Simulation of Semipolar InGaN Laser Diodes

Outline

- Model
- Optical gain without internal field
- Comparison of semipolar, nonpolar and c-plane
- Summary

Hamiltonian

PRB vol59 p4725 1999

$$H(\mathbf{k},\epsilon)=\begin{pmatrix} F & -K^* & -H^* & 0 & 0 & 0 \\ -K & G & H & 0 & 0 & \Delta \\ -H & H^* & \lambda & 0 & \Delta & 0 \\ 0 & 0 & 0 & F & -K & H \\ 0 & 0 & \Delta & -K^* & G & -H^* \\ 0 & \Delta & 0 & H^* & -H & \lambda \end{pmatrix} \begin{matrix} |U_1\rangle \\ |U_2\rangle \\ |U_3\rangle \\ |U_4\rangle \\ |U_5\rangle \\ |U_6\rangle, \end{matrix}$$

$$|U_1\rangle=-\frac{1}{\sqrt{2}}|(X+iY)\uparrow\rangle,$$

$$|U_2\rangle=\frac{1}{\sqrt{2}}|(X-iY)\uparrow\rangle,$$

$$|U_3\rangle=|Z\uparrow\rangle,$$

$$|U_4\rangle=\frac{1}{\sqrt{2}}|(X-iY)\downarrow\rangle,$$

$$|U_5\rangle=-\frac{1}{\sqrt{2}}|(X+iY)\downarrow\rangle,$$

$$|U_6\rangle=|Z\downarrow\rangle.$$

$$F=\Delta_1+\Delta_2+\lambda+\theta,$$

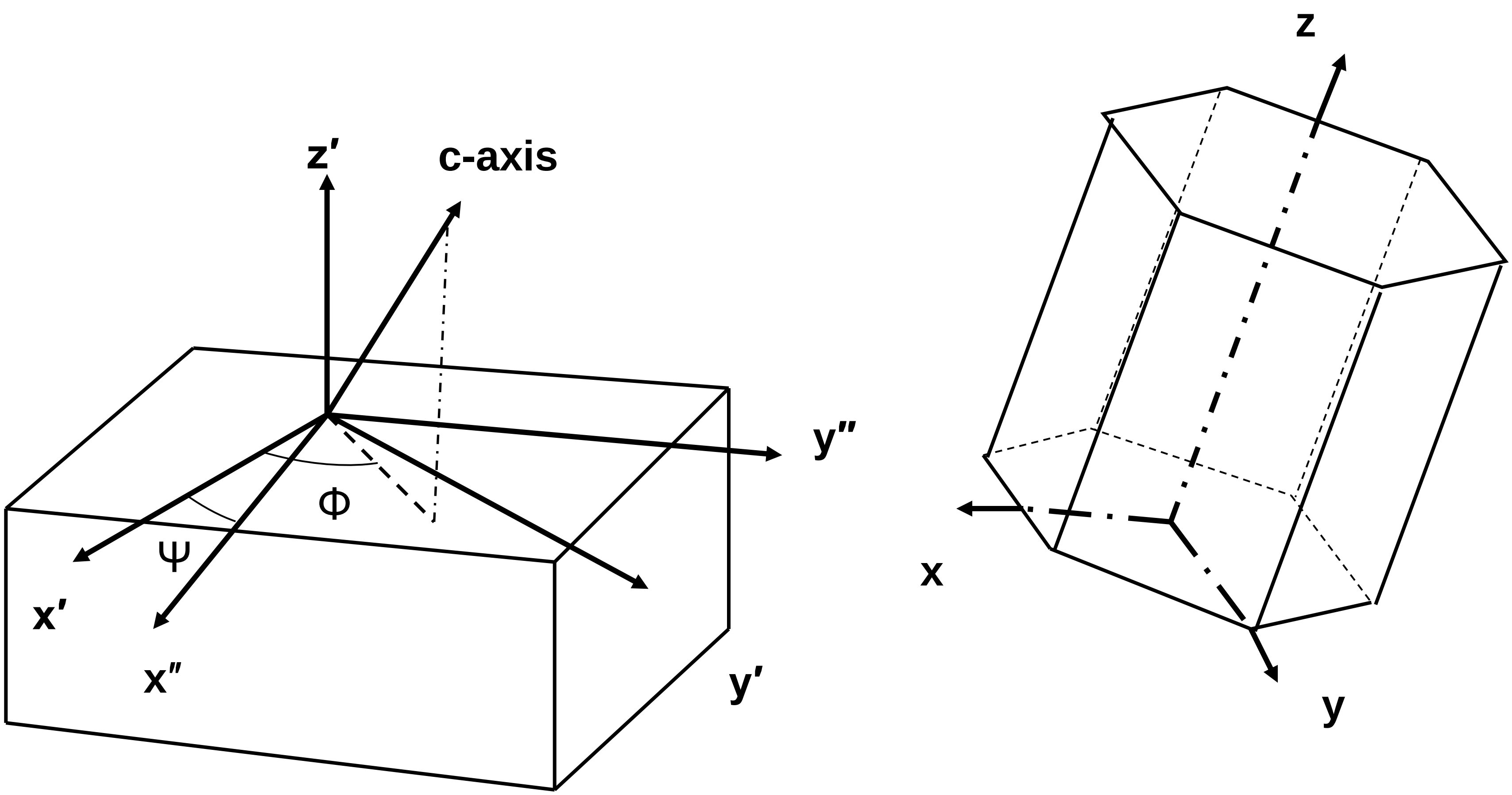
$$G=\Delta_1-\Delta_2+\lambda+\theta,$$

$$\lambda=\frac{\hbar^2}{2m_o}[A_1k_z^2+A_2(k_x^2+k_y^2)]+\lambda_\epsilon,$$

$$\theta=\frac{\hbar^2}{2m_o}[A_3k_z^2+A_4(k_x^2+k_y^2)]+\theta_\epsilon,$$

… etc

Coordinate system



(x,y,z) – crystal coordinate where original Hamiltonian defined
(x',y',z') – growth coordinate system; z'=MQW normal
(x'',y'',z'') – waveguide system; z''//z'; y''=wave propagation direction

