Quantum and Non-local Transport Models in Crosslight Device Simulators

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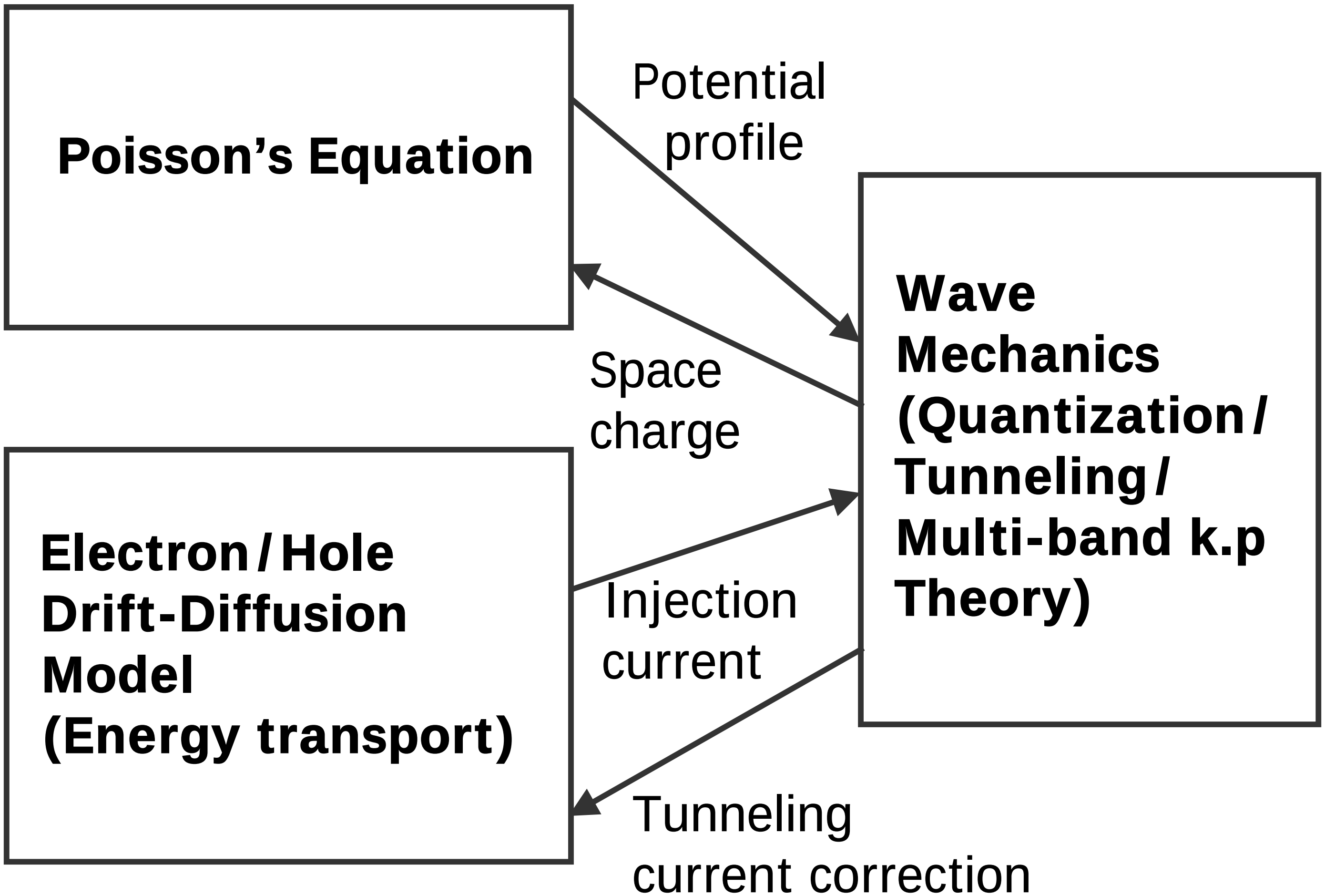
Content

- **Introduction**
- **Quantization effects**
  - Self-consistent charge-potential profile.
  - Space charge distribution and recombination.
- **Non-local quantum transport models**
  - Intraband tunneling.
  - Interband tunneling (tunneling junction).
  - Mini-band tunneling (superlattice).
  - Two-Fermi-level quantum well trapping model.
  - Mean free path-controlled quantum escape.

Introduction:Device evolution

- **Optoelectronic devices:**
  - Laser diode: from double heterostructure laser to quantum well laser and VCSELs.
  - LED: from bulk to MQW and quantum dots. From red (GaAs) to blue (GaN) emissions.
  - Solar cell: from single crystalline cell to tandem thin film and multiple junction cells.
- **Silicon IC:**
  - CMOS gate length from several microns down to deep submicrons.
  - Semiconductor from pure Si to strained Si on SiGe and with various dielectric/drain contact materials.
- **Modeling techniques:**
  - Inclusion of quantum mechanics (QM) into classical drift-diffusion equation solvers.
  - Modification of local drift-diffusion transport to include non-local quantum transport effects.

Integrated Quantum-Drift-Diffusion Model



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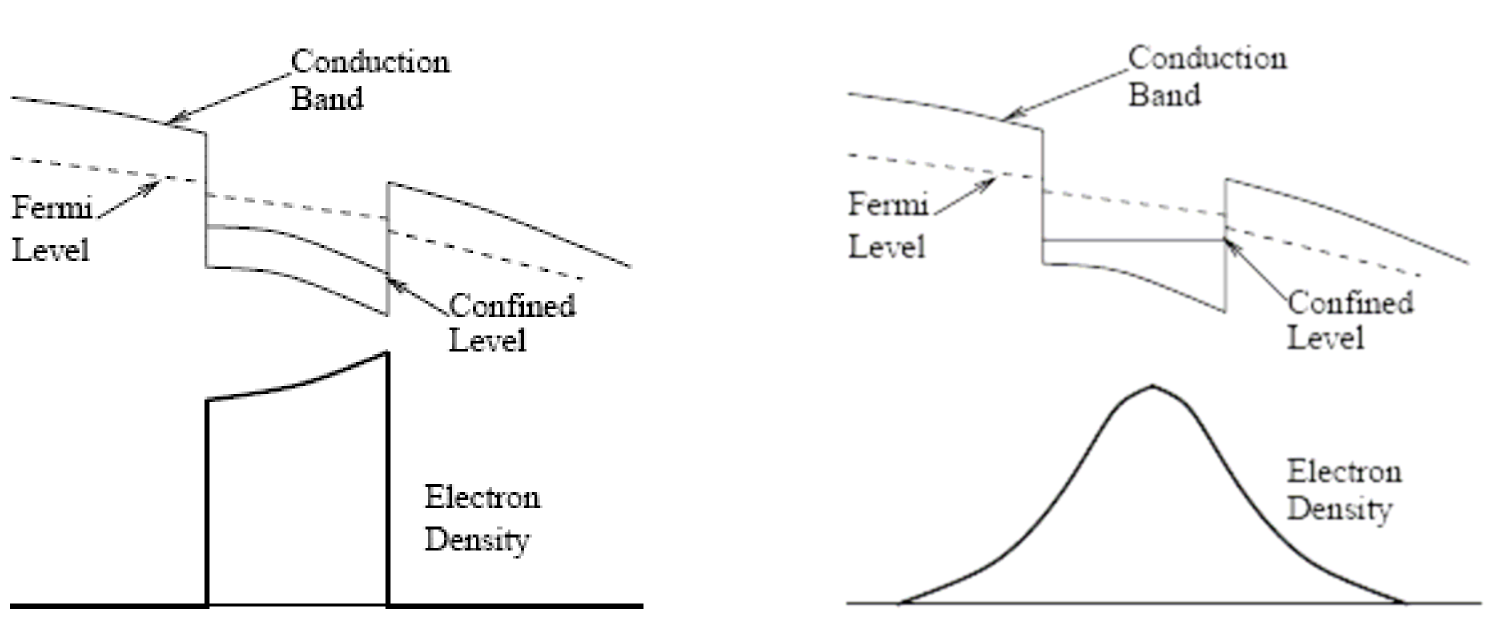
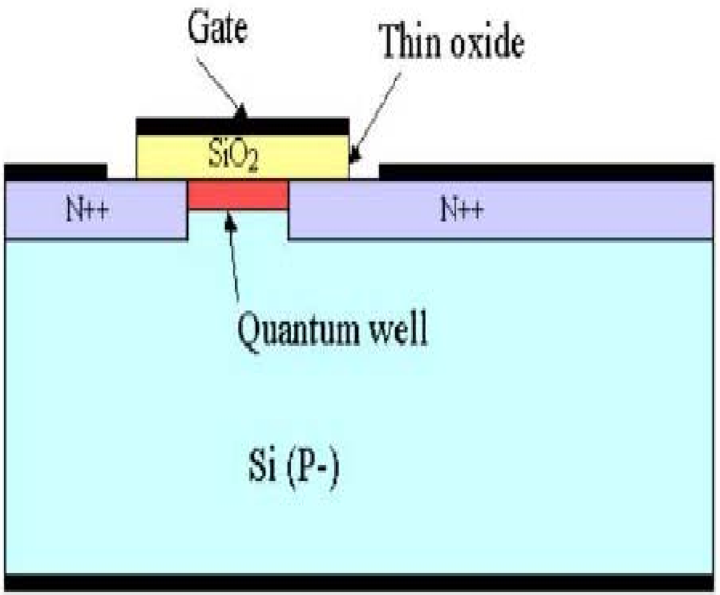
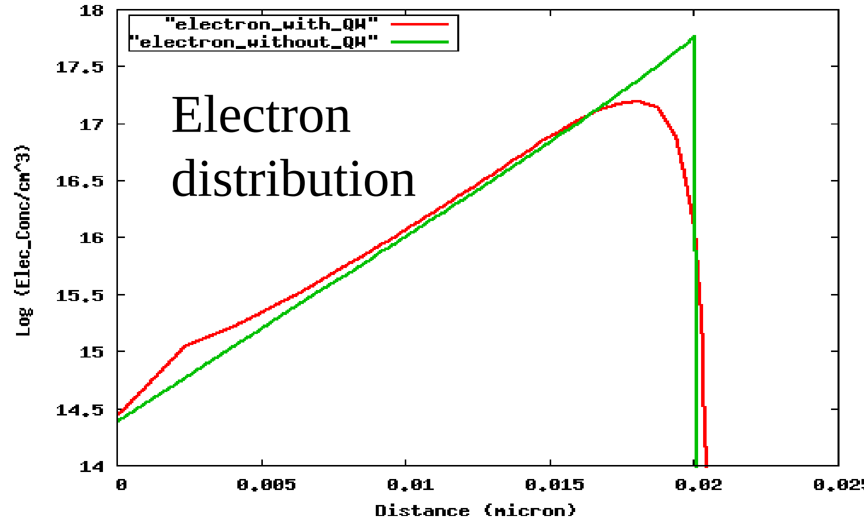
Quantization and quantum confinement in a quantum well

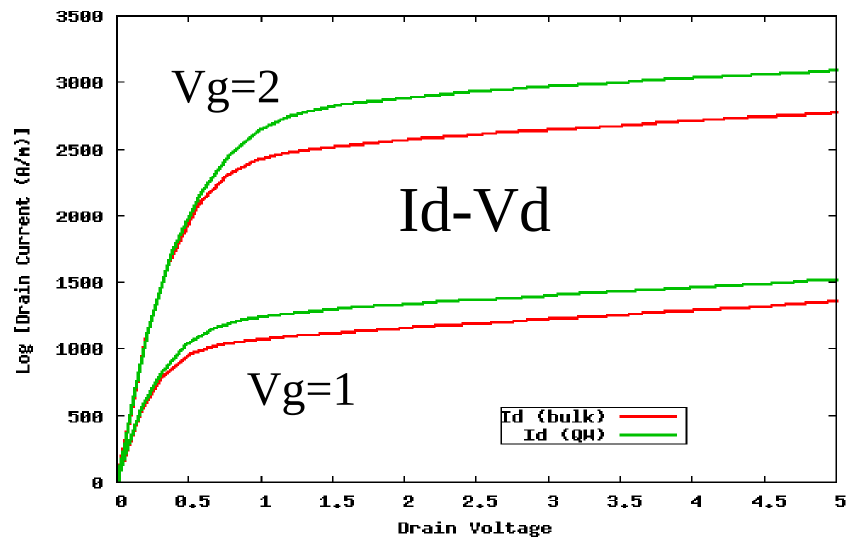


Schematics of quantized state of a quantum well with (a) 2D concentration distributed entirely within the well and (b) concentration modulated by the envelop wave function.

