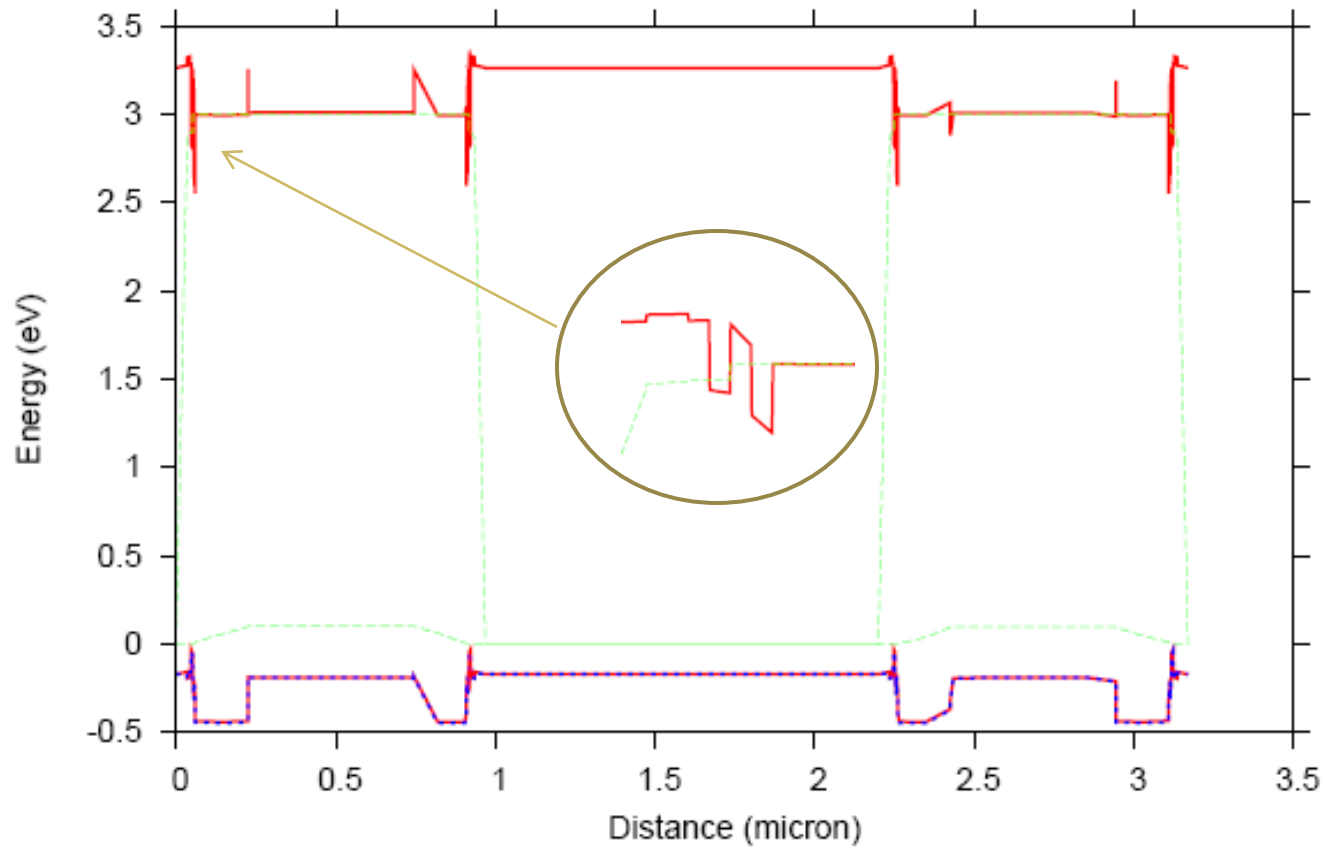
Potential and current flow



Nanowire LED power and IQE

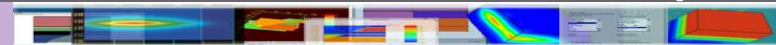


Band diagram of MQW



Conclusions

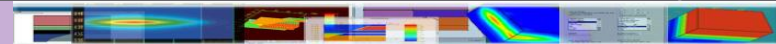
- Efficient numerical simulation with advanced physical models established for GaN-based nanowire or nanotube LED.
- Initial simulation studies show promising results with much optimization needed ahead.
- Electron current overflow has been determined to be the main limitation in such devices.



A Glimpse

Crosslight Software

- 🏠 A leading TCAD provider since 1993
- 🏠 The world's No.1 TCAD simulator for optics and photonics application
- 🏠 The world's first commercialized TCAD for Laser Diode
- 🏠 Customer list extends to hundreds of companies, research institutions and universities world wide.
- 🏠 Originally licensed from the National Research Council Canada and later from Stanford University
- 🏠 Complete product portfolio for 2D/3D semiconductor device simulation
- 🏠 *Café-time Simulator*. Windows based, user friendly graphic user interface makes simulation more enjoyable.



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