Detection Wavelength Tuning and Dark current modeling for GaAs/AlGaAs Quantum Well Infrared Photodetectors using MATLAB and Synopsys ISE TCAD

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Simulation Overview

- Band Structure
  - E Vs k
  - E Vs z
  - Subbands
    - eigenvalues, eigenfunctions
- Optical simulation
  - Absorption coefficient due to intraband transitions
  - Optical generation rate
- Electrical simulation
  - Dark I-V Characteristics

Detection wavelength tuning involves simulation of Band structure by changing x and L_w

Simulation can be used to design a QWIP structure: x, L_w, L_b, N_D, N_w, device geometry

Software Tools used for Simulation

- MATLAB
- MATHEMATICA
- Synopsys ISE TCAD

Band Structure Calculation

- Band Structure Calculation using k.p method which includes strain and many-body effects with its 4x4, 6x6, or 8x8 Hamiltonian matrix
- Subbands in Square wells can be calculated by using 1D Schrodinger solver to calculate eigenfunctions and eigenvalues

Optical Device Simulation

Optical device simulation is split into two distinct models that are calculated simultaneously at each DC bias point.

1. Optical ray trace or FDTD using real component of refractive index (n) to calculate the Electric field and hence the optical intensity at each grid point
2. Absorption or photogeneration model using the imaginary component of refractive index (k) to calculate carrier concentration at each grid point.

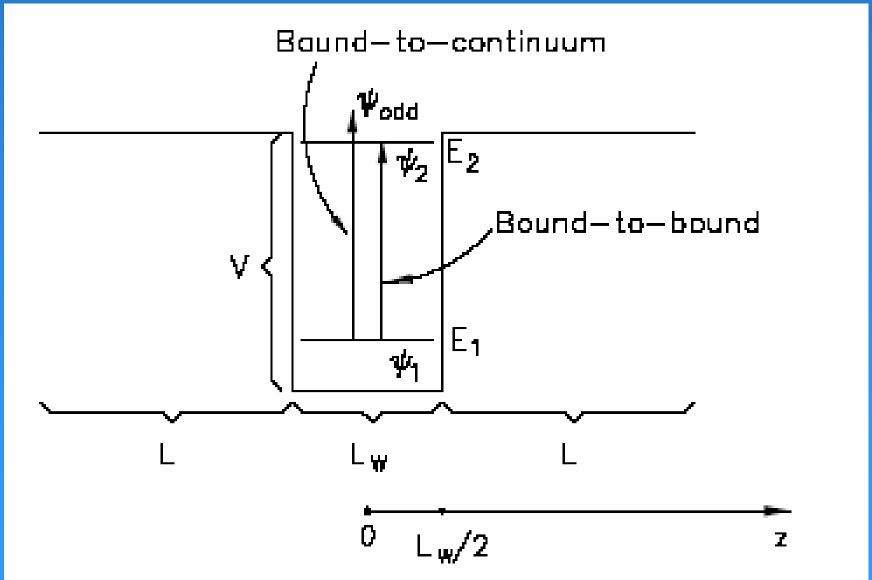
Design device structure

- FDTD solver solves Maxwell's equations to calculate Electric field at each grid point inside the device. Direction of electric field vector with respect to growth direction as well as electric field intensity are calculated. Can be used to simulate optical generation due to IT transitions and hence design **C-QWIP** and **Diffraction Grating coupled QWIPs**.
- Ray Tracing can be used to simulate **45^0 edge-coupled QWIPs**
- Contains extensive library of optical properties (n, k) of materials. Optical properties can also be specified as tabular data. Absorption coefficient values are based on interband transitions.
- TCL scripting language is incorporated. Can be used to extend the capabilities of Synopsys ISE TCAD. Useful for calculation of absorption coefficient due to intraband transitions.

Calculation of Conduction Subband Energy levels for an AlGaAs/GaAs/AlGaAs structure

Theory

- Analytical solution of Schrodinger Equation for Square well potential was used
- The transcendental equations were solved using FindRoot function of Mathematica
- Parameters:
  - Al mole fraction: x
  - Well width: Lw
  - Well depth: V = ΔEc



$$m_b^* = (0.0665 + 0.0835x)m_0$$

$$m_w^* = 0.0065 m_0$$

$$E_g(x) = 1.424 + 1.247x$$

$$\Delta E_g(x) = 1.247x$$

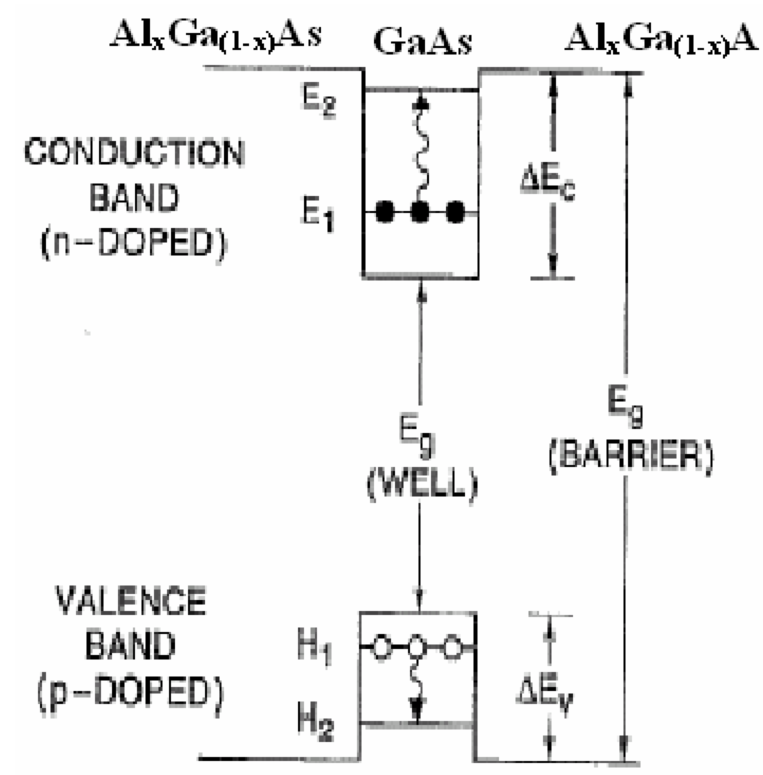
$$\Delta E_c = 0.76x$$

$$\frac{d^2\psi}{dx^2} + k^2\psi(x) = 0 \quad |x| < \frac{L_w}{2}$$

$$\frac{d^2\psi}{dx^2} - \alpha^2\psi(x) = 0 \quad |x| > \frac{L_w}{2}$$

$$\sqrt{2m_w^*\Delta Ec}\left(\frac{L_w}{2\hbar}\right) < N\frac{\pi}{2}$$

$$\alpha = \sqrt{\frac{2m_b^*(V_0 - E)}{\hbar^2}} \qquad k = \sqrt{\frac{2m_w^* E}{\hbar^2}}$$



