CHAPTER 3

Theoretical Background

This chapter focuses over the theoretical detail for calculation of optical properties of the heterostructures under study. To find the optical gain and other lasing parameters of the heterostructures under study, first the behavior of carriers in QW (i.e. wave functions associated with it and corresponding energy states) was studied and then transition matrix elements calculations is designed to perform calculations of momentum matrix elements and dipole moments of selected transitions and finally the optical gain, differential gain, gain compression and anti-guiding factor of the lasing heterostructure is simulated.

The optical gain is the fundamental characteristic of the quantum well heterostructures. To determine the optical response such as the optical gain or optical absorption, the knowledge of the conduction and valence bands structure is essential, which have been discussed in the following sections.

4.1 Calculation of Energy Levels in Conduction and Valence Bands

Assuming the semi parabolic band nature of the conduction band, the discrete energy levels within the conduction band can be evaluated by using the single band effective mass equation as [1, 2];

\[- \frac{\hbar^2}{2m_e^*} \nabla^2 \psi + V_c \psi = E_c \psi\]  

(1)

where \(\hbar\) is reduced Planck’s constant divided by \(2\pi\), \(\psi\) is envelope function, \(m_e^*\) is the effective mass of electron in conduction band, \(V_c\) stands for potential of conduction band, \(E_c\) stands for conduction band electron energy.
The heterostructure in the present work has been studied taking in account the strain effects. The strain can be compressive or tensile. In 1, the effect of strain on the conduction and valance band in a strained quantum well heterostructure is illustrated.

![Figure 1. Effect of strain on conduction and valance bands in quantum well structure.](image)

For a strained quantum well, the conduction band potential is:

\[
V_c = \begin{cases} 
\frac{2\delta_h}{3} & \text{Quantumwell} \\
\Delta V_{bc}, \text{Barrier} & \\
\Delta V_{cc}, \text{Cladding} & 
\end{cases}
\]

(2)

where \(\Delta V_{bc}\) and \(\Delta V_{cc}\) are the conduction band offsets of barrier and cladding layers, respectively; and \(\delta_h\) is the hydrostatic potential that can be defined as [3]:

\[
\delta_h = 2a \left(1 - \frac{C_{12}}{C_{11}}\right) \varepsilon
\]

(3)
where, $a$ is the hydrostatic deformation potential, $C_{11}$ and $C_{12}$ are the elastic stiffness coefficients; $\varepsilon$ stands for the strain constant of the quantum well layer that can be given as:

$$\varepsilon = \frac{a_s - a_q}{a_s}$$

(4)

where $a_s$ and $a_q$ are the lattice constants of substrate and quantum well layers; and the strain in barrier layer can be given as

$$\varepsilon = \frac{a_s - a_b}{a_s}$$

(5)

where $a_b$ is the lattice constants of barrier. In case, if the barrier has no strain, the lattice constant of barrier will be equal to that of substrate, then the strain in quantum well will be given as [1];

$$\varepsilon = \frac{a_s - a_q}{a_b}$$

(6)

Next, for the calculation of energy levels in valence band, the multiband effective mass theory can be used due to its non-parabolic valence band structure that give the coupled differential equations for heavy and light holes. In order to calculate the envelope functions and the energies of heavy holes and light holes in valence energy bands, the Kohn-Luttinger Hamiltonian can be solved. The Schrödinger equation within the Kohn-Luttinger Hamiltonian for heavy and light holes can be given as:

$$\hat{H} \psi = E \psi$$

(7)

where

$$H = -\frac{\hbar^2}{2m_0} \left[ k_x^2 + k_y^2 \right] (\gamma_1 + \gamma_2) - \frac{\gamma_1 - 2\gamma_2}{\delta} \frac{\partial^2}{\partial \zeta^2} + V_{hh,hl}$$

(8)
\[ L = -\frac{\hbar^2}{2m_b} \left[ (k_x^2 + k_y^2) (\gamma_1 - \gamma_2) - (\gamma_1 + 2\gamma_2) \frac{\partial^2}{\partial z^2} \right] + V_{hh, lh} \]  
\[ M = \frac{i\sqrt{3}\hbar^2}{2m_0} (-k_y - ik_x) \gamma_3 \frac{\partial}{\partial z} \]  
\[ N = -\frac{\sqrt{3}\hbar^2}{2m_0} \left[ \gamma_3 (k_x^2 - k_y^2) - 2i\gamma_3 k_x k_y \right] \]  

where \( \psi \) is the envelope function, \( E_v \) is the energy Eigen values of heavy and light holes in valence sub-bands, \( m_b \) is the mass of free electron, \( k_x \) and \( k_y \) are the transverse wave vector components, \( \gamma_1, \gamma_2 \) and \( \gamma_3 \) are the Luttinger parameters, the potential of valence sub-band for heavy hole is \( V_{hh} \), \( V_{lh} \) is the potential of the valence sub-band for light hole.