Quantum / classical regions in a MOSFET







Electron distribution and Id-Vd showing effect of quantum confinement.
Lg=0.17 um

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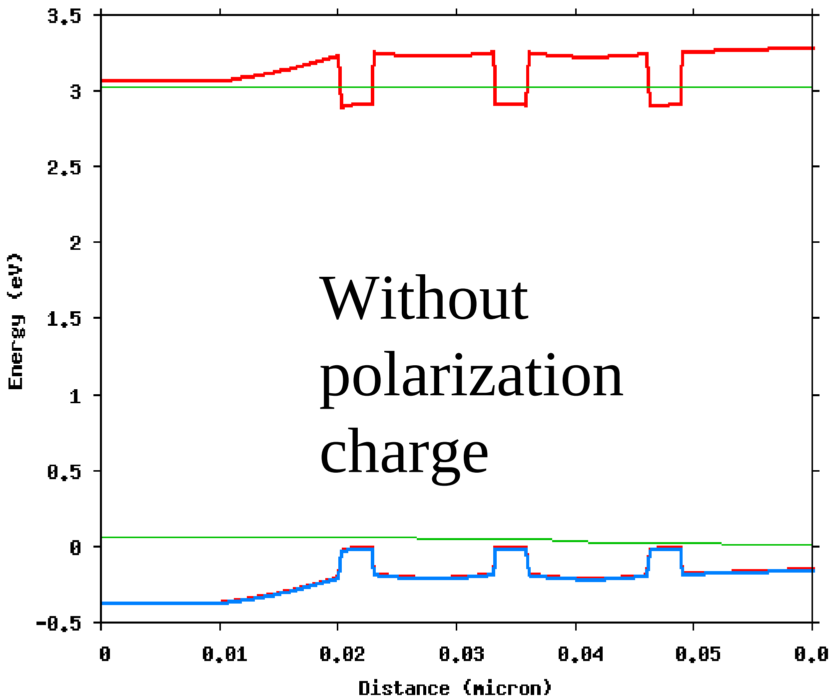
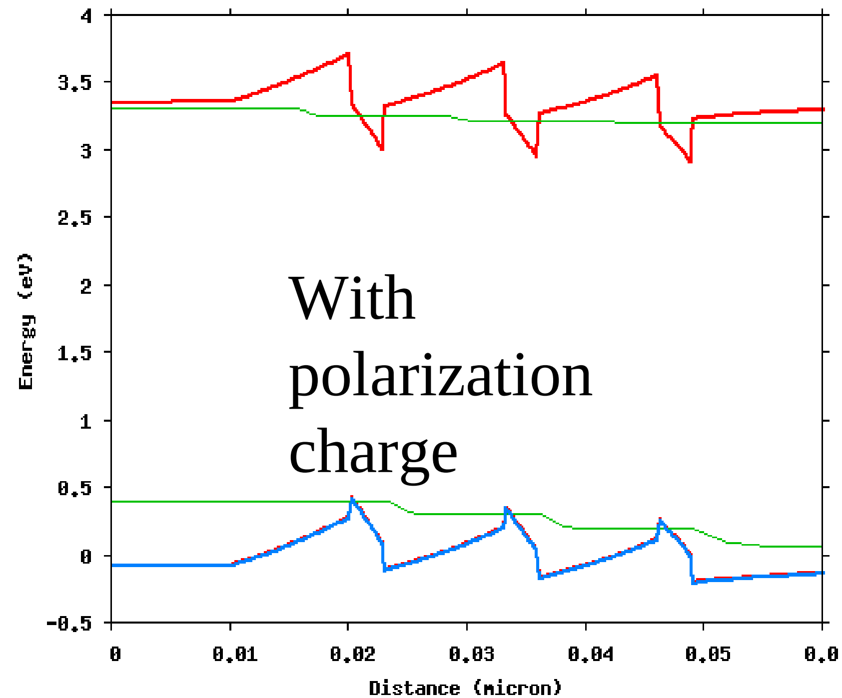
Example: self-consistent solution in InGaN / GaN MQW LED





Remark: well known situation in MQW LED and LD using InGaN/GaN QW

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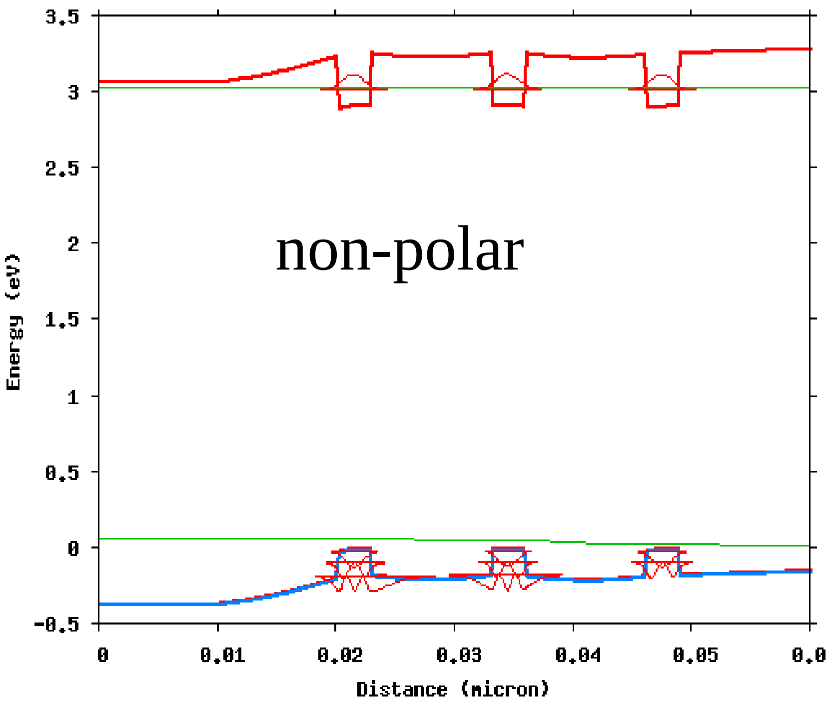
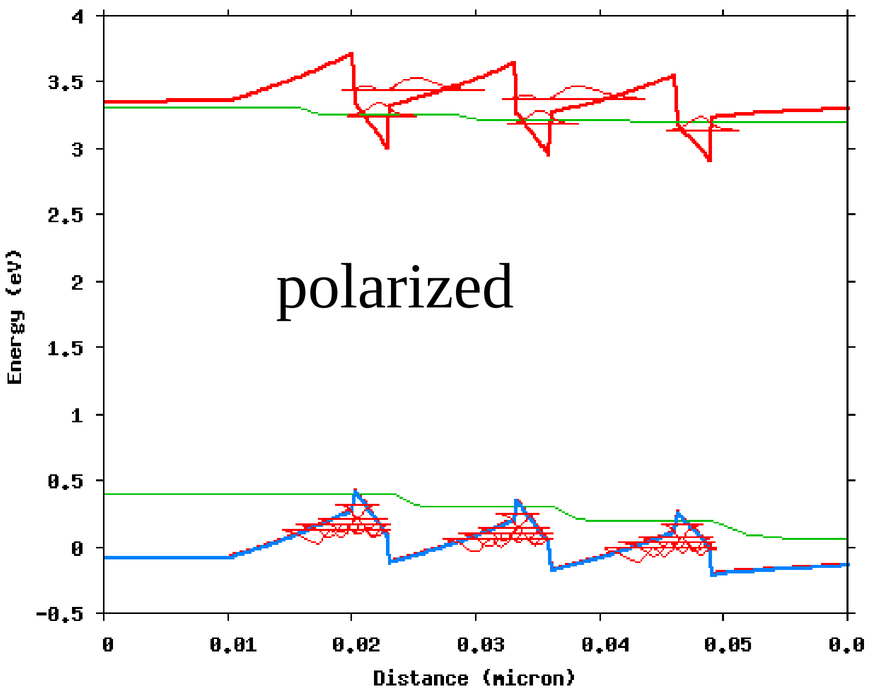
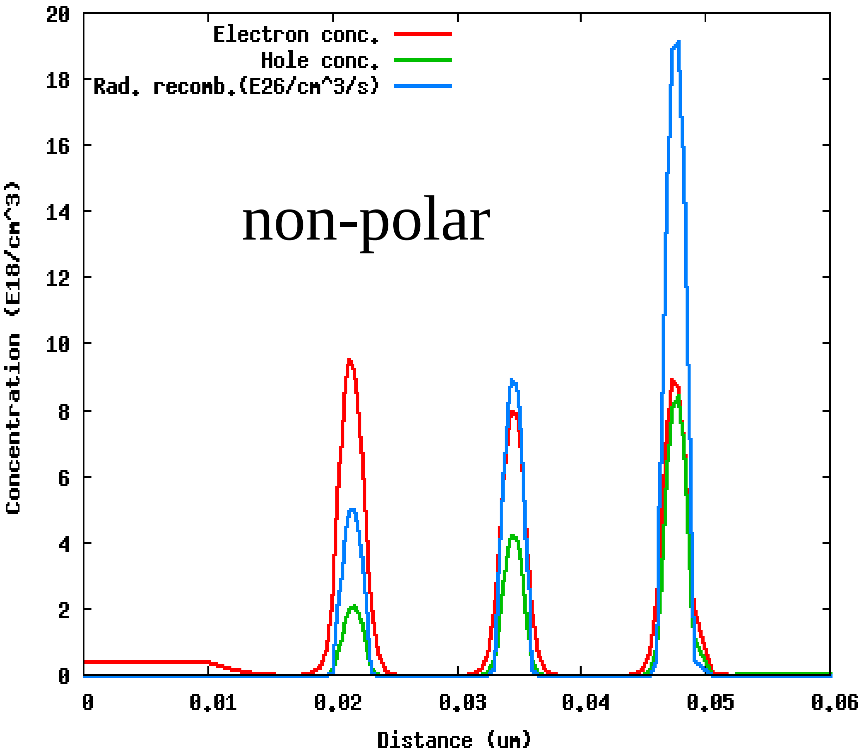
Quantized levels

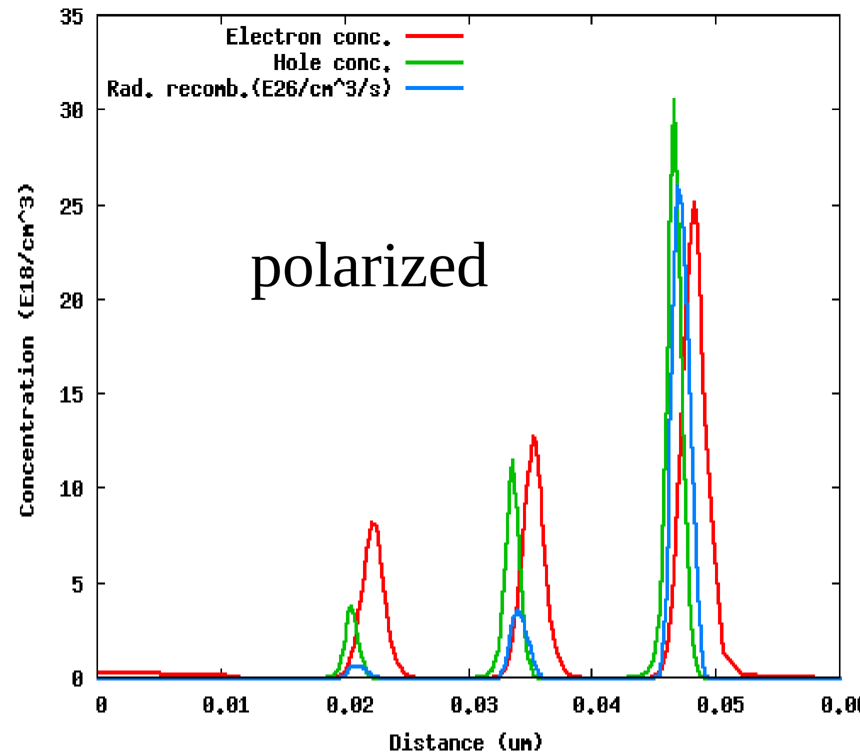




Remark: notice the difference in elec/hole wave function peak positions.