$$\Delta E = E2 - E1 = \frac{h \cdot c}{\lambda}$$

For energy level E1

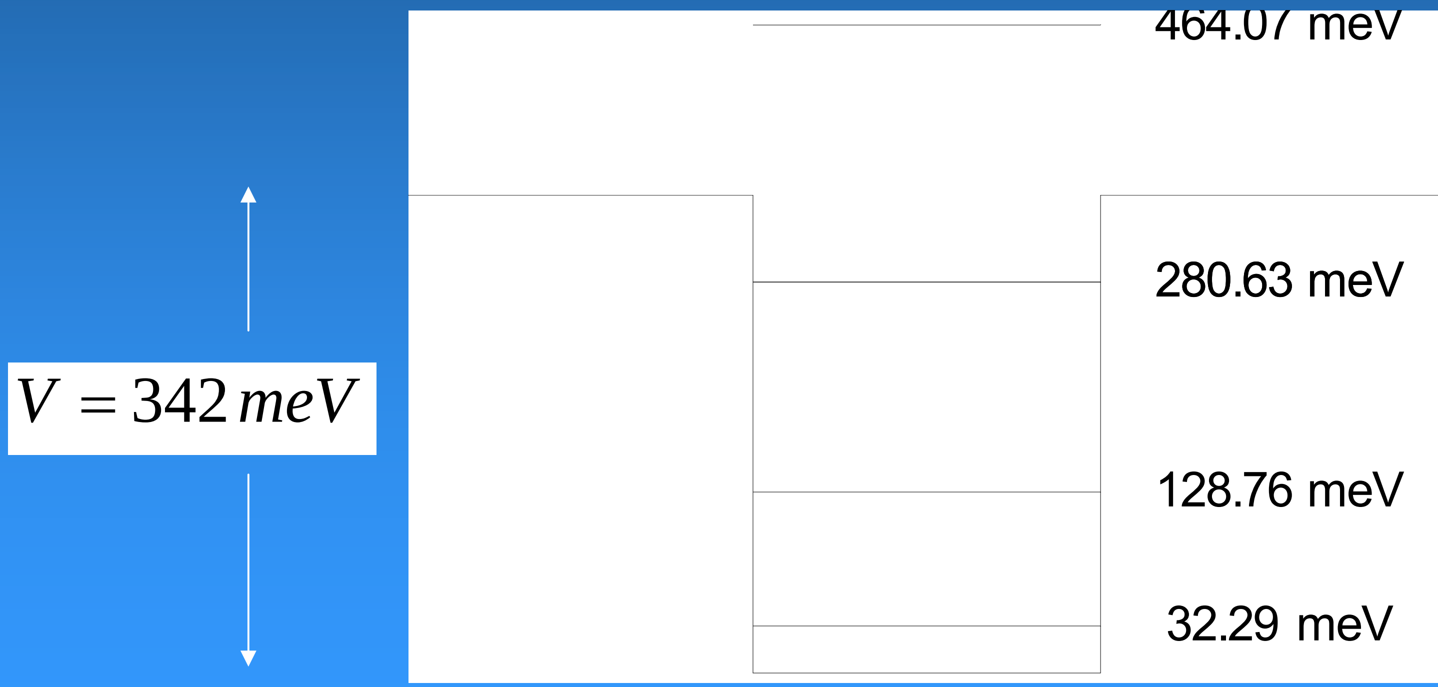
$$\alpha = \frac{m_b^*}{m_w^*} k \tan\left(k\frac{L_w}{2}\right)$$

For energy level E2

$$\alpha = \frac{m_b^*}{m_w^*} k \cot\left(k\frac{L_w}{2}\right)$$

Eigenvalues for a AlGaAs/GaAs/AlGaAs structure (Mathematica calculations)