The potentials of heavy and light holes sub-bands can be expressed as follows;

\[ V_{hh} = \begin{cases} 
\frac{1}{3}\delta_h + \delta_s, \text{Quantumwell} \\
-\Delta V_{bh}, \text{Barrier} \\
-\Delta V_{cv}, \text{Cladding} 
\end{cases} \]  
\[ V_{lh} = \begin{cases} 
\frac{1}{3}\delta_h - \delta_s, \text{Quantumwell} \\
-\Delta V_{bh}, \text{Barrier} \\
-\Delta V_{cv}, \text{Cladding} 
\end{cases} \]  

In the expressions (12) and (13), \( \Delta V_{bh} \) and \( \Delta V_{cv} \) quantities are valence band offset values for barrier and cladding layers, respectively. The quantity \( \delta_s \) represents the shear potential, can be expressed as follows;

\[ \delta_s = 2b \left( 1 + \frac{2C_{12}}{C_{11}} \right) \varepsilon \]  

where \( b \) is shear deformation potential.
3.2 Optical Gain

The optical gain is the fundamental characteristic of the quantum well heterostructures. According to the theory of density matrix, the optical gain can be determined by summing up contribution from overall transitions in between the electrons and holes in the conduction and valence sub-bands, respectively. In the present work, the optical gain is simulated with the help of GAIN simulation package. The simulation of the optical gain of lasing nano-heterostructure is complicated in the quantum well (active region) region. Actually, the GAIN package utilizes the accurate model for optical gain as a function of the photon energy as [3-5];

\[
G(E) = \frac{q^2 |M_B|^2}{\varepsilon_0 m_e^2 c h n_{eff}} \sum_{i,j} \int_{E_g}^{E_{gb}} \int m_{r,ij} C_{ij} A_y (f_e - f_v) L(E - E') dE
\]  

(15)

The integration performed in equation (15) extends from \(E_g\) (band gap of quantum well) to \(E_{gb}\) (band gap of barrier). In equation (15), \(\varepsilon_0\) is free space permittivity, \(c\) stands for speed of light in vacuum, \(q\) is elementary charge, \(W\) is width of quantum well, \(n_{eff}\) is the effective refractive index, \(i\) and \(j\) represent quantum numbers of conduction and valence band, \(m_{r,ij}\) spatially weighted reduced mass for transition, the quantities \(f_e\) and \(f_v\) are the quasi Fermi functions of electrons and holes with in the conduction and valence bands, respectively; the function \(L(E)\) refers to the Lorentzian Lineshape function that convolves with gain spectra to determine the effects the interband transitions [6], \(|M_B|^2\) is the bulk momentum transition matrix element for the dipole transition [7], which can be expressed as [3];

\[
|M_B|^2 = (2/3) |M|^2
\]  

(16)

where

\[
|M|^2 = \left( \frac{m_o}{m_e} - 1 \right) \left[ \frac{E_g + \Delta}{2(E_g + \frac{\Delta}{3})} \right] m_o E_g
\]  

(17)
where \( \Delta \) is the spin orbit interaction energy of the quantum well (active) material, \( m_o \) refers to the rest mass of the electron, \( m_c \) refers the effective mass of the electron in conduction band.

In equation (15), the quantity \( C_{ij} \) represents the spatial overlap factor between \( i \) and \( j \) states which is defined as follows;

\[
C_{ij} = \begin{cases} 
1 & (\text{when } i = j) \\
0 & (\text{when } i \neq j) 
\end{cases}
\]  

(18)

The quantity \( A_{ij} \) represents the angular anisotropy factor and it is normalized so that the angular average becomes unity.

In the transverse electric (TE) polarizations mode, the quantity \( A_{ij} \) can be given as [3, 8];

\[
A_{ij} = \begin{cases} 
(3/4)(1 + \cos^2 \theta), (\text{heavy} - \text{hole}) \\
(1/4)(5 - 3\cos^2 \theta), (\text{light} - \text{hole}) 
\end{cases}
\]

(19)

In the transverse magnetic (TM) polarizations mode, it can be given as;

\[
A_{ij} = \begin{cases} 
(3/2)(\sin^2 \theta), (\text{heavy} - \text{hole}) \\
(1/2)(4 - 3\sin^2 \theta), (\text{light} - \text{hole}) 
\end{cases}
\]

(20)

where the angular parameter \( \cos \theta \) is;

\[
\cos^2 \theta = \frac{E'}{E}
\]

(21)

where \( E \) represents the photonic energy and; \( E' \) the transition energy between \( i \) and \( j \) states.