Strain and stress

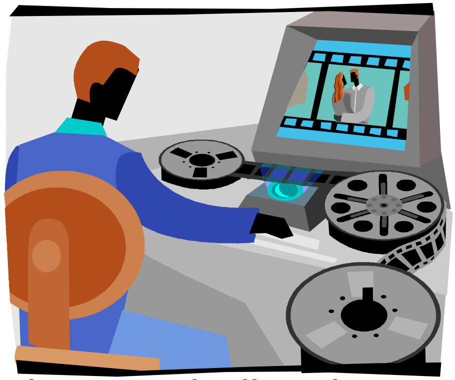
Principle: Pseudomorphic growth; minimization of elastic energy with one degree of freedom being the displacement along the growth direction. Ref: PRB vol59 p4725 1999

Elastic energy density:

$$W=\frac{1}{2}[C_{11}\epsilon_{xx}^2+C_{11}\epsilon_{yy}^2+C_{33}\epsilon_{zz}^2+2C_{12}\epsilon_{xx}\epsilon_{yy}+2C_{13}\times(\epsilon_{xx}\epsilon_{zz}+\epsilon_{yy}\epsilon_{zz})+4C_{44}\epsilon_{xz}^2].$$

Modeling approach:

Handling of coordinate systems



- Transforming k.p Hamiltonian and dipole moment from (x,y,z) to (x',y',z').
- Minimize elastic energy and obtain strain tensor in primed System.

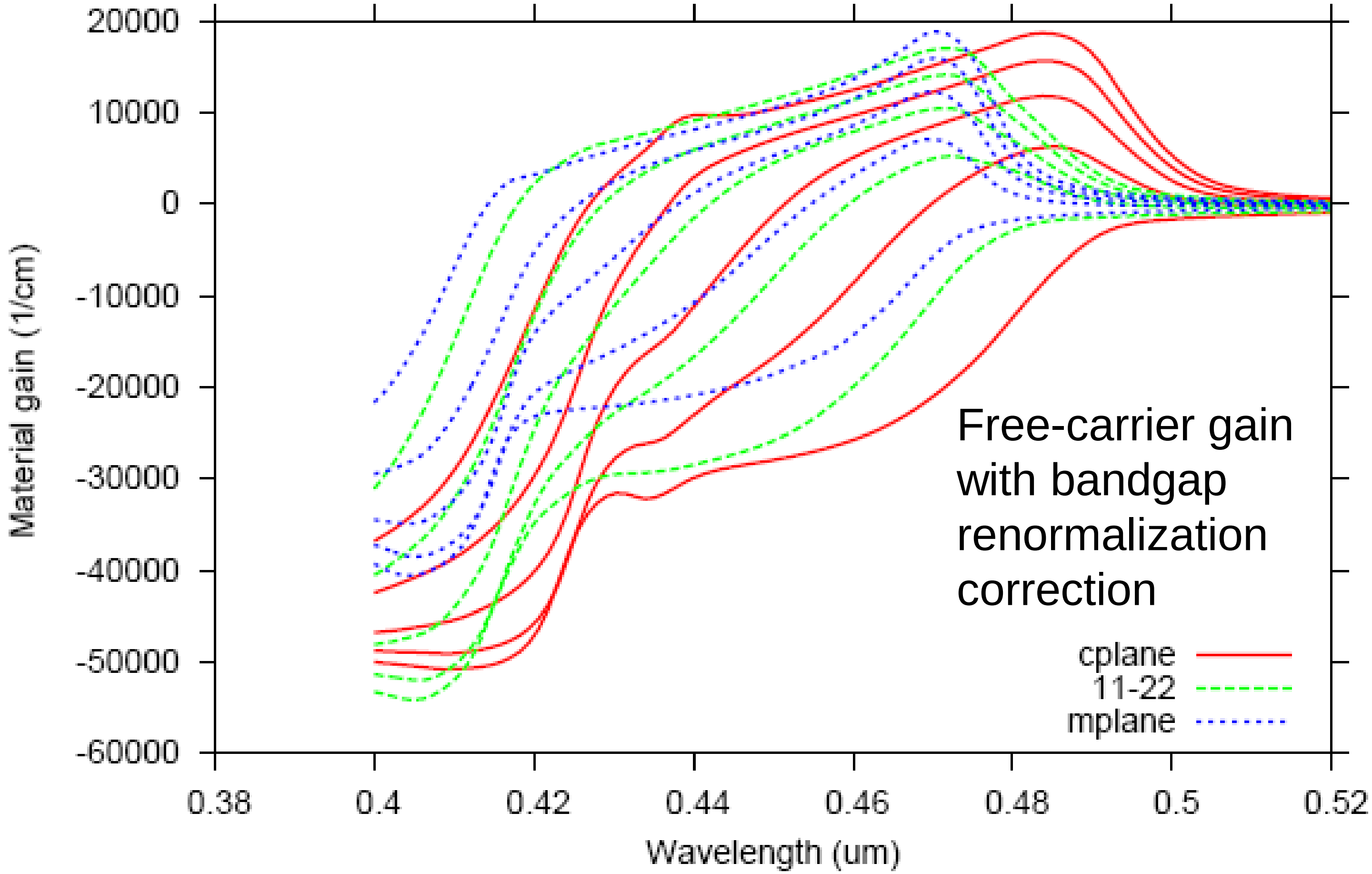
Solution of k.p Hamiltonian in (x',y',z')

- 1D finite difference method used to discretize 6x6 k.p system in the growth direction.
- Rigorous solution of sparse eigen system to obtain envelop wave functions and subband energies.

Optical gain and lasing characteristics

- Integrate carrier density and free carrier gain (with manybody correction) in all directions on (x',y') plane.
- Optionally, full manybody gain model maybe turned on at cost of longer CPU time.
- Optionally, turn on/off internal polarization field.
- Optical dipole moment evaluated for arbitrary E-field polarization in (x'',y'',z'').
- Optical birefringence taken into account using two sets of refractive indices for EO/O.
- Import of field dependent optical gain into LASTIP/PICS3D simulator to compute electrical and optical characteristics in a self-consistent manner.