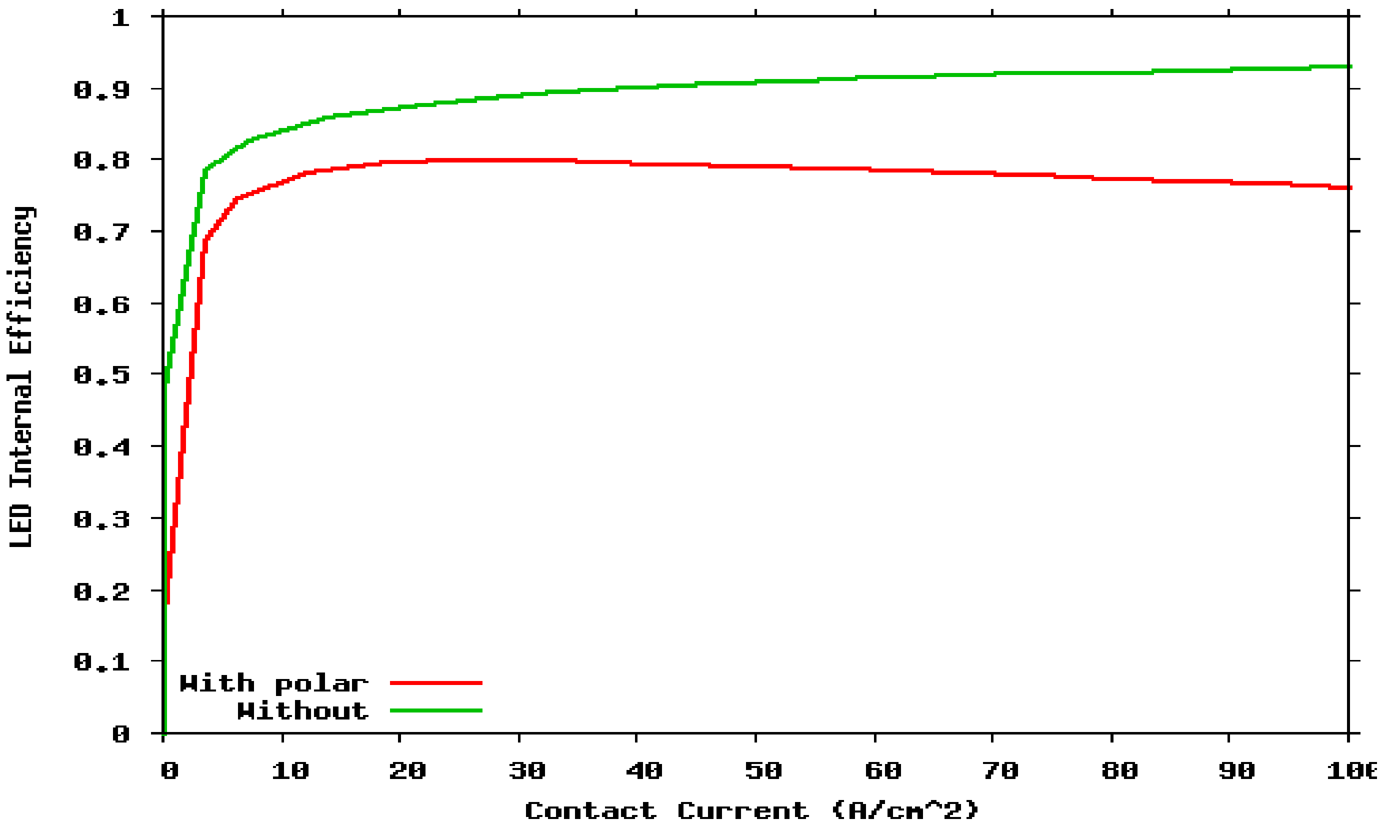
Carrier profile and radiative recombination





Remark: notice that the good overlap of electrons and holes results in larger radiative recombination and emission

IQE vs. current for typical MQW



Remark: the well-known IQE droop effect can easily be simulated using polarization charge on MQW and heterojunction interfaces.

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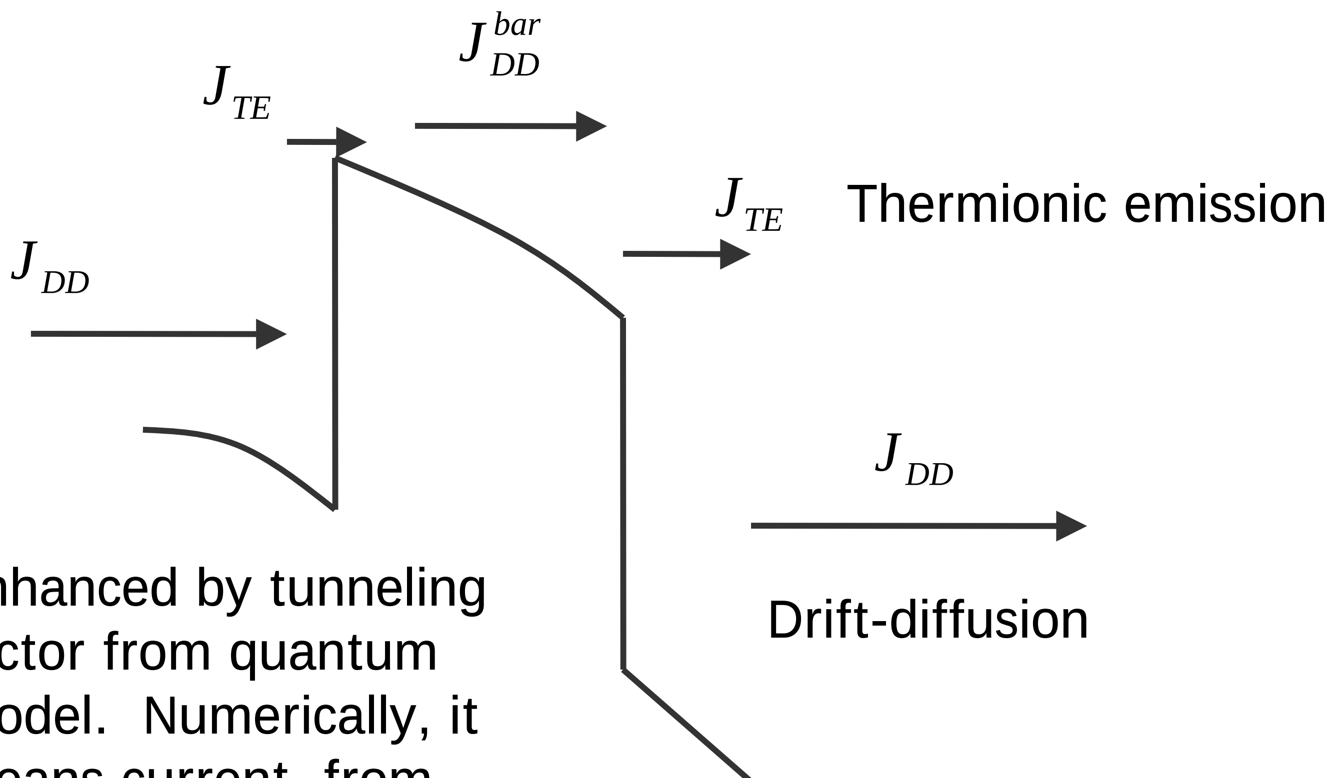
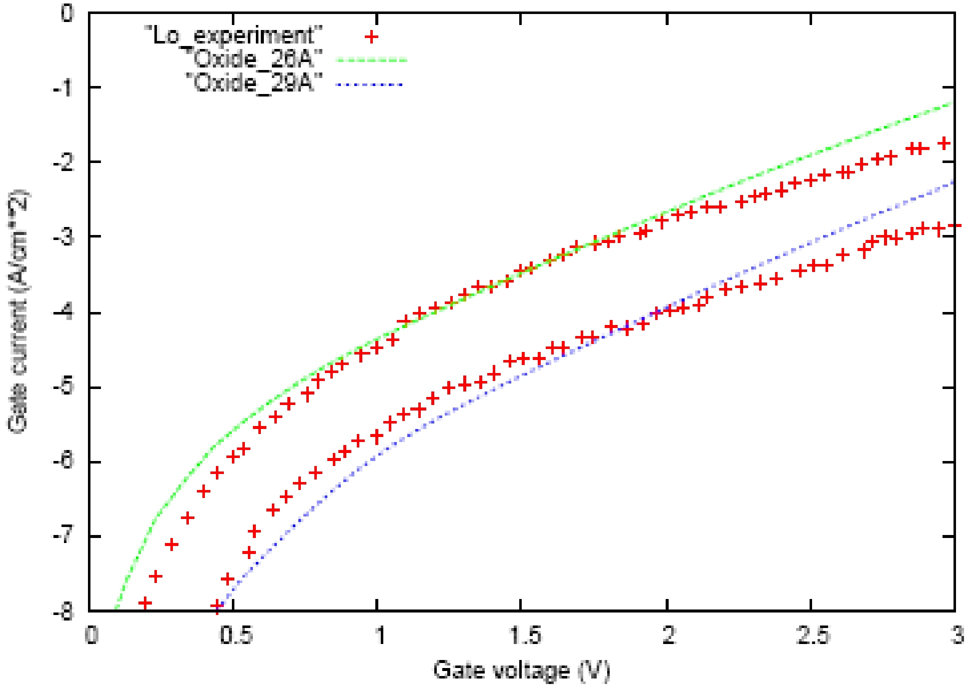
Quantum tunneling correction



J_{TE} J_{DD}^{bar} Enhanced by tunneling factor from quantum model. Numerically, it means current from one mesh point goes to a remote mesh point.

Quantum-DD model works!



Comparison of APSYS simulation of gate leakage current of an NMOS with thin gate oxide with experimental data (ref: IBM J. Res. Develop., vol. 43, No. 3, pp. 327-337, May 1999.).