- For x=0.45, Lw = 100 A^0

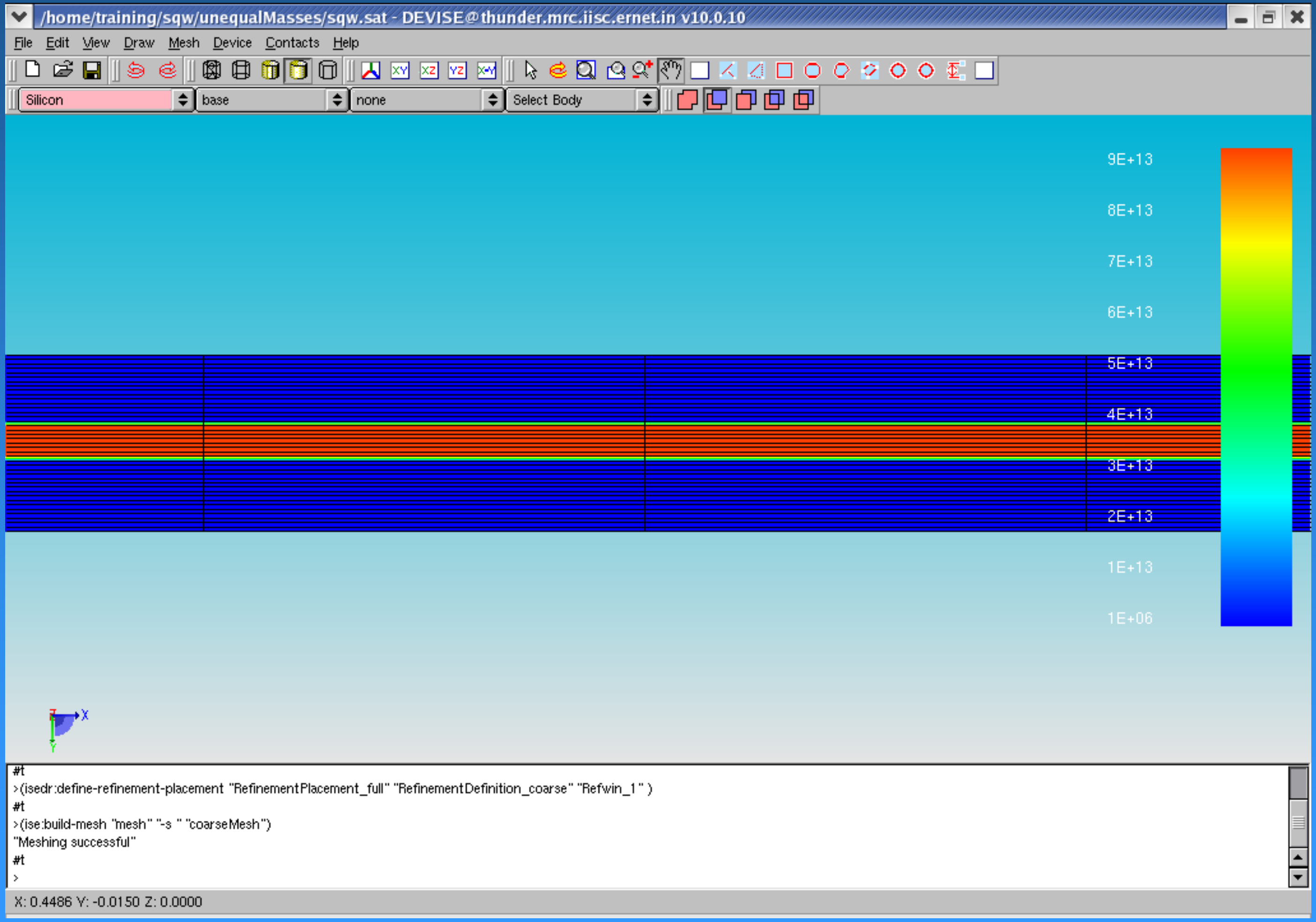


Eigenvalue and Eigenfunction calculation using Synopsys ISE TCAD

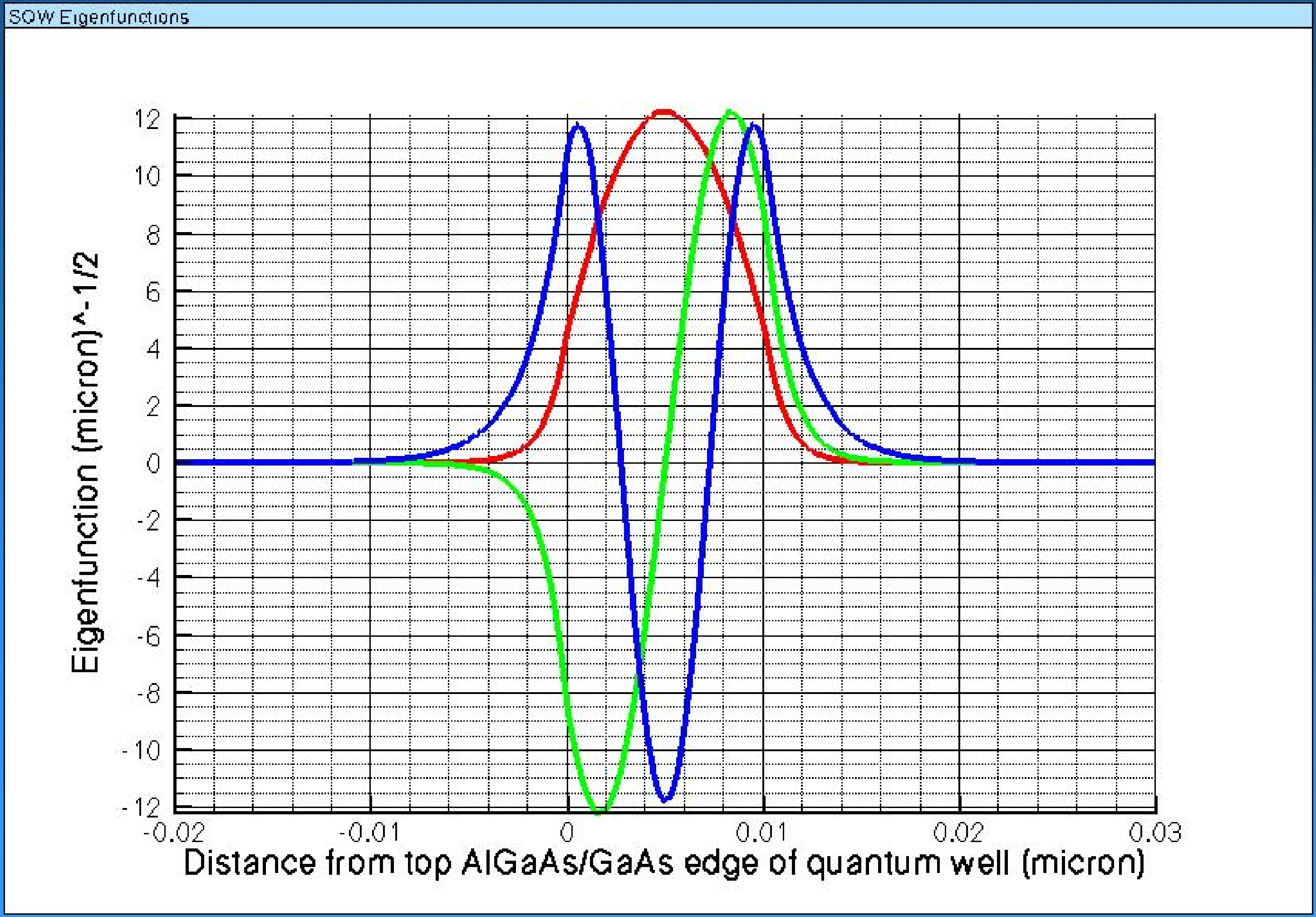
- Synopsys ISE TCAD was used to numerically solve 1D Schrodinger equation for AlGaAs/GaAs/AlGaAs square well
- The structure was drawn in DEVISE (Structure editor) and DESSIS (device simulator) was used to solve Schrodinger equation