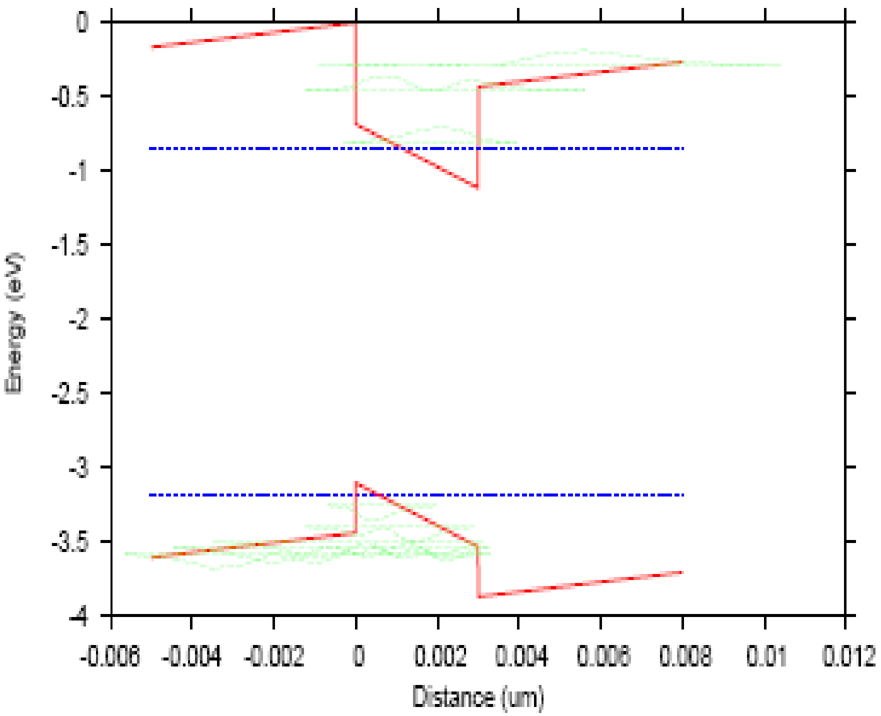
Optical gain without internal field:

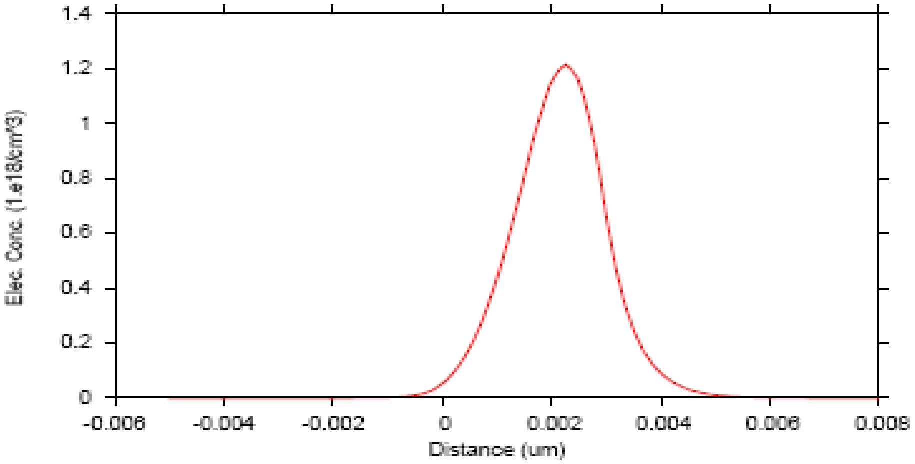


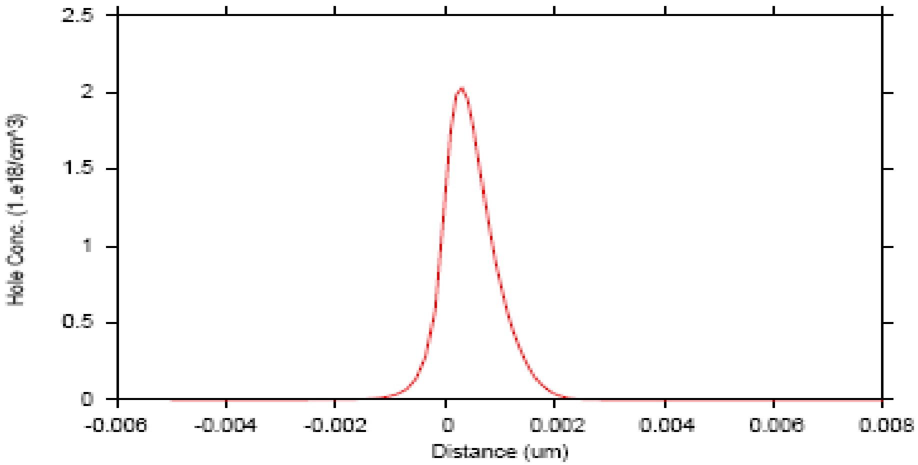
InGaN/GaN well with 20 percent indium; 3 nm well
Well concentration from 3.e12 to 3.e13 (1/cm^2) in equal intervals
Waveguide ridge parallel to projection of c-axis, TE polarization

