THEORETICAL DETAIL

The heterostructures, which consists of different kinds of semiconductor layers having different energy bandgap, can be realized with the help of quantum wells. When one semiconductor material of small bandgap is squeezed in between other semiconductor material of greater bandgap, a well is formed. Hence, to study the behavior of particles (electrons or holes) in the heterostructures, the study on physics of quantum well is necessary.

It confirms from the well known fact that when the thickness of the quantum well is equivalent to the De Broglie’s wavelength of the carriers (electrons and holes), “quantum confinement” takes place leading to the formation of energy levels called “energy subbands” which suggests that the carriers can occupy discrete energy levels only (discretization of energy levels). This is precisely the reason why a quantum well is considered as a potential well having only the discrete energy values. Quantum confinement of charge carriers gives the peculiarities to the QW. We can also observe and control and manipulate optical and electrical properties of heterostructure which is commonly referred to as “bandgap engineering”. In order to find the optical gain and other lasing parameters of the heterostructures under study, first we study the behavior of carriers in QW (i.e. wave functions associated with it and corresponding energy states) and then transition matrix elements calculations is designed to perform calculations of momentum matrix elements and dipole moments of selected transitions and finally we simulate the optical gain, differential gain, gain compression and anti-guiding factor of the lasing heterostructure.

The optical gain is one of the fundamental distinctive features 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.
3.1 Calculation of Energy Levels in Valence and Conduction Bands

The discrete energy levels within the conduction band can be evaluated (if we assume the semi parabolic band nature of the conduction band), by using the single band effective mass equation as [1, 2];

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

(3.1)

where \( \hbar \) is reduced Planck’s constant (which is Planck’s constant by \( 2\pi \)), \( m^*_c \) is the electron’s effective mass in conduction band, envelope function is represented with \( \psi \), \( V_c \) stands for the potential of conduction band and \( E_c \) is the electron energy in conduction band.

The heterostructure in the present work has been studied taking into account the strain effects. The strain can either be compressive or tensile. In the figure 3.1, the effect of strain on the conduction and valence band structure in a strained quantum well heterostructure can be seen.

For a strained quantum well the conduction band potential is given as

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

(3.2)

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

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

(3.3)

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

\[ \varepsilon = \left( \frac{a_s - a_t}{a_t} \right) \]  

(3.4)

where \( a_s \) and \( a_t \) are the lattice constants of substrate and quantum well layers; while the barrier layer’s strain is given as

\[ \varepsilon = \left( \frac{a_s - a_b}{a_b} \right) \]  

(3.5)
where the lattice constants of barrier is represented as $a_b$. In a situation where there is no strain in the barrier, the lattice constant of substrate represents the lattice constant of barrier and so the quantum well’s strain will be given as [1]:

$$\varepsilon = \left( a_b - a_q / a_b \right)$$

(3.6)

**Figure 3.1** Visualisation of effect of strain, on the CB and VB in a quantum well structure.

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

$$\hat{H} \psi = \begin{bmatrix} H & M & N & 0 \\ M^* & L & 0 & N \\ N^* & 0 & L & -M \\ 0 & N^* & -M^* & H \end{bmatrix} \psi = E \psi$$

(3.7)
where

\[ H = -\frac{\hbar^2}{2m_0} \left[ (k_x^2 + k_y^2)\gamma_1 + \gamma_2 \right] - (\gamma_1 - 2\gamma_2) \frac{\partial^2}{\partial z^2} + V_{hh, lh} \]  
(3.8)

\[ L = -\frac{\hbar^2}{2m_0} \left[ (k_x^2 + k_y^2)\gamma_1 - \gamma_2 \right] - (\gamma_1 + 2\gamma_2) \frac{\partial^2}{\partial z^2} + V_{hh, lh} \]  
(3.9)

\[ M = i\frac{\sqrt{3}\hbar^2}{2m_0} (\gamma_3 \partial_z - ik_y) \gamma_3 \frac{\partial}{\partial z} \]  
(3.10)

\[ N = -\frac{\sqrt{3}\hbar^2}{2m_0} \left[ \gamma_2 (k_x^2 - k_y^2) - 2i\gamma_3 k_x k_y \right] \]  
(3.11)

where \( \psi \) is the envelope function, \( E_\nu \) is the energy Eigen values of heavy and light holes in valence sub-bands, \( m_0 \) is the mass of free electron, \( k_x \) and \( k_y \) are the transverse wave vector components, the Luttinger parameters are given as \( \gamma_1, \gamma_2 \) and \( \gamma_3 \), \( V_{hh} \) and \( V_{lh} \) respectively are the heavy hole and light hole’s potential of the valence sub-band which are represented as

\[
V_{hh} = \begin{cases} 
\frac{1}{3} \delta_3 + \delta_2, \text{Quantumwell} \\
-\Delta V_{pv}, \text{Barrier} \\
-\Delta V_{cv}, \text{Cladding} 
\end{cases}
\]  
(3.12)

\[
V_{lh} = \begin{cases} 
-\frac{1}{3} \delta_3 - \delta_2, \text{Quantumwell} \\
-\Delta V_{pv}, \text{Barrier} \\
-\Delta V_{cv}, \text{Cladding} 
\end{cases}
\]  
(3.13)