Device Structure after meshing (AlGaAs/GaAs/AlGaAs)

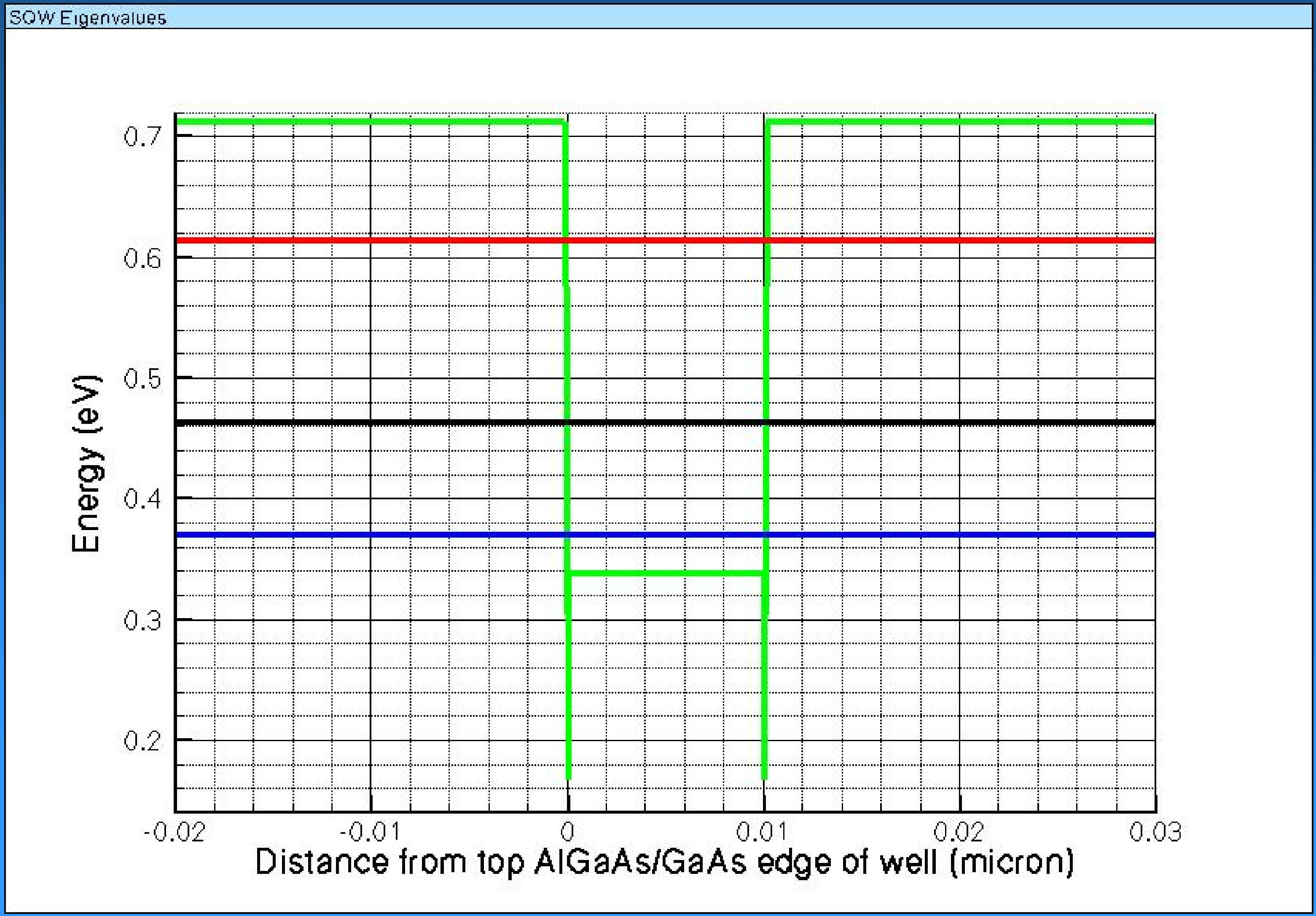
$x=0.45$, $L_w=100\ A^0$, $L_b=200\ A^{0,}$ $N_D = 10^{18}\ /cm^3$



Eigenfunctions of Square Well



Eigenvalues of Square Well



Comparison of Eigenvalues calculated using Mathematica and ISE TCAD

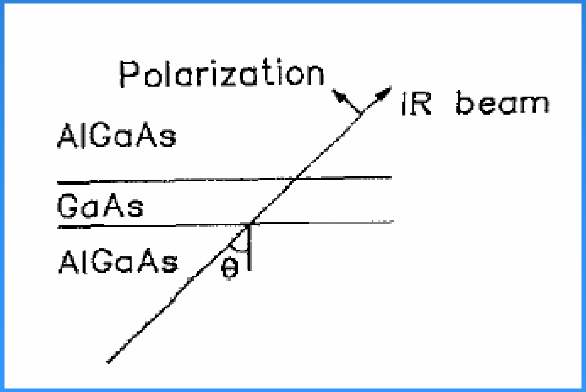
Energies (meV)	Mathematica	ISE TCAD
V	360	373.26
E1	32.69	31.001
E2	130.42	124.3
E3	285.47	275.38

- The results match well
- A more precise match can be achieved by tuning material parameters in ISE TCAD with experimental values (Band gap or Electron affinity, effective mass, etc.)