C-plane with internal field

HH is plotted

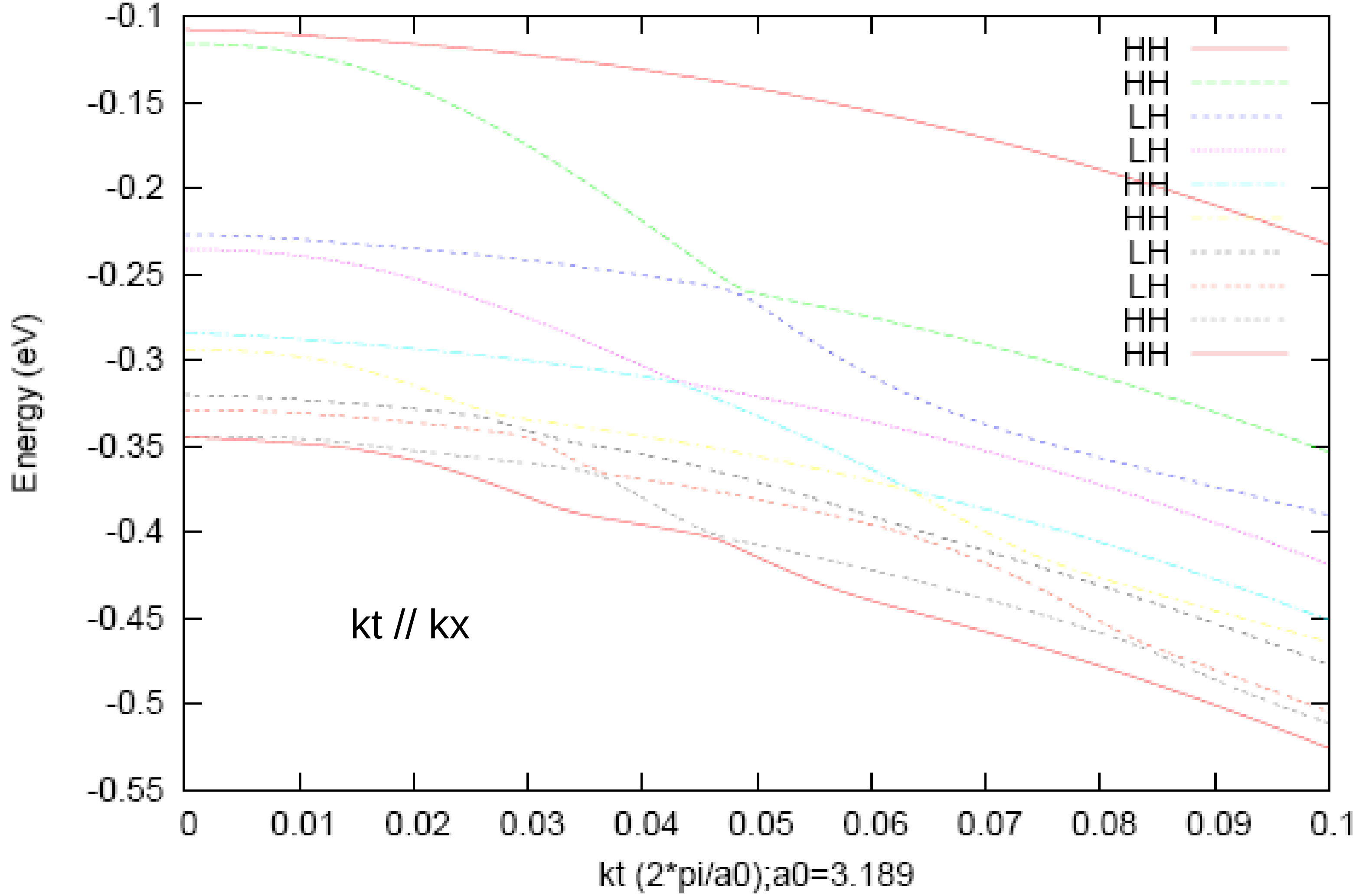






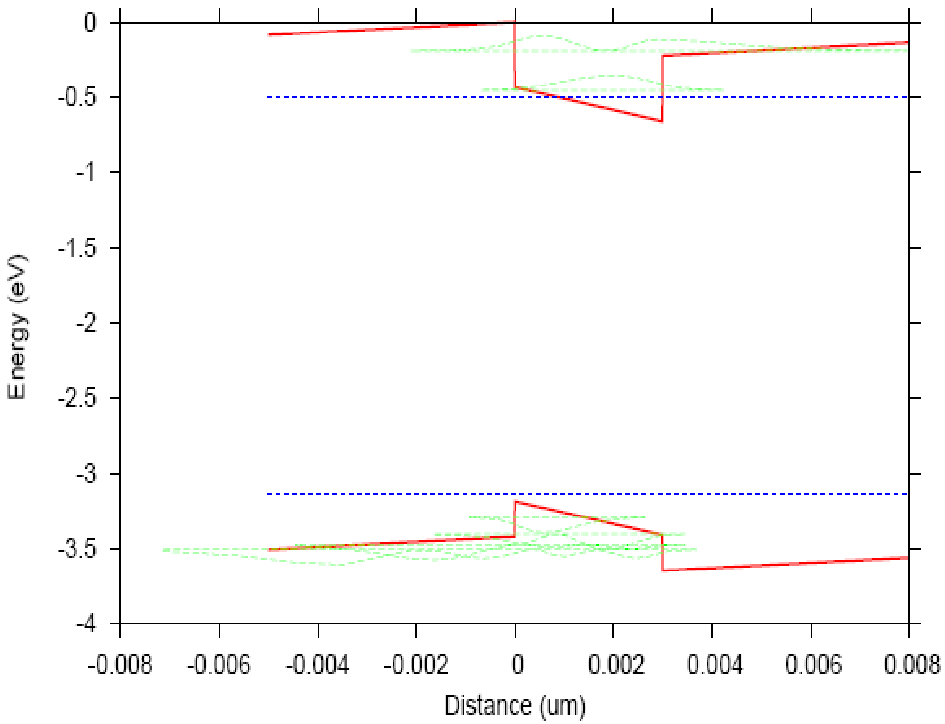
Conc=1.e12 1/cm^2

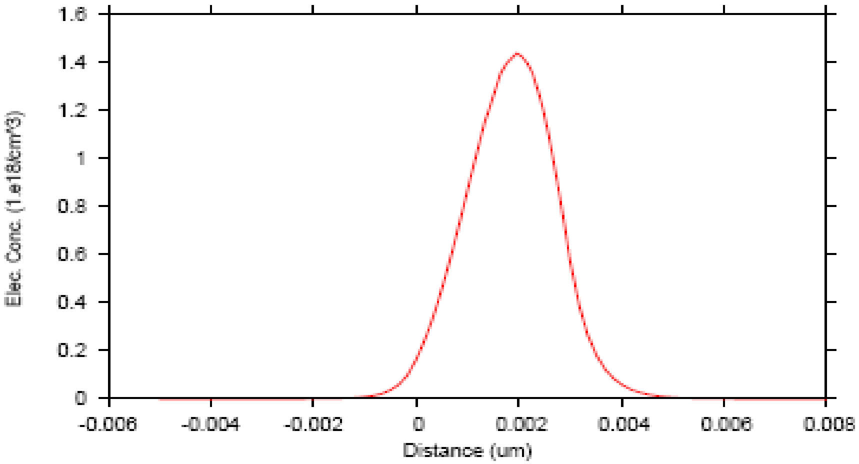
C-plane with internal field