Next, in equation (15), the function \( L(E) \) can be used as;

\[
L(E - E') = \frac{\hbar}{\pi (E - E')^2 + (\frac{\hbar}{\tau_n})^2}
\]

(22)
where $\tau_i$ represents interband relaxation time having the order of pico-seconds [2].

Further, the temperature dependent optical gain coefficient can be expressed as:

$$G(E) = \frac{\pi \hbar e^2}{n_{\text{eff}} E m^* e_0 c} \left[1 - \exp\left(\frac{E - \Delta f}{k_B T}\right)\right] \times \sum_{n_i, n_v} \frac{|M_{n_i n_v}|^2}{4 \pi^2 W} f_c f_v \times$$

$$\frac{\hbar / \tau_{\text{iso}}}{\pi (E - E)^2 + (\hbar / \tau_{\text{iso}})^2} dk_x dk_y$$

(23)

where $\Delta f$ is the Fermi level separation and $k_B$ is the Boltzmann Constant.

Now again referring to equation (15) for optical gain, the functions $f_c$ and $f_v$ are the Fermi distribution functions for electrons and holes in conduction and valence bands, respectively, are still to be calculated. Actually, the Fermi function gives the occupation probability of energy states in conduction and valence bands as [9];

$$f_{cv}(E, E_{fc,fv}) = 1/[1 + e^{(E-E_{fc,fv})/k_B T}]$$

(24)

In equation (24), $E_{fc,fv}$ represents the quasi Fermi levels in conduction and valence bands.

Since the carrier density in an energy band can be given by the integration over of the product of the occupation probability of the carriers and the density of states over the entire band, hence for non-parabolic band structure the carrier density can be given as [10–11];

$$N = \sum_{N} \int_{0}^{\infty} \rho(k) \left[f_c \left(E_{nc}(k), E_{fc}\right)\right] dk$$

(25)

$$P = \sum_{hh,LH} \int_{0}^{\infty} \rho(k) \left[1 - f_v \left(E_{nm}(k), E_{fv}\right)\right] dk$$

(26)

But, for the material systems in the present work, assuming the parabolic conduction bands and non-parabolic valence bands, the carrier density can be expressed as;

$$N = \frac{m^* k T}{\pi \hbar^2 W} \sum_{i} \ln[1 + e^{(E_{fi} - E_i)/k_B T}]$$

(27)
\[ P = \frac{m_n^* kT}{\pi \hbar^2 W} \sum_i \ln[1 + e^{(E_{n_i} - E_0)/k_BT}] + \frac{m_{hh}^* kT}{\pi \hbar^2 W} \sum_i \ln[1 + e^{(E_{hh} - E_0)/k_BT}] \]  

(28)

where \( m_n^* \), \( m_{hh}^* \) and \( m_{lh}^* \) are the effective masses of the electrons and holes.

3.3 Modal Gain

The modal (or mode) gain can be calculated by multiplying the material (or optical) gain of single quantum well with the optical confinement factor associated with it, hence the modal gain as a function of current density is given as;

\[ G_m(J) = \Gamma G(J) = \Gamma G_o(J) [\ln\left(\frac{J}{J_o}\right) + 1] \]  

(29)

In equation (29), \( G_m(J) \) is the modal gain, \( G(J) \) is the material gain, \( G_o(J) \) is optimum gain and \( J_o \) is the current density at \( G(J) \). Now refer to equation (29), the appearance of +1 in right hand side parentheses ensures existence of optimum gain at \( J = J_o \). Moreover, in terms of transparency current density \( J_{tr} \), the modal gain is given as [12, 13];

\[ G_m(J) = \Gamma G(J) = \Gamma G_o(J) \ln\left(\frac{J}{J_{tr}}\right) \]  

(30)

where \( \Gamma \) represents optical confinement factor associated with the single quantum well, can be given as;

\[ \Gamma = \frac{\int_{-W/2}^{W/2} |\epsilon(z)|^2 \, dz}{\int_{-W}^{W} |\epsilon(z)|^2 \, dz} \]  

(31)

where \( \epsilon(z) \) is the intensity of the electric field of radiation along z-direction. The confinement factor depends on the geometry of the quantum well or active layer, on refractive indices, and on the emission wavelength.

The transparency current density \( J_{tr} \) is related with threshold current density \( J_{th} \) as [13];
\[ J_{th} = J_{\nu} + \frac{eW}{G\Gamma\tau} \left( \alpha_i + \frac{1}{2L} \ln \frac{1}{R_1R_2} \right) \]  

(32)

where \( L \) is the cavity length, \( \alpha_i \) is internal loss due to reflections and \( R_1, R_2 \) are the reflectivities. Here \( \tau \) is carrier life time and \( e \) is the elementary electron charge.