Demonstration: RTD simulation

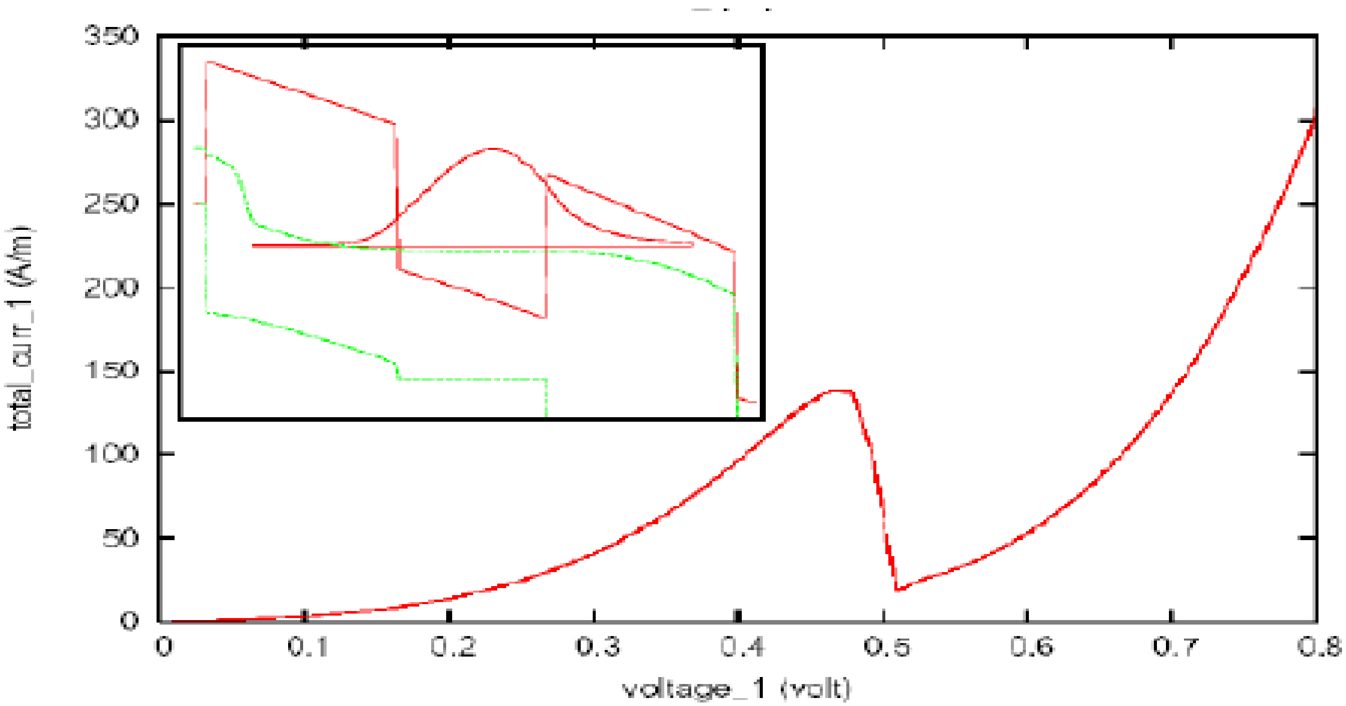
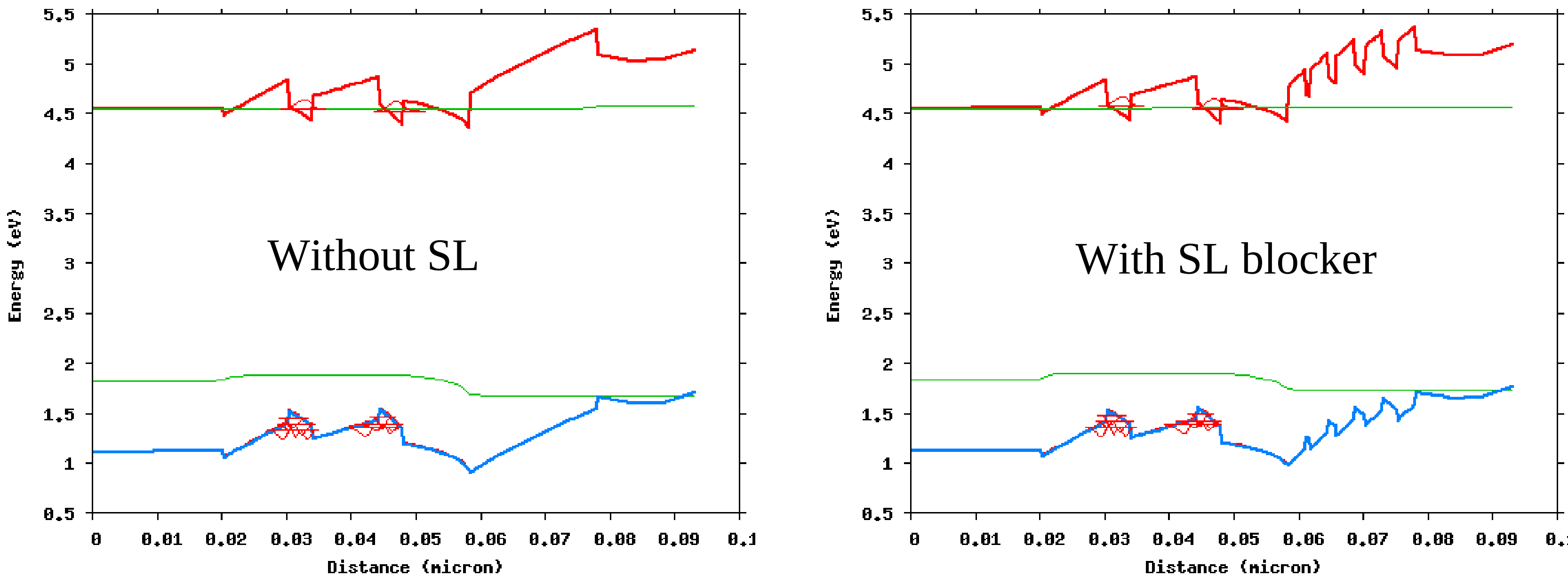


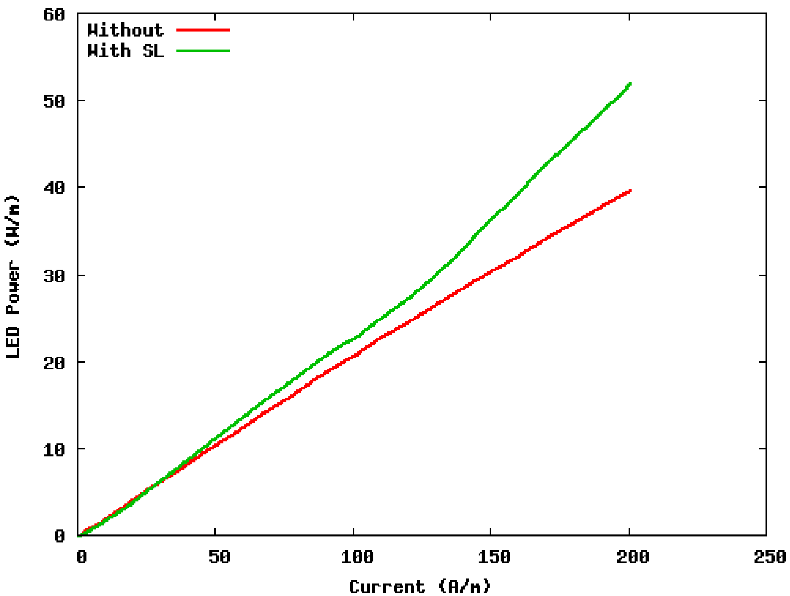
Figure 4. Band diagram, the confined wave function and the resonant I-V characteristics indicating injection carriers are energetically resonating with the confined energy level at a certain bias.

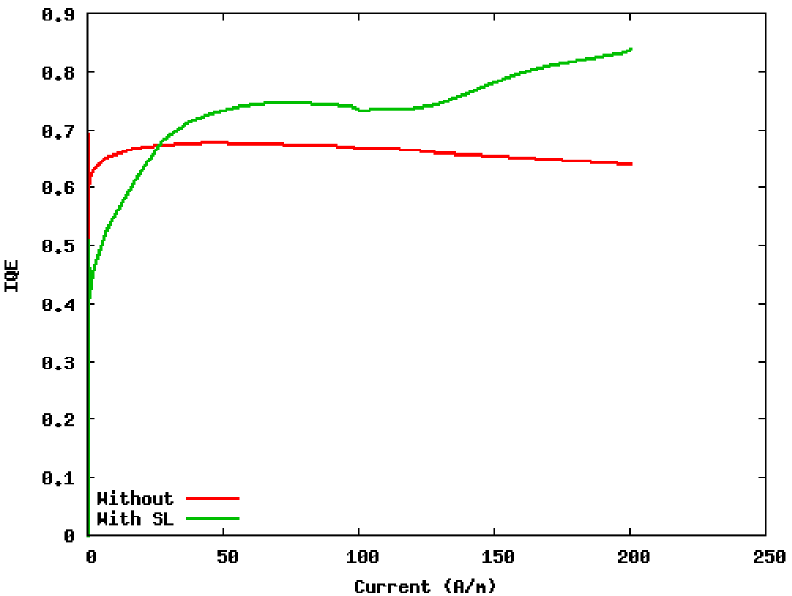
Demonstration: InGaN LED superlattice blocker



Structure based on Ref: Lee et al. Appl. Phys. Lett. 88, p.111101-1 (2006), which experimentally found improved emission power for LED with superlattice blocker.

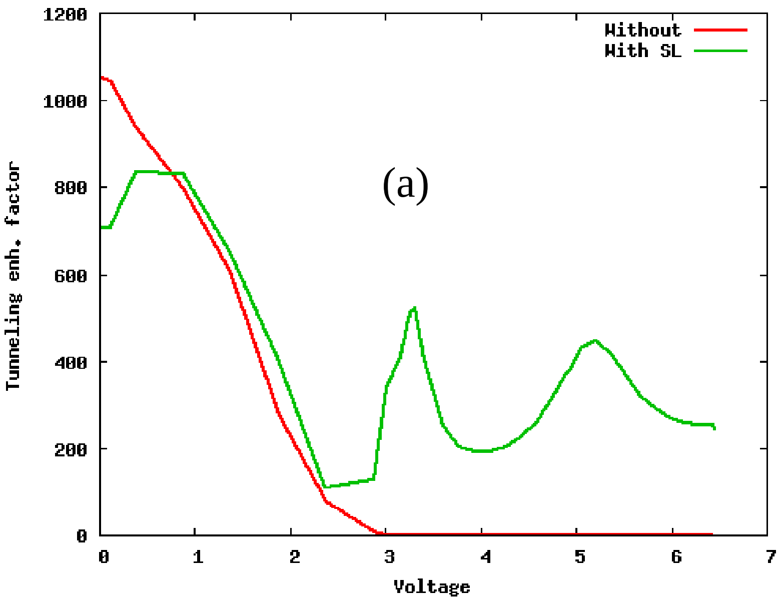
Simulated emission power and IQE

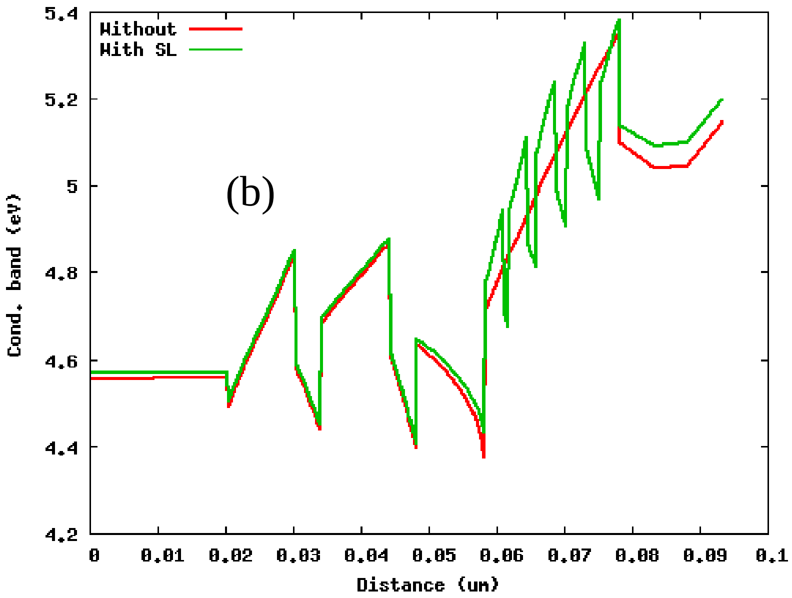




2D Simulation by APSYS indeed shows improved emission power and IQE, similar to experimental observation.

Simulated quantum tunneling effect





Remark: quantum tunneling enhancement factor is actually larger for most of bias ranges. So the SL LED performed better NOT because of quantum interference effect as originally designed [see (a)]. Instead, the SL countered the internal fields and helped increase the overall barrier potential (b).