Calculation of absorption coefficient due to intraband transitions in GaAs/AlGaAs QWIPS

Intraband transitions (IT)

- Transition from a quantized level to the continuum
- Calculation done for a single pass of light through the structure



$$\eta = \frac{e^2 h}{4\epsilon_0 n_r m c} \frac{\sin^2\theta}{\cos\theta} n_{2D} \frac{1}{\pi \Delta E} \left[\frac{1}{1+[(E_2-E_1-\hbar\omega)/\Delta E]^2} f_{B-B} + \right.$$
$$\left. + \frac{L\sqrt{2m}}{2\pi\hbar} \int_V^\infty \frac{dE_z}{\sqrt{E_z - V}} \frac{1}{1+[(E_z-E_1-\hbar\omega)/\Delta E]^2} f_{B-C} \right].$$

Ref: H.C.Liu, J. Appl. Phys. 73 (6), pp. 3062-3066, 1993

Calculation of absorption coefficient due to intraband transitions (IT)

Calculate Eigenenergies, eigenfunctions

Calculate BB and BC oscillator strengths, f_{BB}, f_{BC}

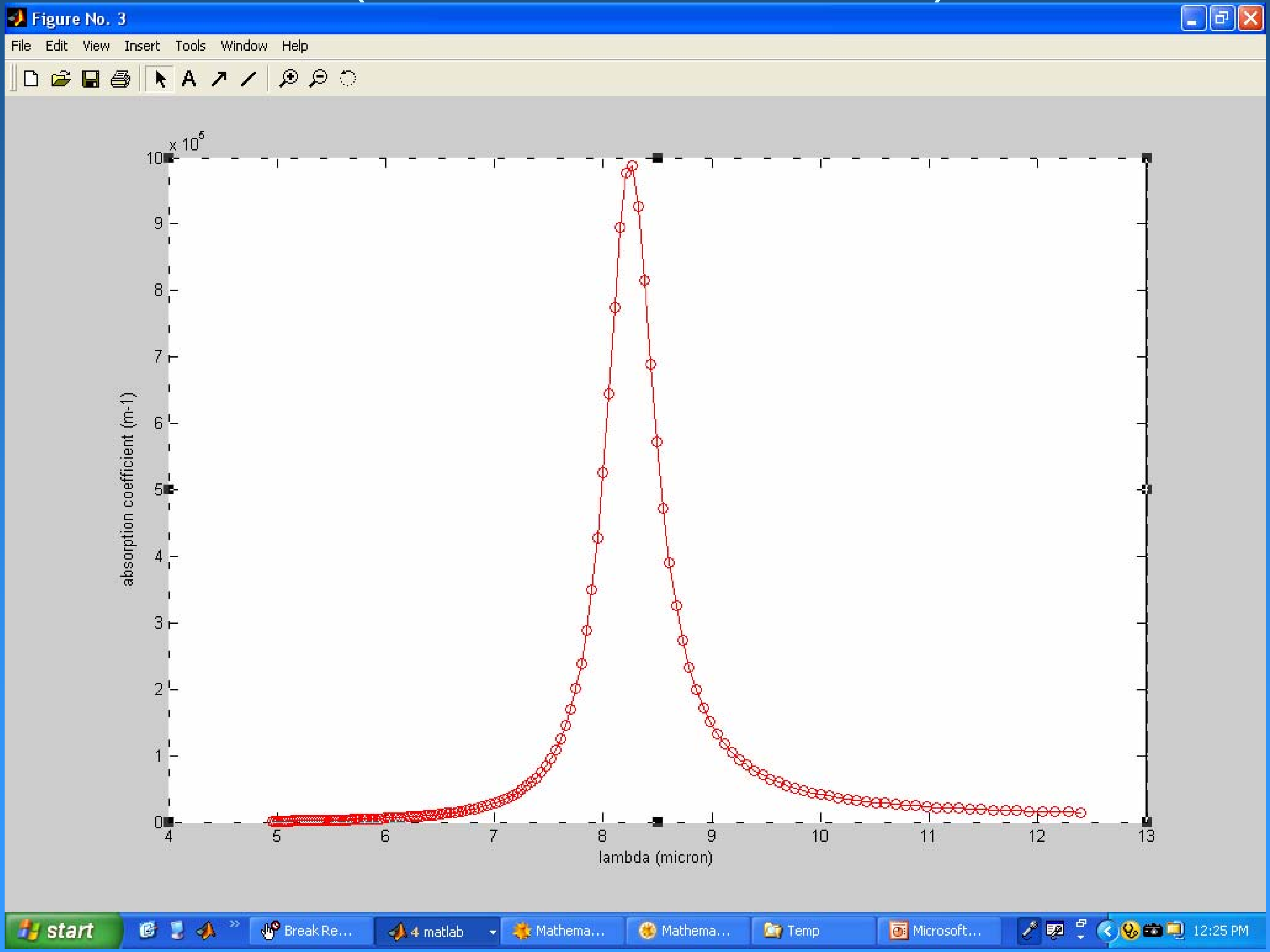
Calculate absorption efficiency, η

Calculate absorption coefficient

$$\eta = \frac{I_{in} - I_{out}}{I_{in}}$$

$$\alpha = \frac{\eta \cos(\theta)}{L_w}$$

Absorption coefficient as a function of wavelength for x=0.3, Lw = 65 A^0 (MATLAB calculation)