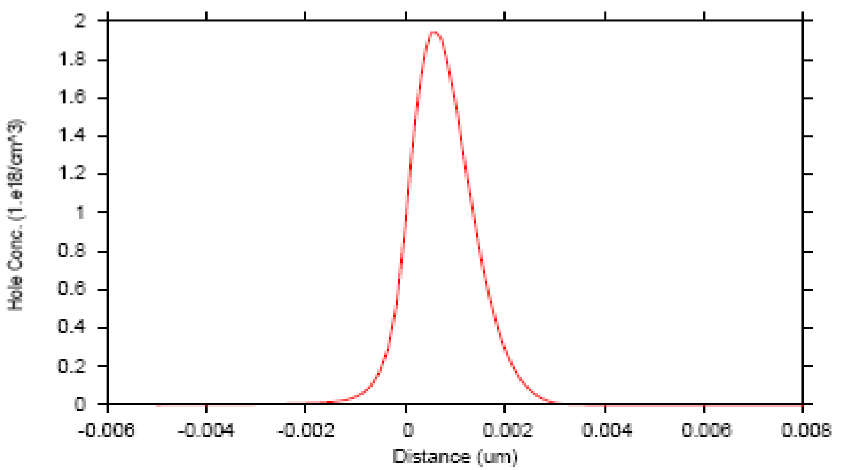


Semipolar (1 1 -2 2) with internal field

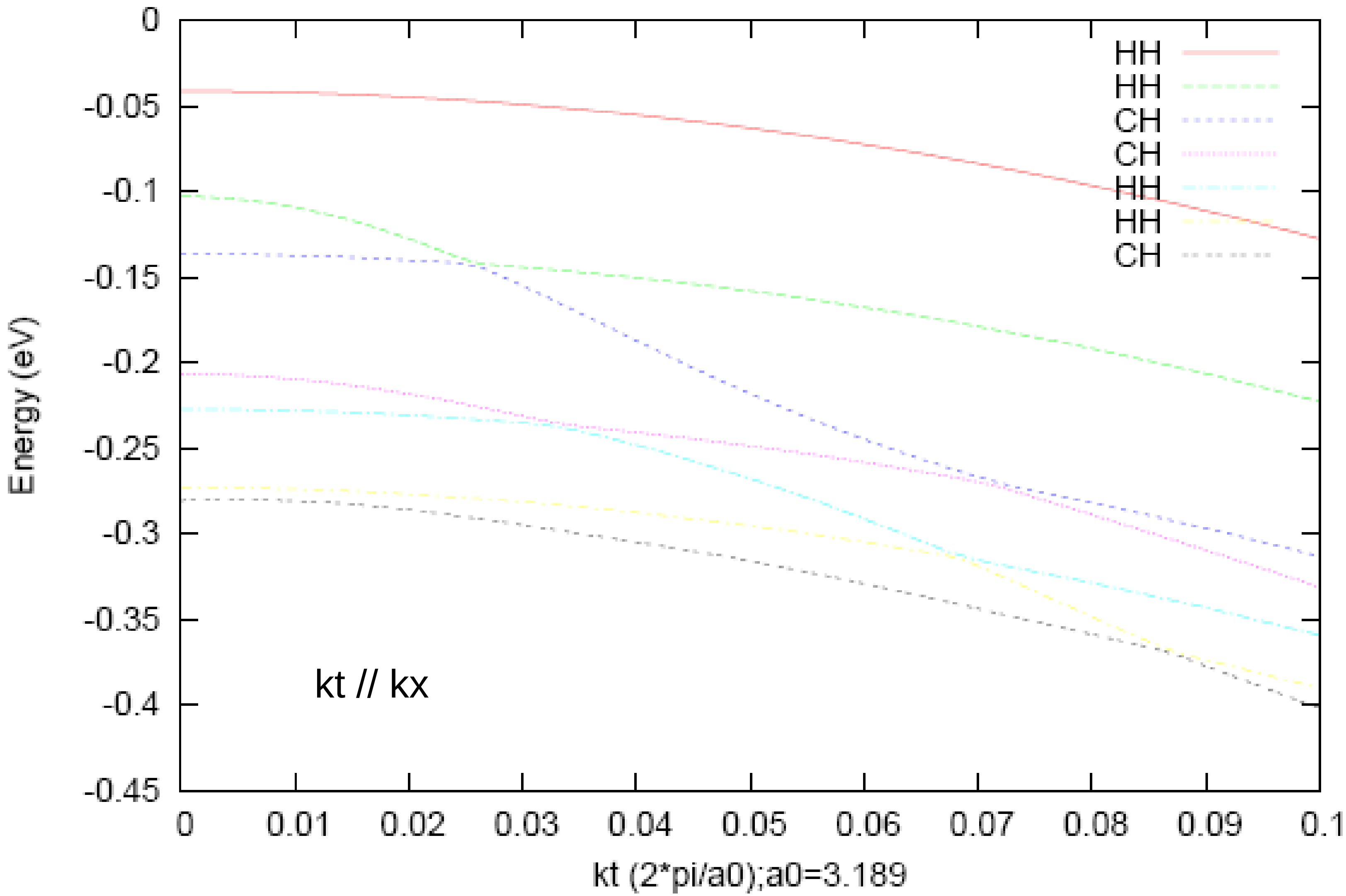
HH is plotted



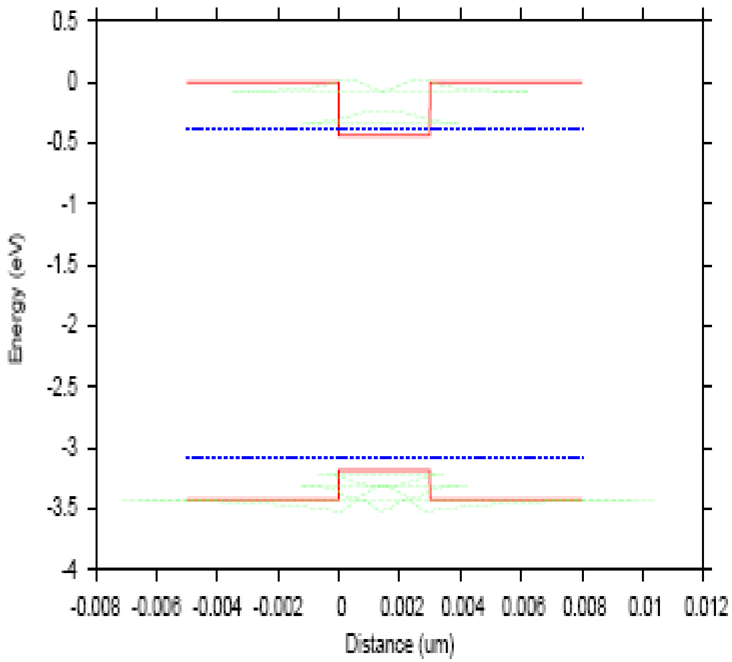




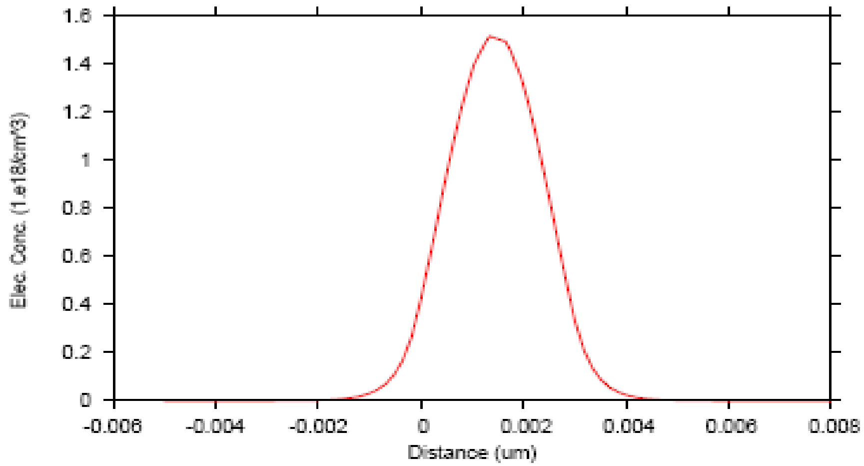