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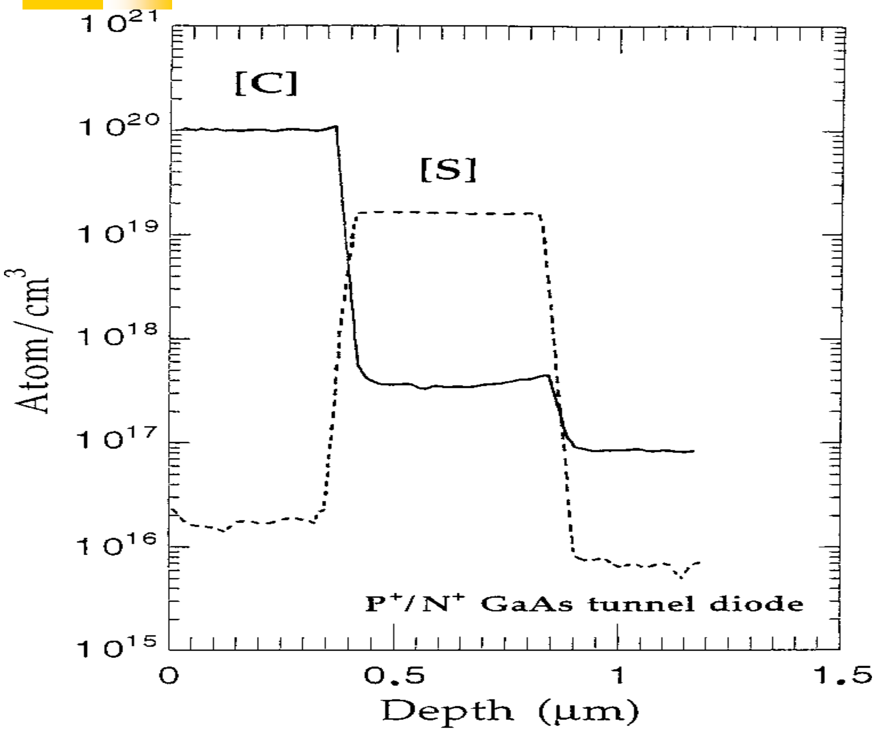
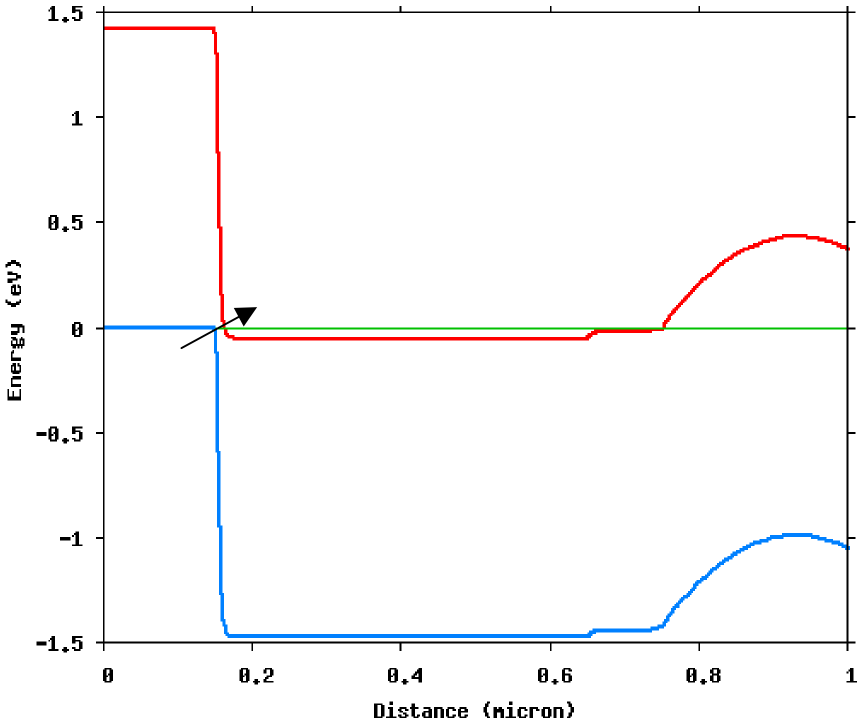
About tunneling junction model

- **Application:**
  - Solar cell, VCSEL, bipolar cascade laser, LED.
  - Critical for design of many devices.
- **Numerical issues:**
  - Equivalent carrier local generation has convergence issues.
  - Improved convergence using equivalent mobility which is difficult to estimate.
  - New approach: physically based TJ current across junction implemented within drift-diffusion solver.

Tunneling junction lets e<-->h non-locally

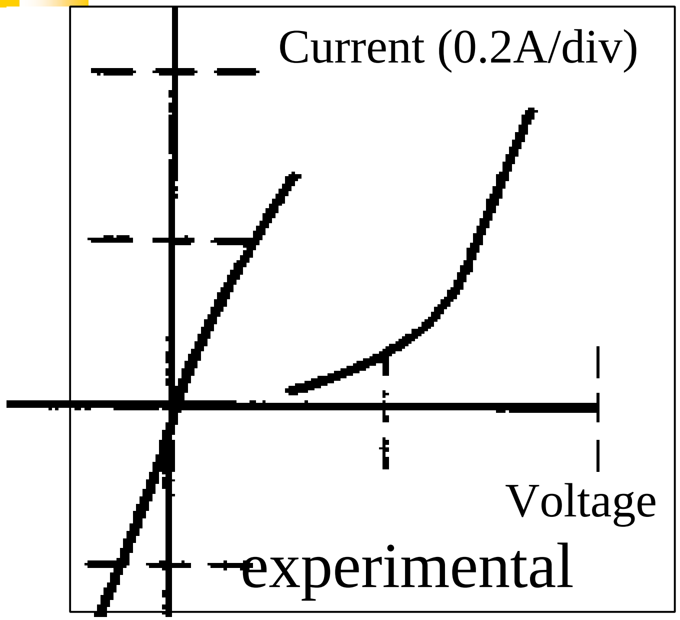


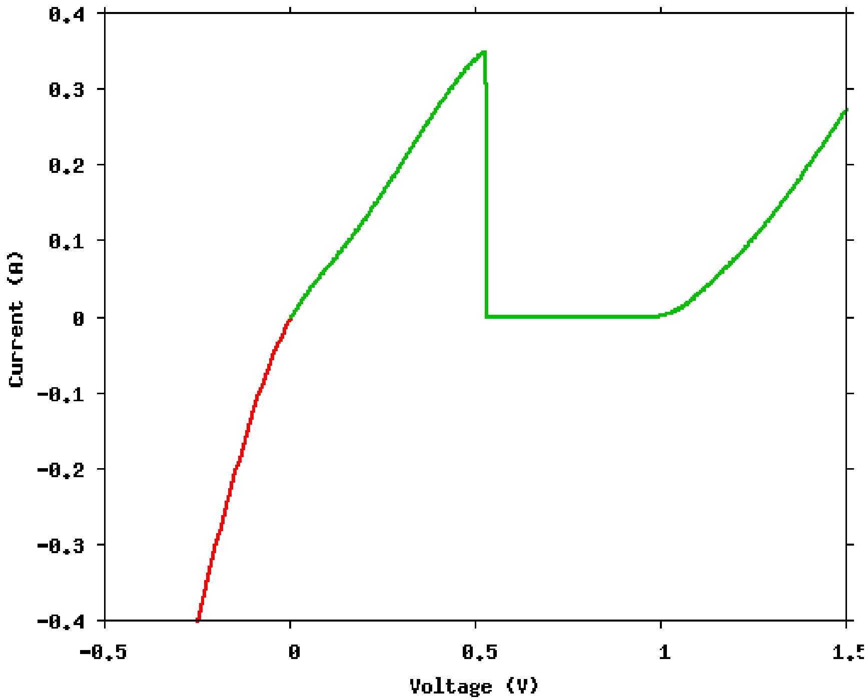


Numerical challenge: current flow across p-n junction through many mesh points.

Example structure Ref: APL, 71, p3752, (1997)

Simulated I-V in both forward and reverse dir





Remark: careful adjustment of contact resistance is necessary to get a good fit of experimental data.

Negative resistance only appears within rather small range of contact resistance.

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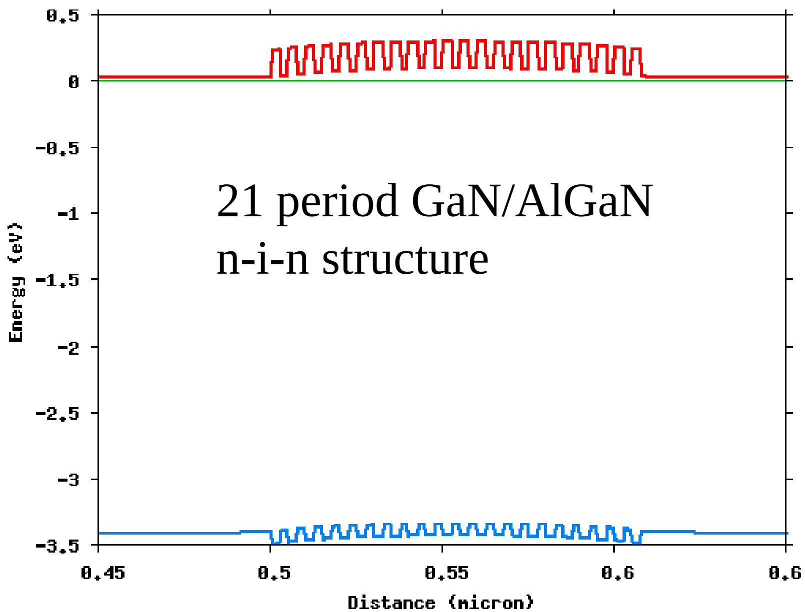
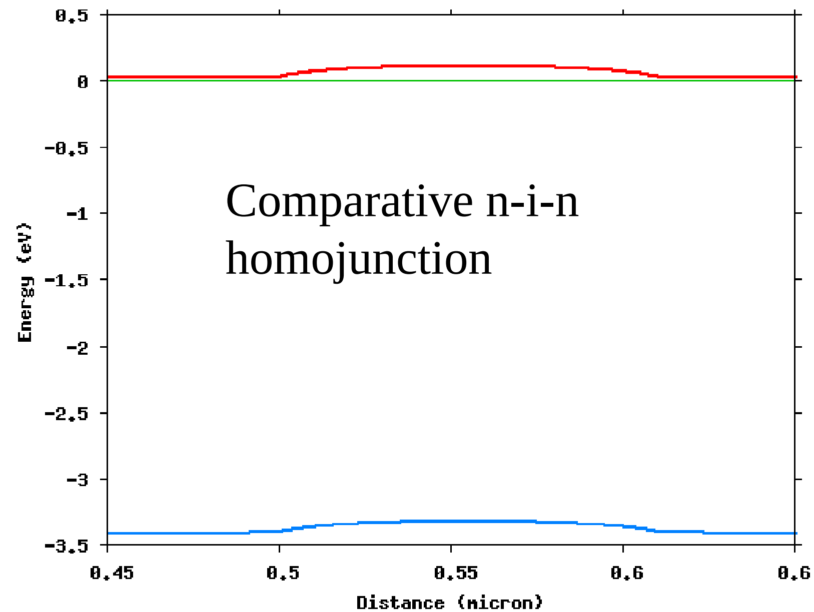
Mini-band tunneling in Crosslight

- **Application:**
  - When supperlattice used as part of cathode/anode.
  - May be used to alter potential profile (e.g., to reduce overall polarization field).
- **Implementation:**
  - Included as part of non-local tunneling.
  - Requires a single representative period for mini-band computation --> So choose a period carefully.
  - Theory based on Ref: Physics Reports 357 (2002) 1-111

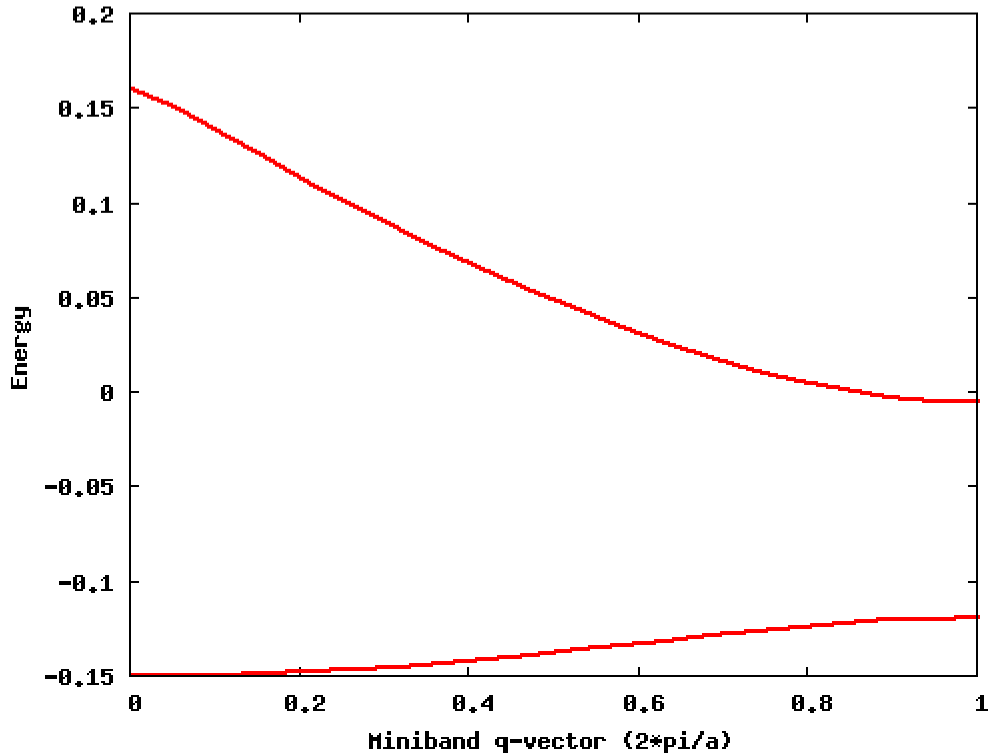
Simple test structures





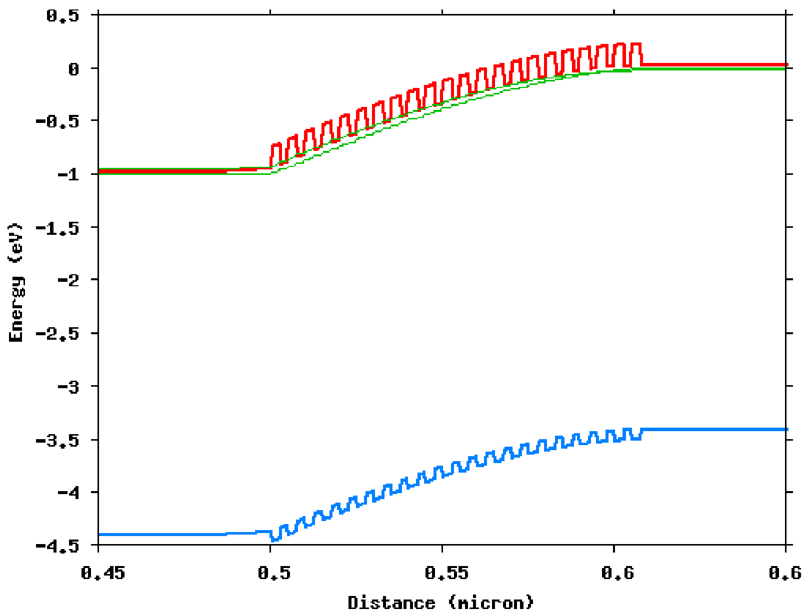
Remark: tunneling region defined from n to n regions. Al fraction is 16 percent for the barriers and well/barrier width is 2.5nm. Polarization charge ignored for simplicity.