$L_w = 60\ A^0$

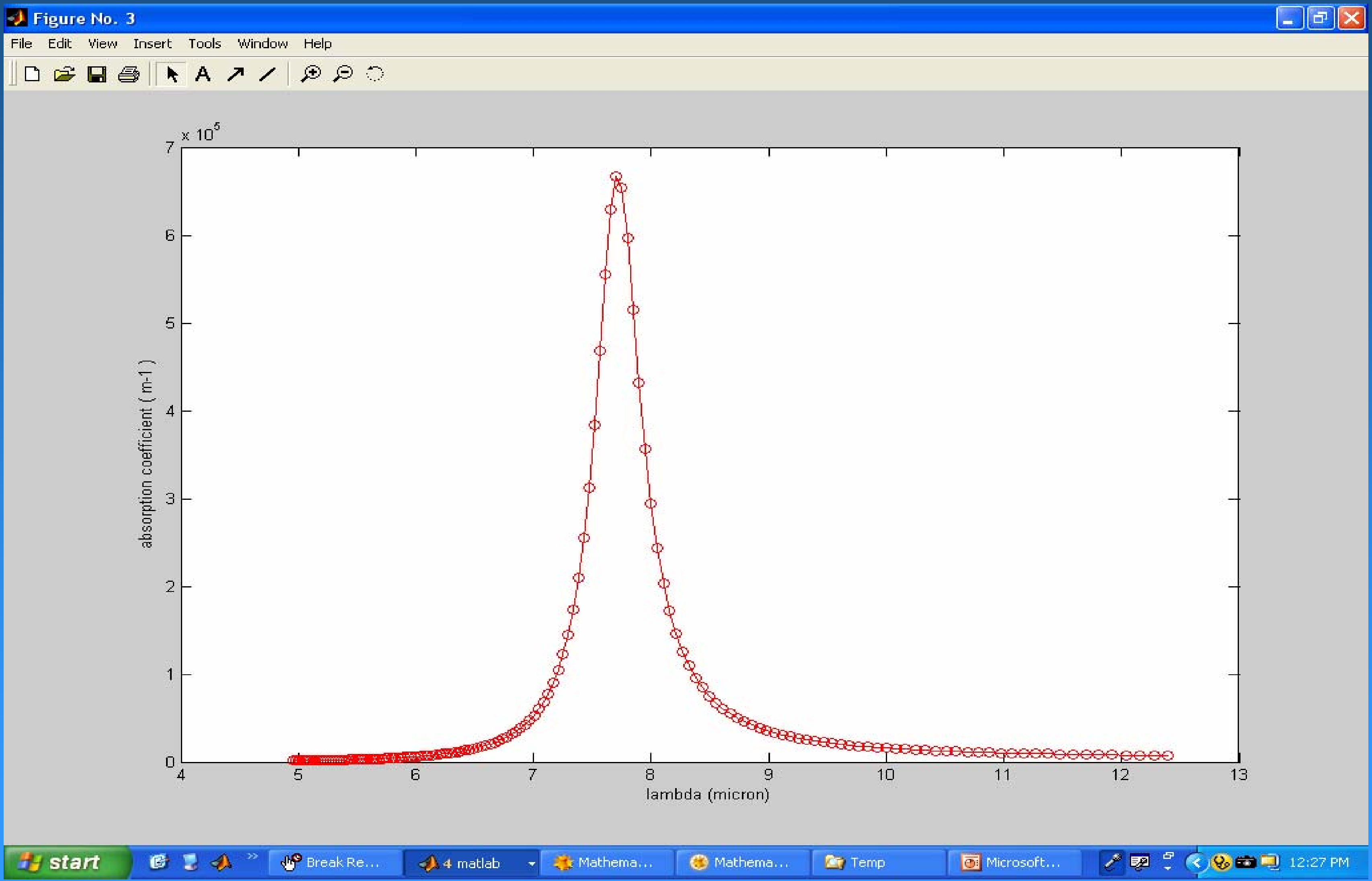


Figure No. 3
File Edit View Insert Tools Window Help
x 10^5
absorption coefficient (m-1)
lambda (micron)
0
1
2
3
4
5
6
7
4
5
6
7
8
9
10
11
12
13

Lw (Angstrom)	Peak detection wavelength (micron)
60	7.7
65	8.3

Peak detection wavelength can be tuned by using proper x and L_w values

Simulation of optical generation rate using Synopsys ISE TCAD

Theory

Theory

Schrodinger solver in Dessis

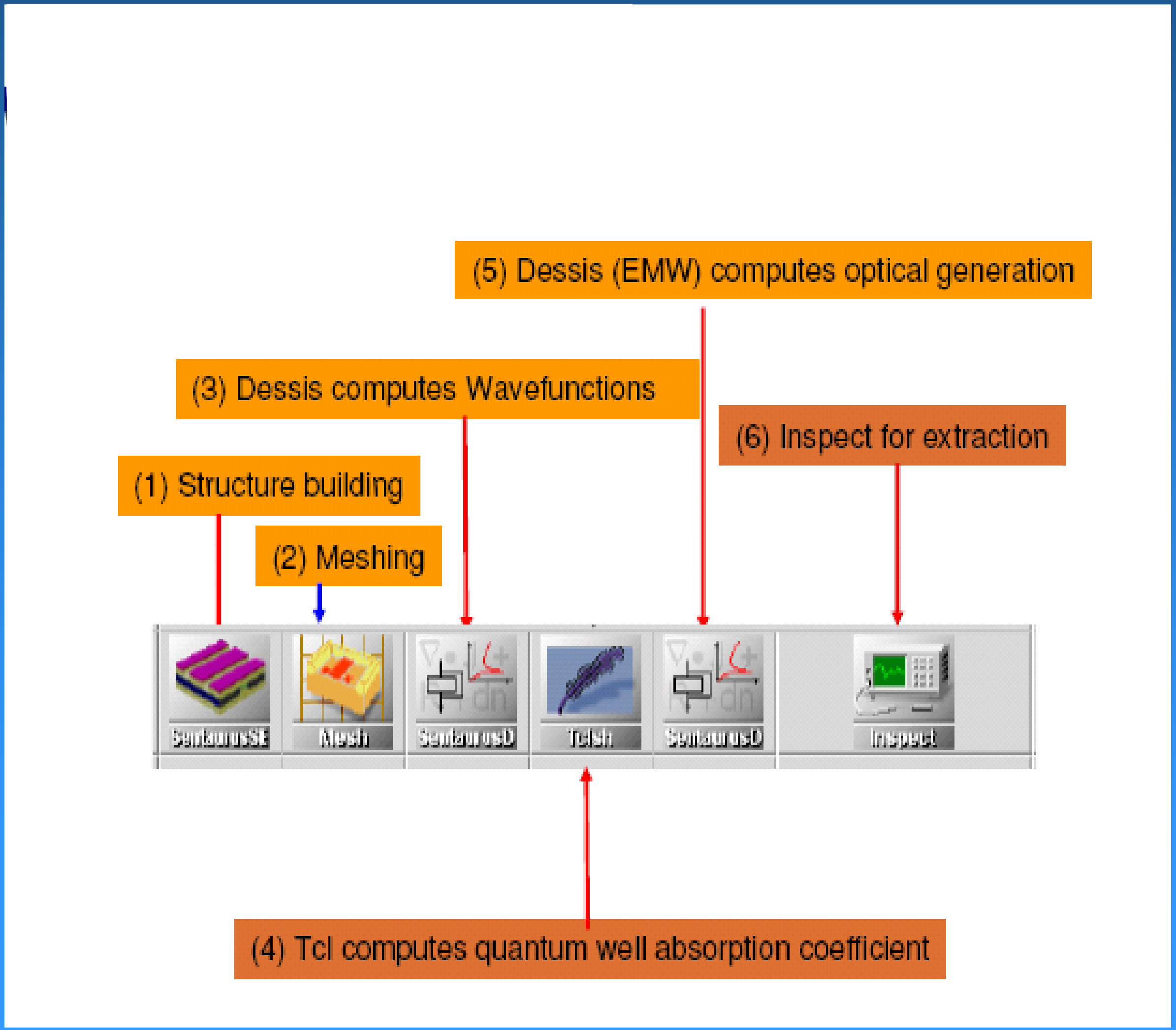
$$\frac{-\hbar^2}{2}\frac{\partial}{\partial z}\left(\frac{1}{m_e^*(z)}\frac{\partial}{\partial z}\phi_{n,q}(z)\right) + V(z)\phi_{n,q}(z) = E_{n,q}\phi_{n,q}(z)$$