Semipolar (1 1 -2 2) with internal field



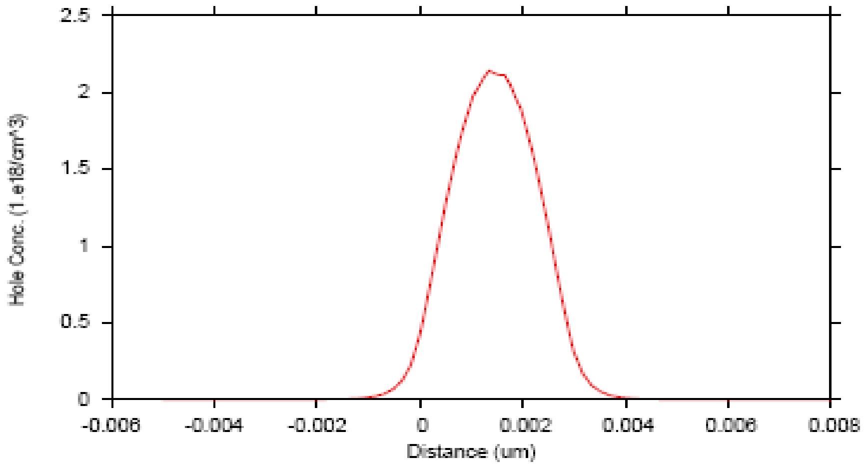
mplane



0.5
0
-0.5
-1
-1.5
-2
-2.5
-3
-3.5
-4
Energy (eV)
-0.008 -0.006 -0.004 -0.002 0 0.002 0.004 0.006 0.008 0.01 0.012
Distance (um)