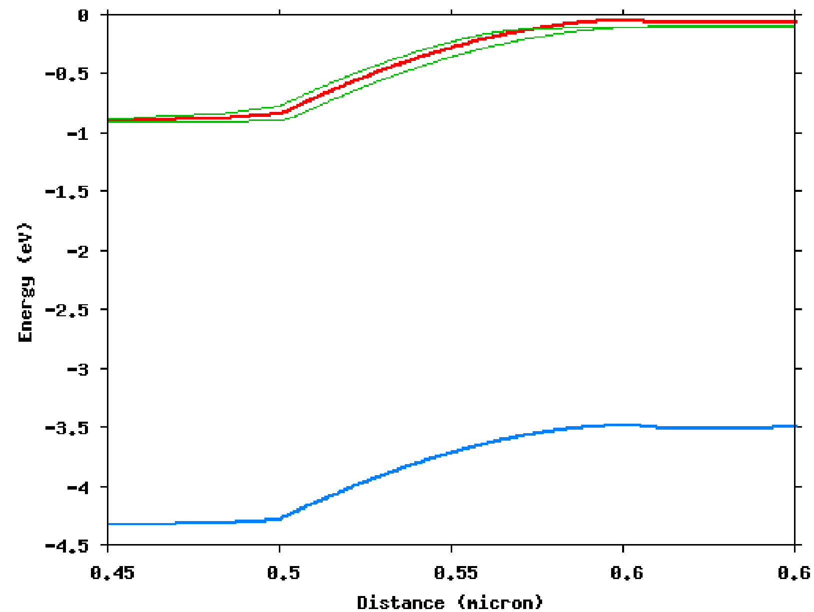
First two mini-bands



Remark: mini-band calculated according to a reference period in the middle at bias of one volt. Energy referenced to the potential of the above reference period.

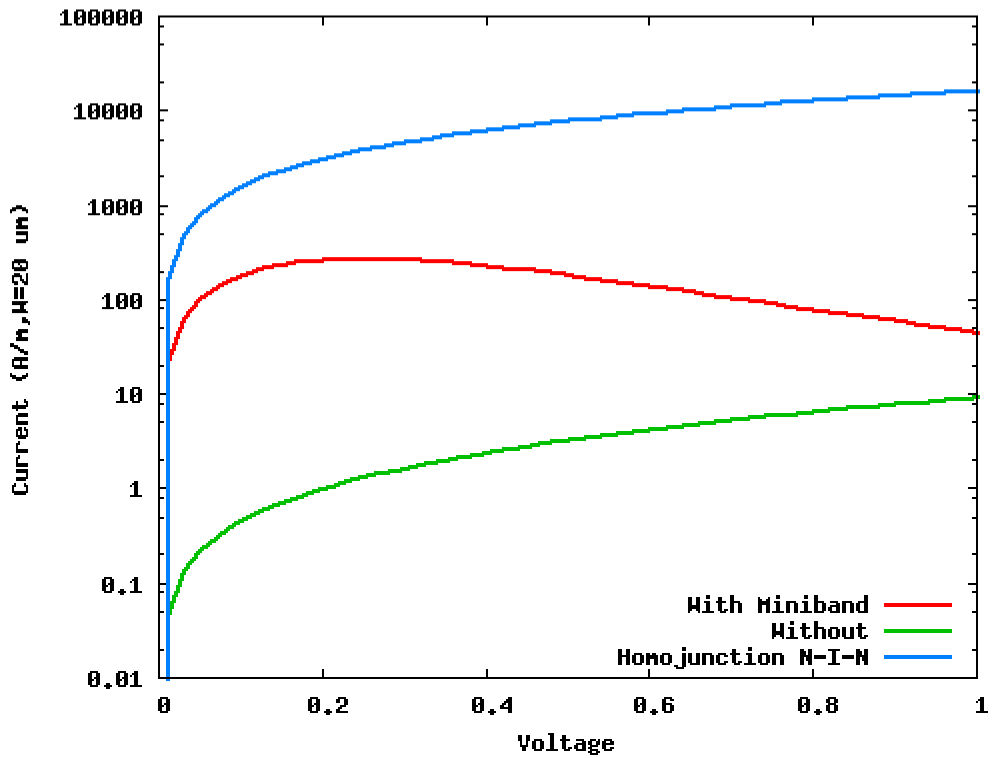
Band diagrams at one volt bias





Remark: mini-band structure is recalculated at all small bias steps to ensure self-consistency.

Calculated I-V curves



Remark: homojunction with no barriers has the highest current as expected. Without miniband transport, superlattice has low current based on thermionic emission only. Resonance between injection current and miniband states caused enhanced carrier transport in superlattice.

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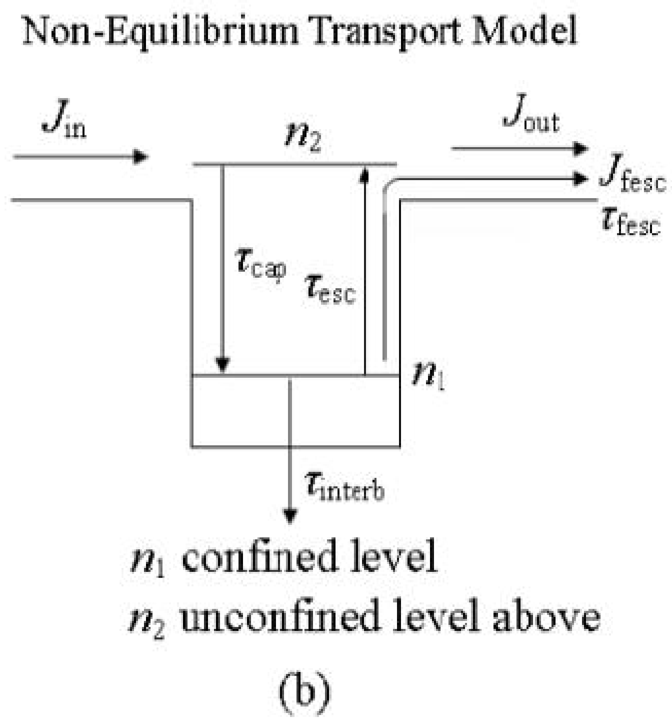
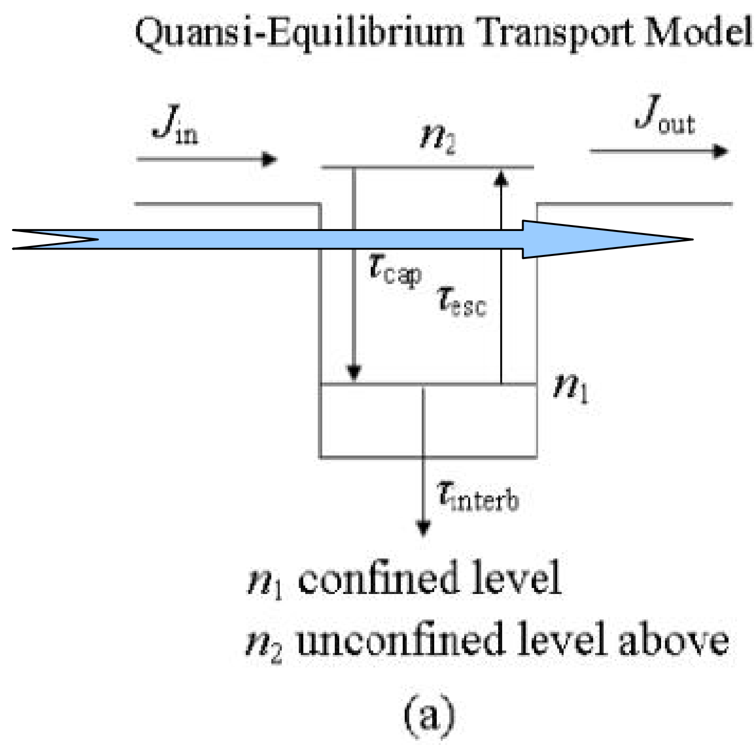
Two-Fermi-level quantum well trapping model



When the well is really narrow and deep, carriers may not reach local equilibrium. Treat it as a carrier trap, with trapping rates determined by phonon scattering theory.

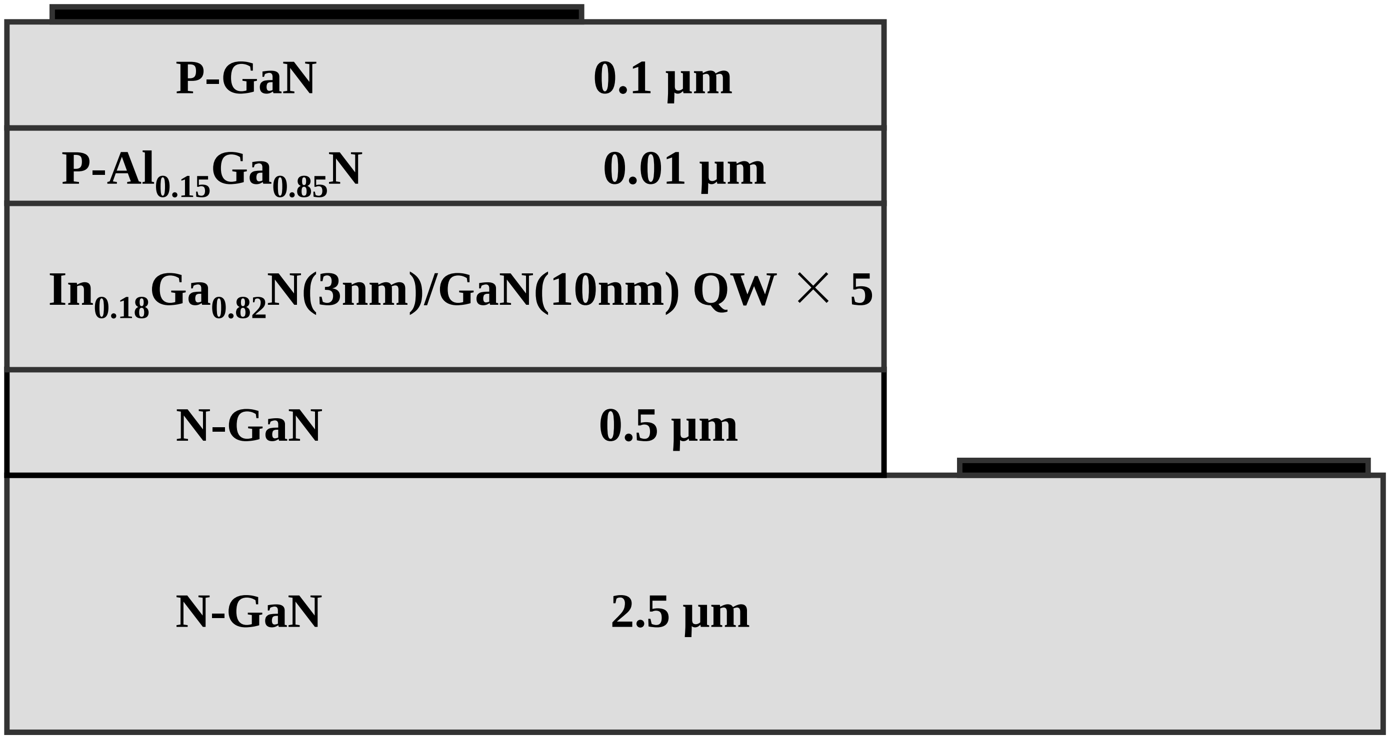
Alam, Hybersten & al., IEEE Tran. Elec. Dev., Vol.. 47, No. 10, Oct. 2000, p. 1917

Mean free path-controlled quantum escape



Given the mean free path of carrier, we expect direct flying over the quantum well/dot with probability of exp(-D/lambda) where D=well width & lambda=mean free path.