Tcl / MATLAB computation

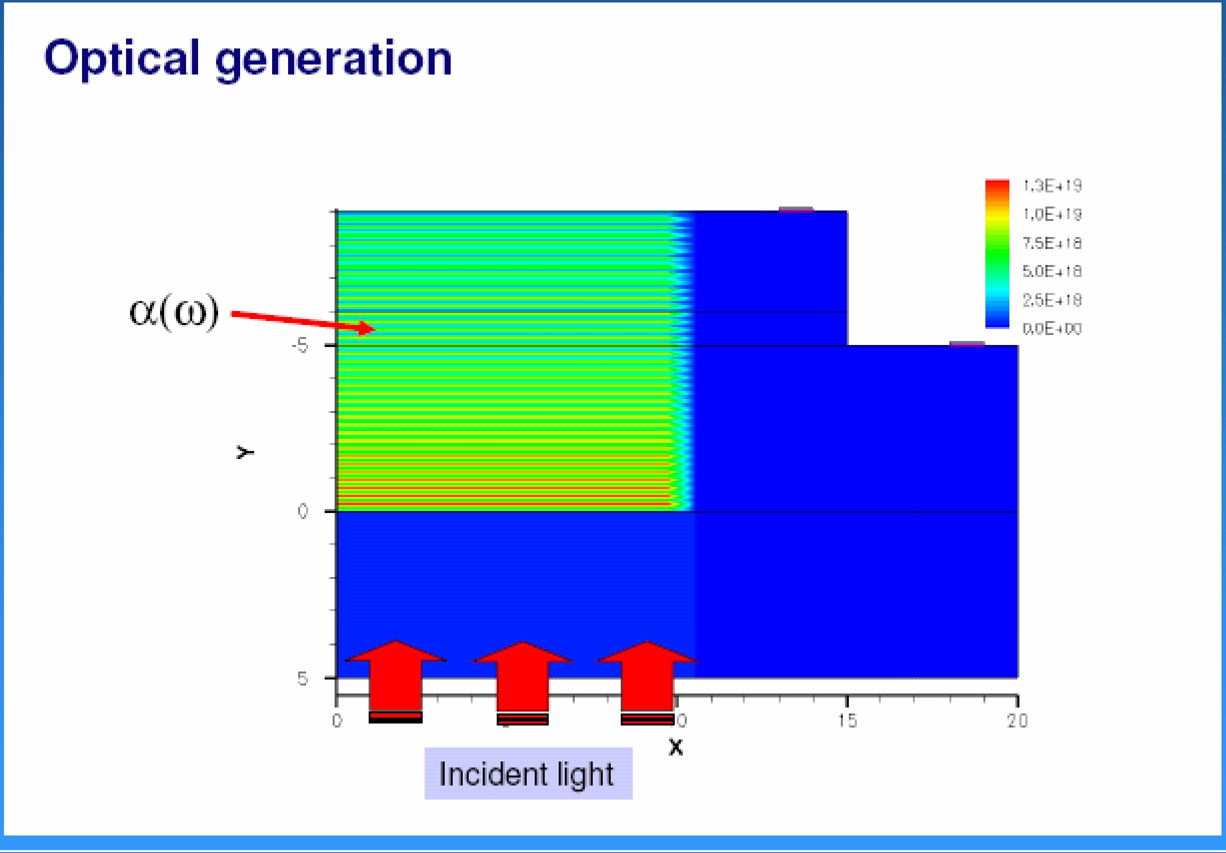
$$\alpha(\omega) = \frac{e^2\pi}{n_r c\epsilon_0 m_0^2(h\omega)}\sum_{n,q}|M_{n,q}|^2 \frac{\Gamma}{(E_{n,q} - E_{1,q} - h\omega)^2 + \left(\frac{\Gamma}{2}\right)^2}(N_{1,q} - N_{n,q})$$

$$M_{n,q} = \left\langle \phi_{n,q}(z) \middle| \frac{-ih}{m_e^*(z)\partial z} \middle| \phi_{1,q}(z) \right\rangle$$

Possible tool flow for QWIP simulation using Synopsys TCAD



Example of optical generation using Synopsys ISE TCAD (interband transitions)



Optical generation due to Intraband transition is yet to be implemented using the suggested tool flow

Simulation of Dark Current-Voltage (I-V)Characteristics

Models

- Thermionic Emission (TE)
- Thermally assisted Tunneling (TAT)
- Sequential Resonant Tunneling (SRT)

- SRT can be neglected for wide barriers. TE and TAT are important at QWIP operating temperatures of 77 K