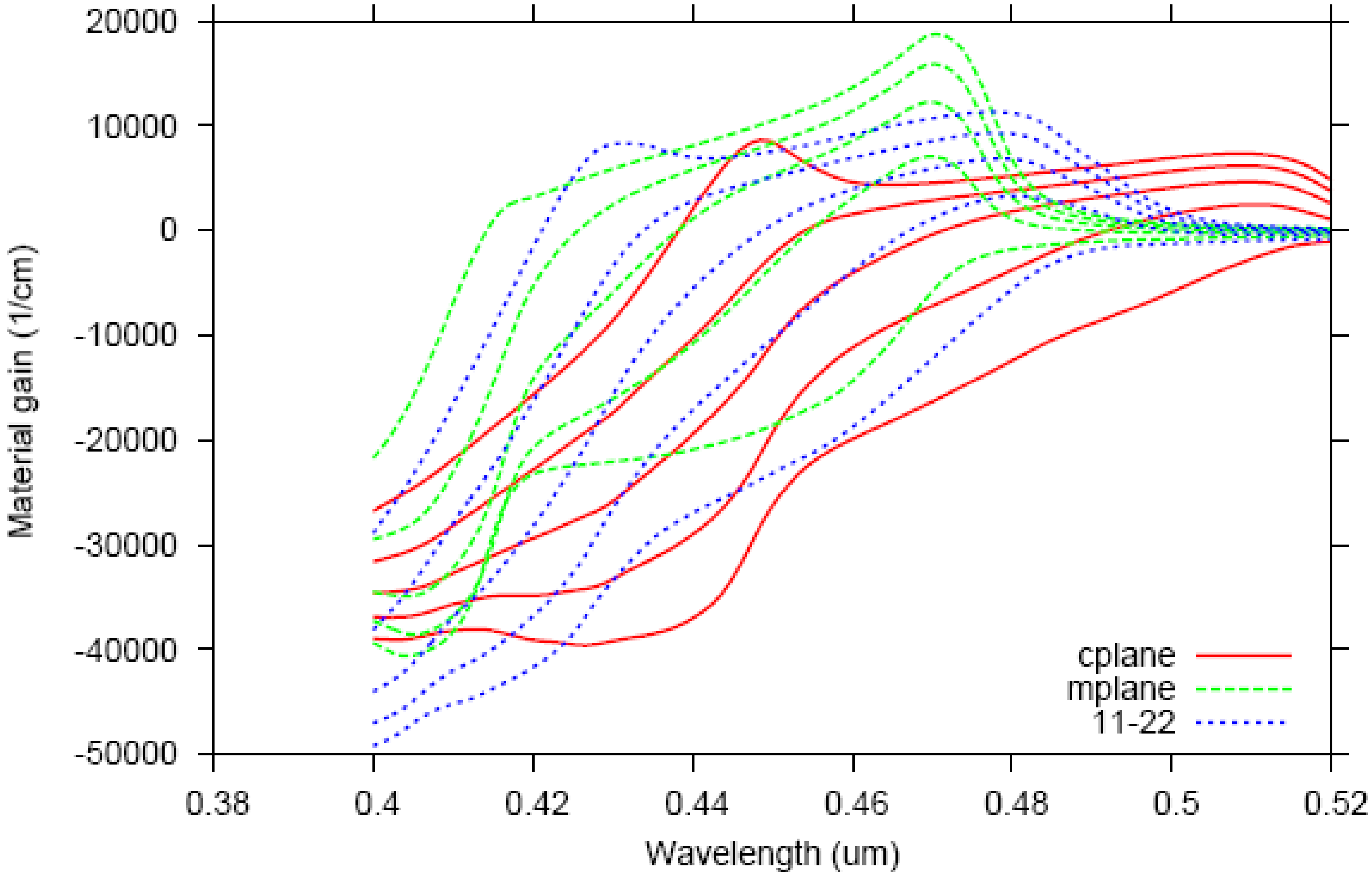


1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
Elec. Conc. (1.e18/cm^3)
-0.006 -0.004 -0.002 0 0.002 0.004 0.006 0.008
Distance (um)



2.5
2
1.5
1
0.5
0
Hole Conc. (1.e18/cm^3)
-0.006 -0.004 -0.002 0 0.002 0.004 0.006 0.008
Distance (um)

Optical gain with internal field:



InGaN/GaN well with 20 percent indium; 3 nm well
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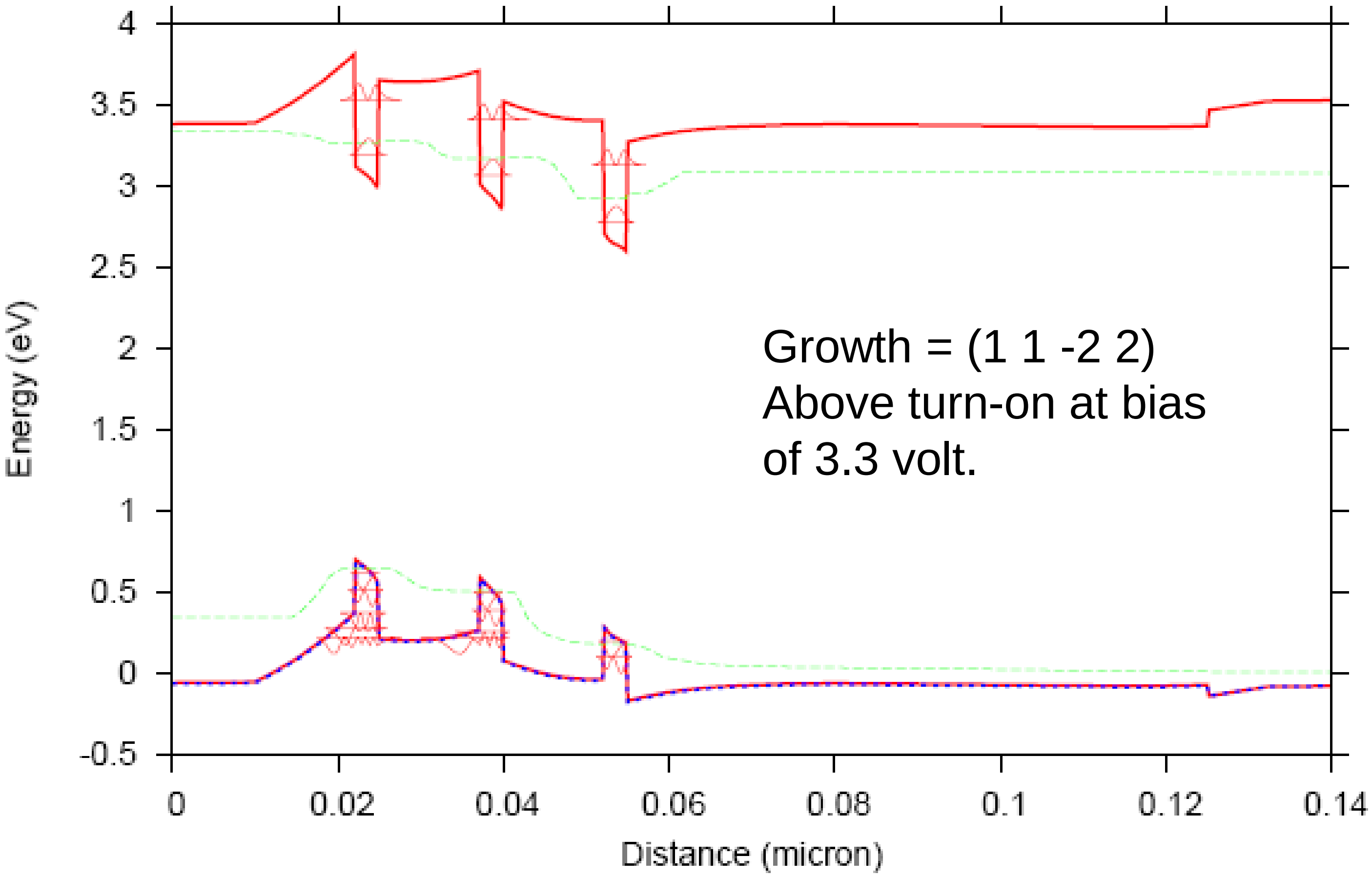
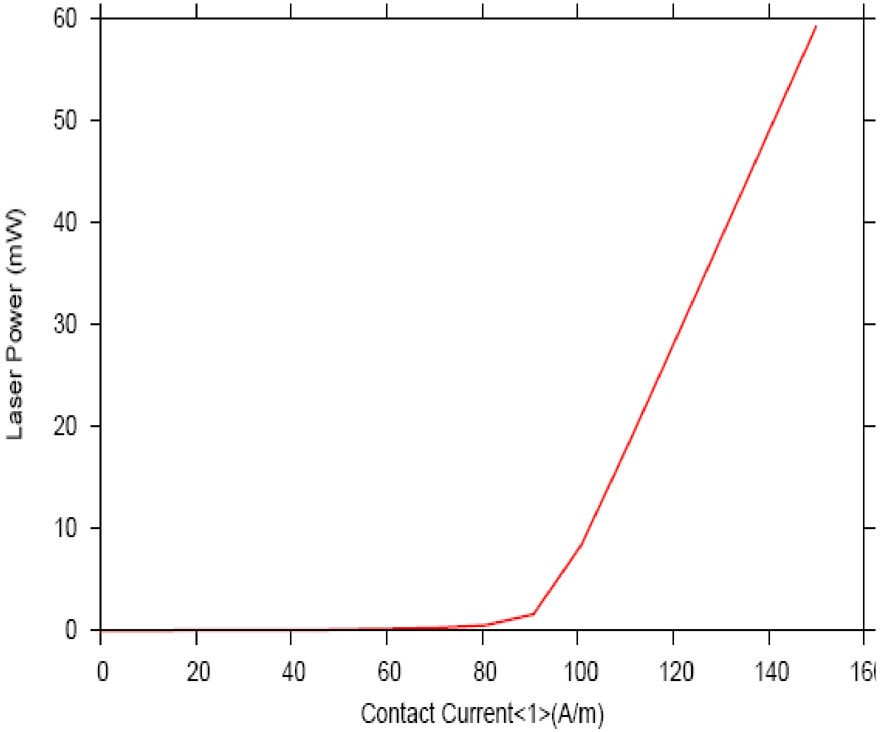
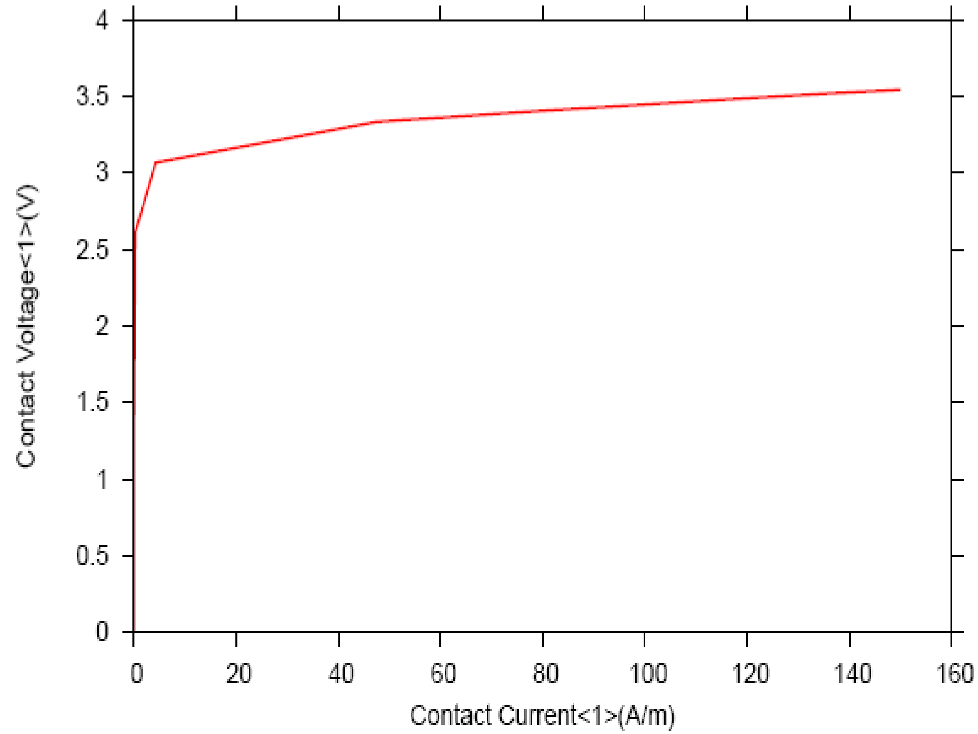
2D simulation using LASTIP



Simple 3MQW with optical gain spectrum imported from a separate active region calculation. Self-consistent simulation performed with internal field effects.

2D simulation using LASTIP





Ridge width = 3 micron; growth=(1 1 -2 2)

Summary

- Using rigorous k.p theory, optical gain spectra (green) of c-plane, semi-polar and non-polar growth are computed and compared.
- Without internal polarization field, MQW optical gain are reasonably isotropic.
- Main difference comes from effect of polarization internal field which strongly reduces c-plane optical gain.
- Semipolar (1 1 -2 2) shows significantly higher optical gain than that of c-plane growth.
- APSYS, LASTIP and PICS3D successfully included k.p based model for wurtzite MQW device with arbitrary crystal growth orientation.

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