Reference Structure

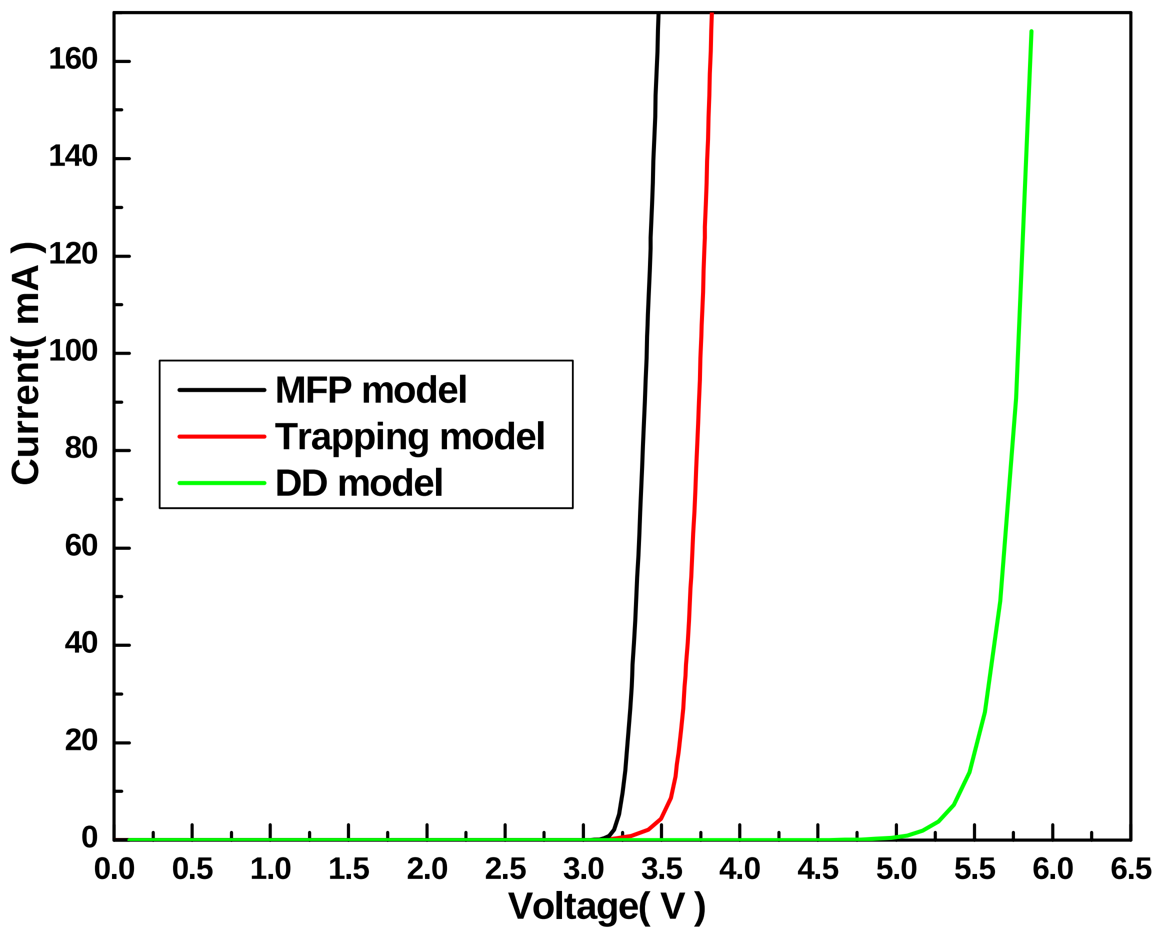


Size: 300 µm × 300 µm

The polarization charge set on the interface of QWs is 80% of the theoretical value calculated based on the Ref. Appl. Phys. Letts, 80, 1204(2002).

Comparing the models

I-V Curve



Drift-diffusion model shows unrealistically high turn-on voltage

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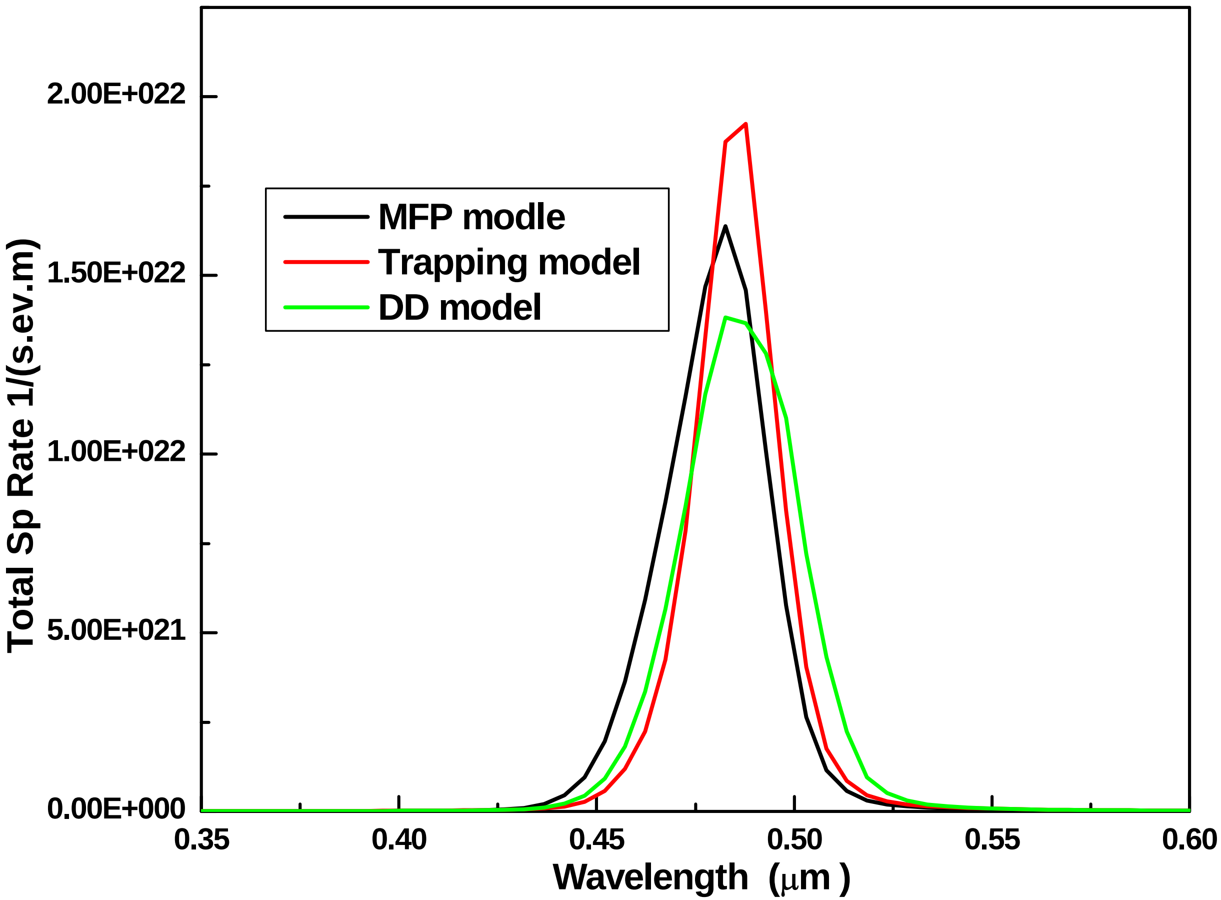
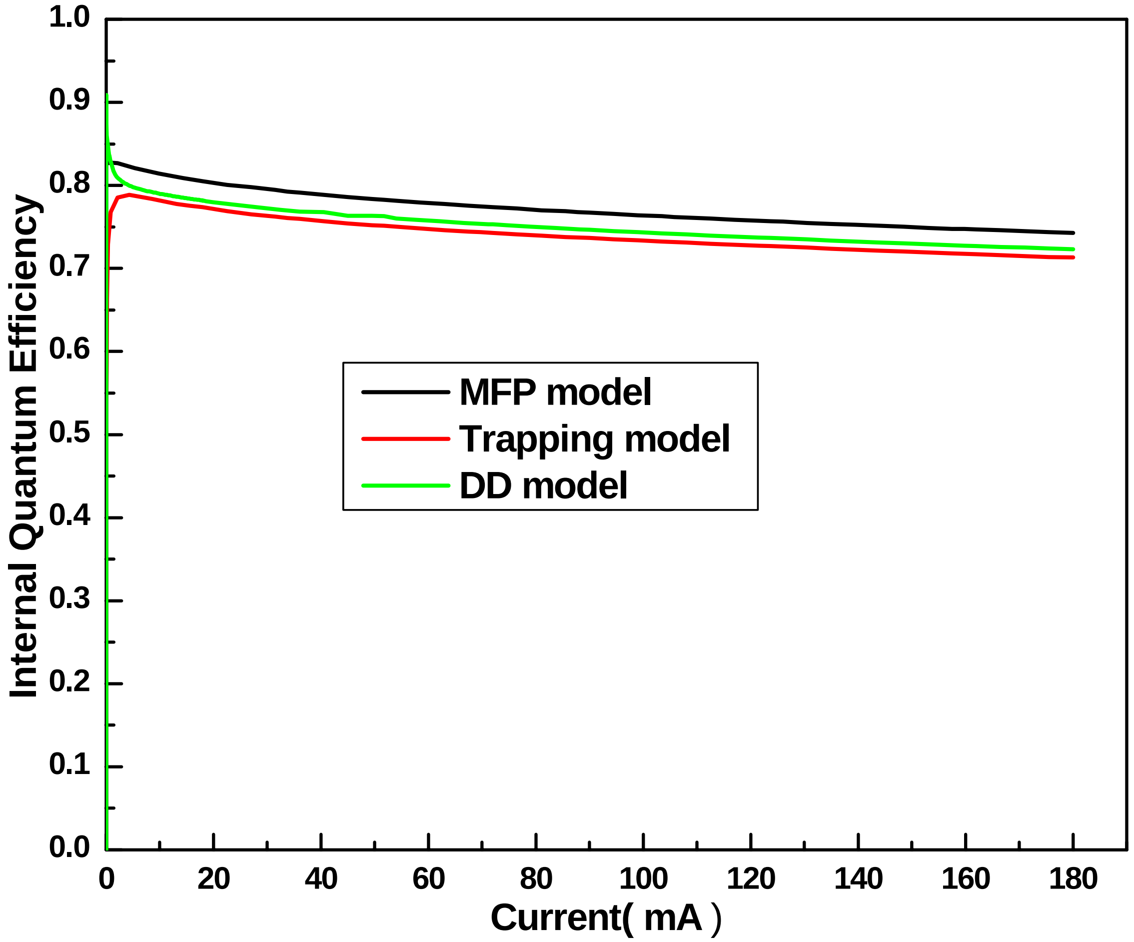
EL Spectrum



MFP modle
Trapping model
DD model
Total Sp Rate 1/(s.ev.m)
2.00E+022
1.50E+022
1.00E+022
5.00E+021
0.00E+000
0.35
0.40
0.45
0.50
0.55
0.60
Wavelength (μm)