Simulation of Dark Current

1. $$I_D(V) = n(V) \cdot e \cdot v(V) \cdot A$$

e → Electronic charge
A → area of the QWIP

3. $$v = \mu F \frac{1}{\sqrt{1 + (\mu F / v_s)^2}}$$

μ → mobility of electron
F → Applied field
ν_s → saturation velocity

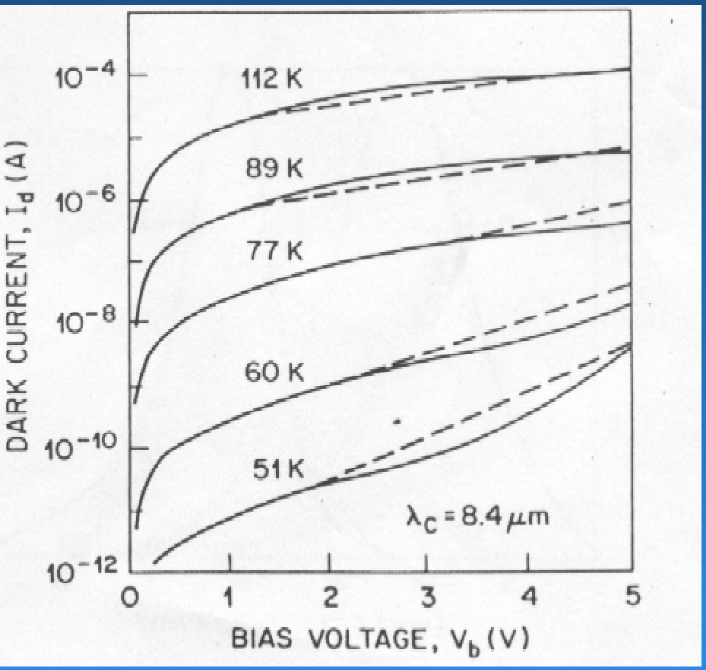
2. $$n(V) = \left(\frac{m^*}{\pi \hbar^2 L_p} \right) \int_{E_0}^{\infty} f(E) T(E,V) dE$$

2.A $$E_f = \frac{n_0 \cdot \pi \cdot \hbar^2 \cdot L_w}{m_w^*}$$ $$f(E) = \frac{1}{1 + e^{\left(\frac{E - E_0 - E_f}{kT} \right)}}$$

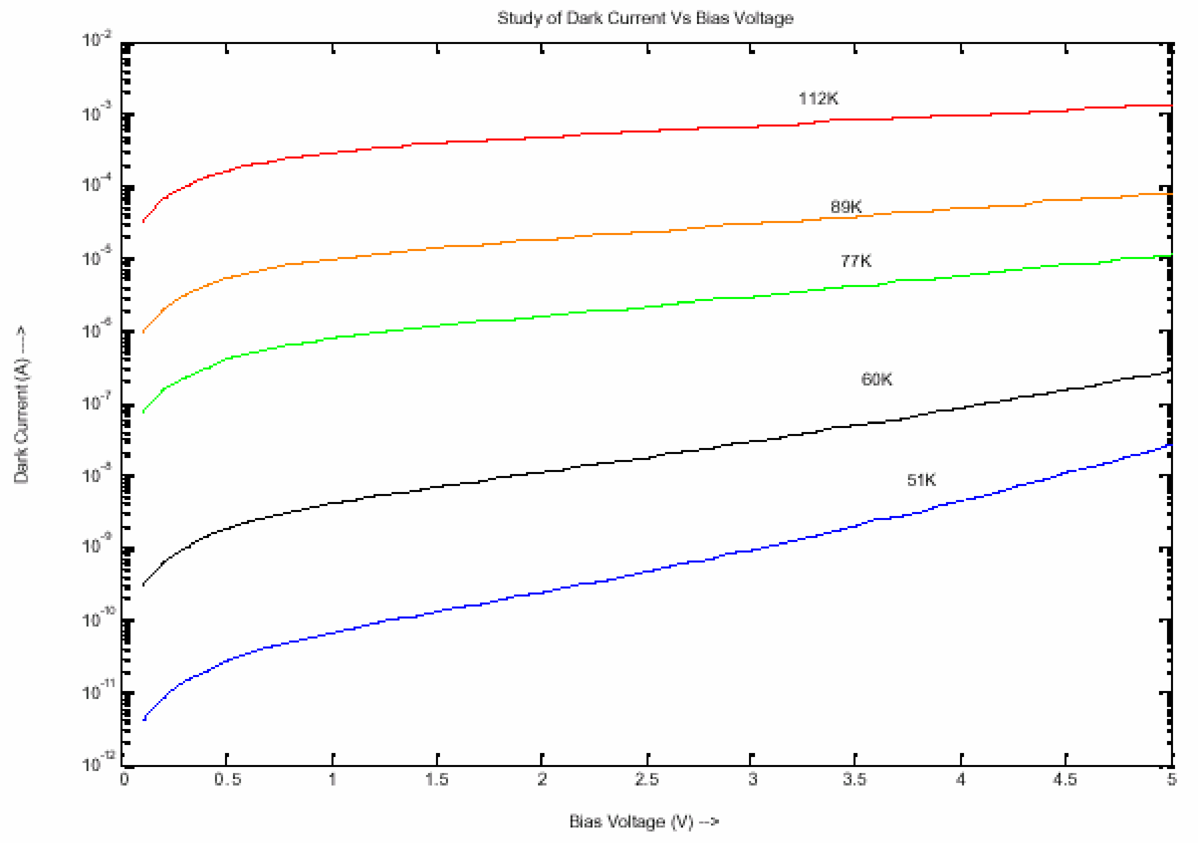
2.B
$$T(E,V) = 1 \qquad E > V_0$$
$$T(E,V) = \exp[(-4L_b / 3eV)(2m/\hbar^2)^{1/2}(V_0 - E)^{3/2}] \qquad V_0 - eV < E < V_0$$
$$T(E,V) = \exp\left[\frac{-4L_b}{3eV} \cdot \left(\frac{2m}{\hbar^2} \right)^{1/2} [(V_0 - E)^{3/2} - (V_0 - E - eV)^{3/2}] \right] \qquad E_0 < E < V_0 - eV$$

Ref: S. R. Andrews and B. A. Miller, J. Appl. Phys., **70** (2), pp. 9931003, 1991

Comparison of Dark current curves (MATLAB)



Experimental Plot



Theoretical Plot

A = 9e-8 /m²
Well width = 40e-10 m
Barrier width = 305e-10 m
x = 0.29
n0 = 1e18 /cm³
No. of wells = 50
Mobility = 1000 cm² /V s
Saturation velocity= 5e6 cm/s

Ref: B. F. Levine, J. Appl. Phys. **74** (8), R1, 1993

Conclusions

- Energy levels in a GaAs/AlGaAs quantum well were calculated using MATHEMATICA and ISE TCAD. There is a close match between both the results
- Detection wavelength can be tuned by varying Al mole fraction and well width
- Absorption coefficient due to IT transitions in QWIP structure were calculated using MATLAB
- Capability of Synopsys ISE TCAD to calculate optical generation rate and hence design a QWIP structure was discussed.
- Dark current simulation was carried out

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