The modal gain in terms of transparency current density for MQWs can be modified as;

\[ n\Gamma G(J) = n\Gamma G_\nu(J) \ln \left( \frac{nJ}{nJ\nu} \right) \]  

(33)

where \( n \) is the number of quantum wells.

The condition of threshold modal gain for lasing can be expressed as;

\[ R_1R_2 \exp[2L(n\Gamma G(J) - \alpha_i)] = 1 \]  

(34)

Therefore, threshold modal gain can be given as;

\[ G_{th}(J) = n\Gamma G(J) = \alpha_i + \frac{1}{2L} \ln \frac{1}{R_1R_2} = \alpha_i + \alpha_m \]  

(35)

In equation (35), \( G_{th} \) represents the threshold modal gain; and \( \alpha_m \) represents the mirror loss.

The threshold current density for lasing is;

\[ J_{th} = J_{\nu} + \frac{G_\nu(J)}{G'(J)} \]  

(36)

where \( G' \) represents the differential gain. The threshold current density in terms of optical losses can be given as;

\[ J_{th} = \left( \frac{nJ\nu}{\eta} \right) \exp \left[ \left( \frac{1}{n\Gamma G_\nu(J)} \right) \times \left( \alpha_i + \frac{1}{2L} \ln \frac{1}{R_1R_2} \right) - 1 \right] \]  

(37)

where \( \eta \) is the quantum efficiency.
3.4 Differential Gain

The derivative of optical gain with respect to carrier density is known as differential gain. It also plays an important role to determine the characteristics of a quantum well based lasing heterostructure. The differential gain coefficient in terms of energy of photon is given as:

\[
G'(E) = \frac{dG(E)}{dN} = \frac{8\pi^2 m_e E}{c\epsilon h^3 W} \int_E^{\infty} \left| M_B \right|^2 \left( \frac{df_i(E)}{dN} - \frac{df_s(E)}{dN} \right) L(E) dE
\]  

(38)

3.5 Gain Compression

The gain compression is substantial parameter to design properly of QW lasing structures. This factor can also be used in shaping the amplitude and frequency modulation of the lasing diodes.

In general, the change in optical gain with respect to photon density is termed as gain compression. In other words, the variation in differential gain with respect to optical gain can be defined a quantity, which is called gain compression. Basically, QW-lasing heterostructure performs above the threshold condition, in this condition, saturation mechanism and small fluctuations of relative intensity of output light are occurred, this type of saturation mechanism is called gain compression and it can be given in terms of carrier density as:

\[
\varepsilon = \left( \frac{1}{P} \right) \left[ \frac{G_s(N) - G(N)}{G(N)} \right] 
\]

(39)

where \( P \) stands for photonic density and the quantities \( G(N) \) and \( G_s(N) \) are gain and saturated gain, respectively.

3.6 Refractive Index Change

The behavior of spectrum of refractive index of QWs in the lasing heterostructure has vital role in the design and implementation of nano-scale opto-electronic equipments. For heterostructure, the most important differences between the quantum well or active region and barrier layers (SCH region) occur normally in the energy of band-gap and the index of refraction. The variation in the energy band-gap permits spatial confinement of injection carriers of electrons and holes in the conduction and valence bands. The variations in index of refraction can be utilized to develop
the optical waveguides, hence, it has essential role to find the explicitly of refractive index change with the carrier density in the quantum region of the nano-scale heterostructure. The coefficient of refractive change with respect to carrier density as function of energy of photon is given as

\[
\frac{dn(E)}{dN} = \frac{4\pi^2 m_e E \lambda \tau}{c \varepsilon h^2 W} \int_{E} [M(E) \left( \frac{df_e(E)}{dN} - \frac{df_h(E)}{dN} \right) \cdot (E - E) L(E)] dE
\]  

(40)

where \( n(E) \) represents the refractive index as a function of energy of photon, the quantity \( N \) stands for the density of carriers (electrons and holes), the physical quantity \( \lambda \) stands for the lasing wavelength and \( \tau \) represents the time of inter-band relaxation.

3.7 Anti-guiding Factor

The anti-guiding factor plays a very crucial role in deciding the optical gain of lasing heterostructure and can be defined in terms of refractive index change and differential gain as;

\[
\alpha = \frac{4\pi (-n')}{\lambda G'}
\]  

(41)

where the quantities \( G' \) and \( n' \) are the differential gain and differential refractive index change with respect to carrier concentration, respectively in the nano-heterostructure, \( \lambda \) is the lasing wavelength.

References