IQE Curve



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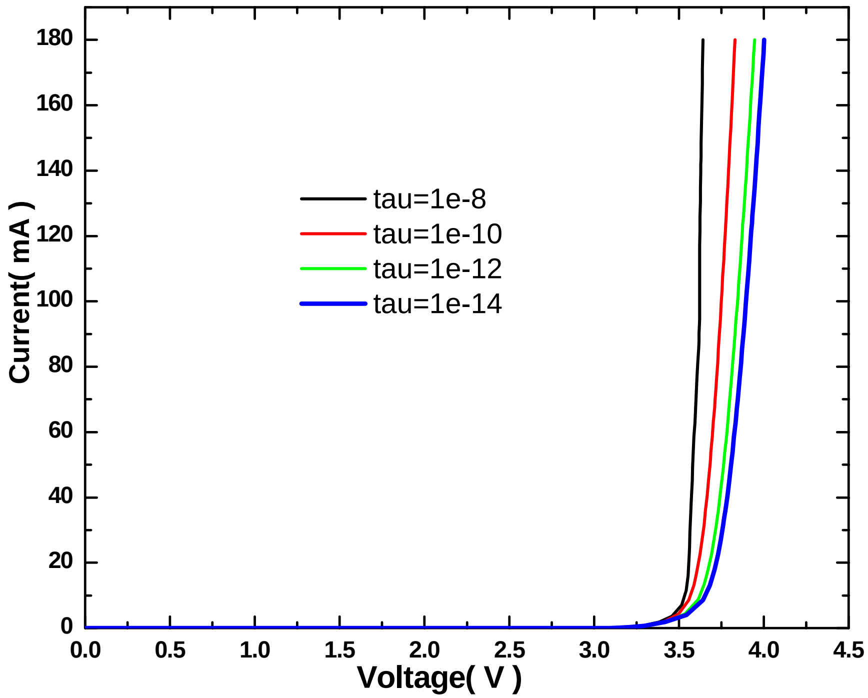
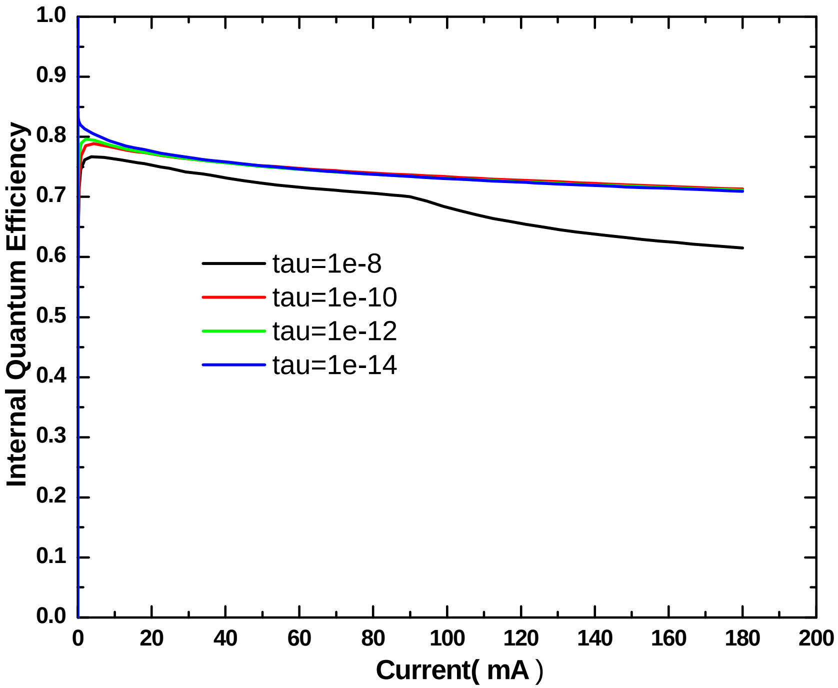
The impact of lifetime parameter in Trapping model

Comparison





q_trap_tau is the time constant for the 2-Fermi level trapping model.
In Crosslight, the default value is 1 ps.

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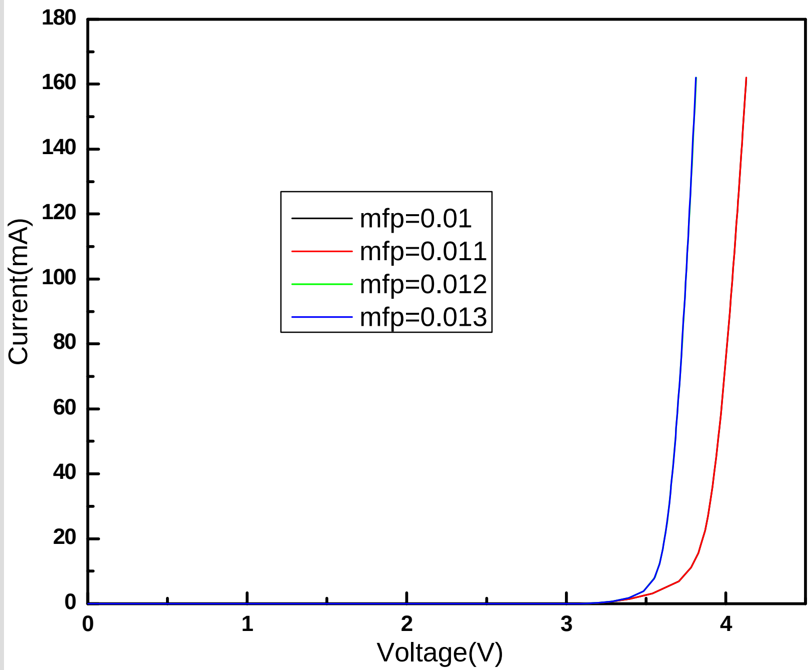
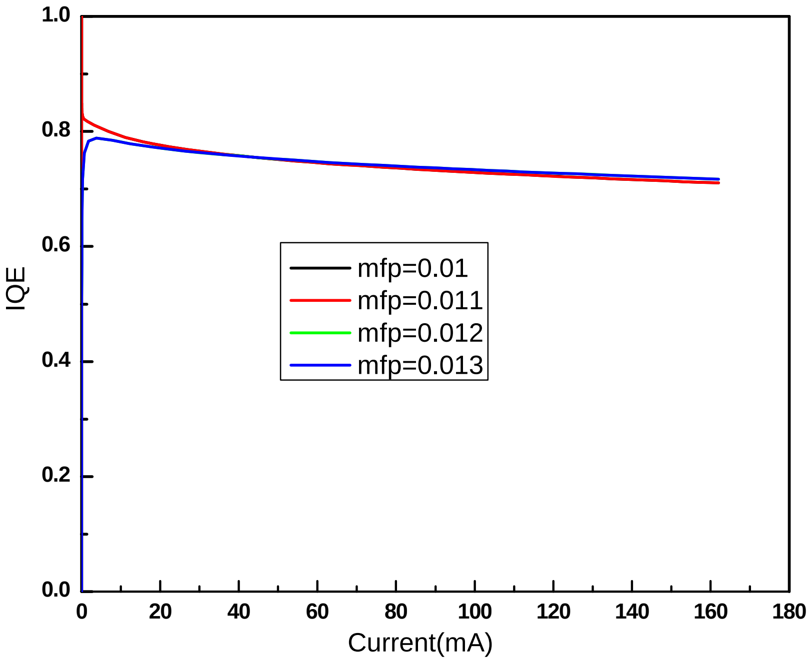
The impact of the mean free path parameter in Trapping model

Comparison





mfp is the electron or hole mean free path. In the trapping model, it controls the transport of carriers that fly-over and are not trapped. In Crosslight, the default value is 0.01 (um).

The impact of the mean free path parameter in MFP model

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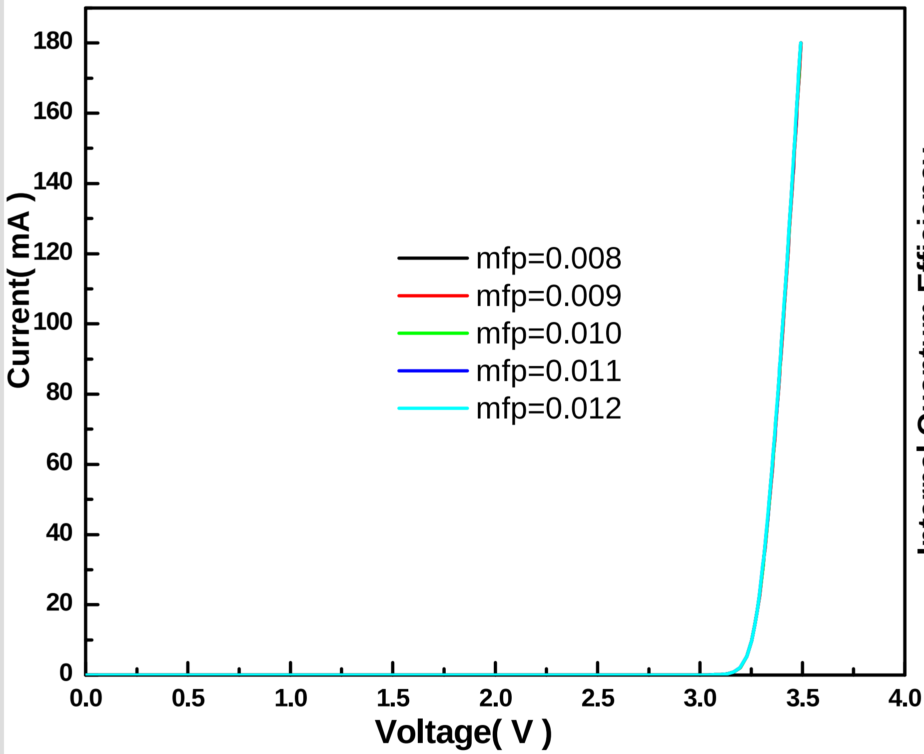
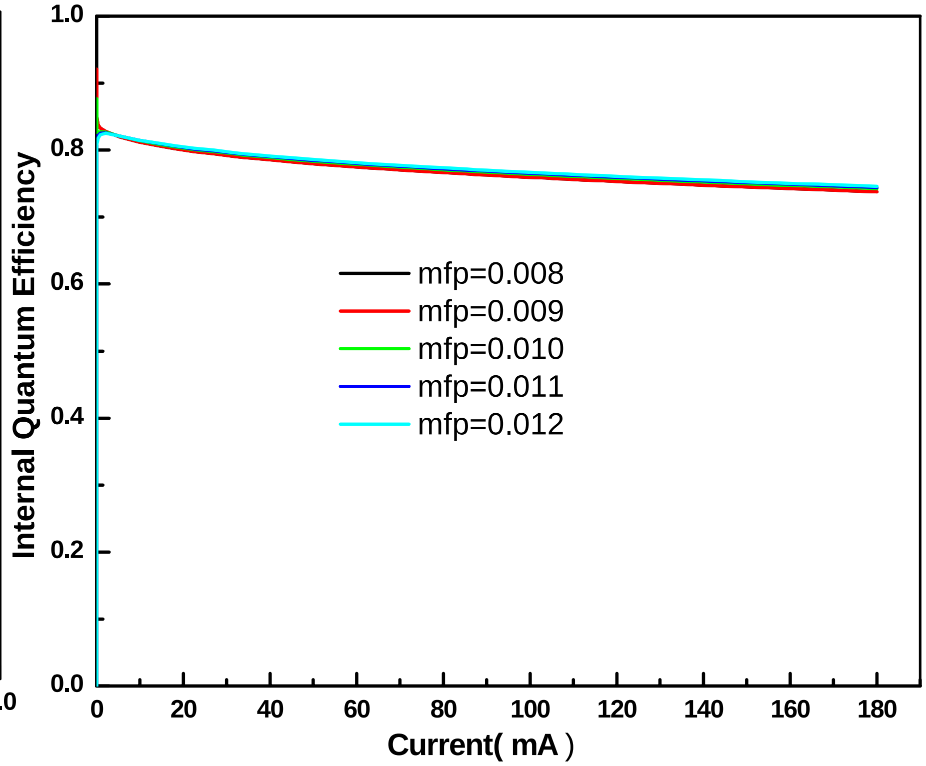
Comparison





In MFP model, **mfp** is used for the exponential factor to control the non-local current flow intensity. In Crosslight, the default value is 0.01 (um).

Summary

- **Conventional drift-diffusion solver has been modified to include various quantum and non-local models.**
- **Such models turn out to be critical when simulating devices involving quantum and non-local physics.**
- **Potential difficulty in such approach: all such advanced treatment require some validity judgment by users.**