In the expressions (3.12) and (3.13), the valence band offset values for barrier and cladding layers, are given as \( \Delta V_{pv} \) and \( \Delta V_{cv} \) respectively. The shear potential \( \delta_s \) is expressed as follows-

\[
\delta_s = 2b \left( 1 + \frac{2C_{12}}{C_{11}} \right) \epsilon 
\]  
(3.14)

here \( b \) is shear deformation potential.
3.2 Material Gain

The material (optical) gain is one of the fundamental distinctive features of the quantum well heterostructures. In other words, the optical or material gain has a crucial role to evaluate the characteristics of a quantum well based lasing heterostructure. According to the theory of density matrix, the optical gain can be determined by summing up contribution from overall transitions of the electrons and holes between 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 a 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 [3-4]:

\[
G(E) = \frac{q^2 |M_B|^2}{\varepsilon_0 \omega^2 n_{\text{eff}} W} \sum_{\ell_1 \ell_2} m_{\ell_1 \ell_2} C_{\ell_1 \ell_2} \langle f_c - f_e \rangle L(E - E') dE
\]  

(3.15)

The integration performed in equation (3.15) extends from \( E_g \) (band gap of quantum well) to \( E_{gb} \) (band gap of barrier). In equation (3.15), \( \varepsilon_0 \) is free space permittivity, \( c \) stands for speed of light in vacuum, \( q \) is elementary charge, \( W \) is width of quantum well, \( n_{\text{eff}} \) is the effective refractive index, \( i \) and \( j \) represent quantum numbers of conduction and valence band, \( m_{\ell_1 \ell_2} \) is spatially weighted reduced mass for transition, the quantities \( f_v \) and \( f_c \) are the quasi Fermi functions of electrons and holes within the valence band and conduction band respectively; the function \( L(E) \) refers to the Lorentzian Lineshape function. This function is convolved with the gain spectra to determine the effects of the interband transitions [5], \(|M_B|^2\) is the bulk momentum transition matrix element for the dipole transition [6], which can be expressed as [3]:

\[
|M_B|^2 = \left( \frac{2}{3} \right) |M|^2
\]  

(3.16)

where

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

(3.17)
where the spin orbit interaction energy of the quantum well is represented as $\Delta$, rest mass of the electron is $m_0$, and the electron’s effective mass in the conduction band is $m_c$.

In equation (3.15), the quantity $C_{ij}$ represents the spatial overlap factor between $i$ and $j$ states which is defined as follows;

$$C_{ij} = \begin{cases} 1 & \text{when } i = j \\ 0 & \text{when } i \neq j \end{cases}$$  \hspace{1cm} (3.18)

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, 7];

$$A_{ij} = \begin{cases} (3/4)(1 + \cos^2 \theta), & (\text{heavy - hole}) \\ (1/4)(5 - 3\cos^2 \theta), & (\text{light - hole}) \end{cases}$$  \hspace{1cm} (3.19)

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

$$A_{ij} = \begin{cases} (3/2)(\sin^2 \theta), & (\text{heavy - hole}) \\ (1/2)(4 - 3\sin^2 \theta), & (\text{light - hole}) \end{cases}$$  \hspace{1cm} (3.20)

where the angular parameter $\cos \theta$ is;

$$\cos^2 \theta = \frac{E'}{E}$$  \hspace{1cm} (3.21)

where $E'$ represents the photonic energy and; $E'$ the transition energy between $i$ and $j$ states.

Next, in equation (3.15), the function $L(E)$ can be used as;

$$L(E-E') = \frac{1}{\pi} \frac{\hbar/\tau_{in}}{(E-E')^2 + (\hbar/\tau_{in})^2}$$  \hspace{1cm} (3.22)

where $\tau_{in}$ represents interband relaxation time having the order of pico-seconds [2].

Further, the temperature dependent optical gain coefficient can be expressed
\[ G(E) = \frac{\pi \hbar e^2}{n_0 \varepsilon_0 E_m \varepsilon_0 e} \left[ 1 - \exp\left( \frac{E - \Delta f}{k_b T} \right) \right] \times \sum_{\mathbf{m}, \mathbf{m}'} \frac{|M_{\mathbf{m}}|^2}{4 \pi^2 W} f_{\mathbf{m}} f_{\mathbf{m}'} \times \frac{\hbar / \tau_{in}}{\pi (E - E)^2 + (\hbar / \tau_{in})^2} \]  

(3.23)

where \( \Delta f \) is the Fermi level separation and \( k_b \) is the Boltzmann Constant.

Referring again to equation (3.15) for optical gain, the functions \( f_{\mathbf{m}} \) and \( f_{\mathbf{m}'} \) and are the Fermi distribution functions for electrons and holes in the valence band and conduction band respectively, which are the parameters to be calculated. Actually, the Fermi function gives the occupation probability of energy states in conduction and valence bands as [8];

\[ f_{\mathbf{m}} (E, E_{f_{\mathbf{m}}, f_{\mathbf{m}'}}) = 1 / [1 + e^{(E - E_{f_{\mathbf{m}}, f_{\mathbf{m}'}}) / k_b T}] \]  

(3.24)

In equation (3.24), \( E_{f_{\mathbf{m}}, f_{\mathbf{m}'}} \) represents the quasi Fermi levels in conduction and valance bands.

Integrating the product of the occupation probability of the carriers and the density of states over the entire band gives the carrier density in an energy band. So for a non-parabolic band structure, the carrier density can be given as [9–10];

\[ N = \sum_{N} \int_{0}^{\pi} \rho(k) \left[ f_{\mathbf{m}} \left( E_{\mathbf{m}}(k), E_{f_{\mathbf{m}}} \right) \right] \cdot dk \]  

(3.25)

\[ P = \sum_{\mathbf{m}, \mathbf{m}} \int_{0}^{\pi} \rho(k) \left[ 1 - f_{\mathbf{m}'} \left( E_{\mathbf{m}}(k), E_{f_{\mathbf{m}'}} \right) \right] \cdot dk \]  

(3.26)

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

\[ N = \frac{m^*_{\mathbf{m}} kT}{\pi \hbar^2 W} \sum_{\mathbf{m}} \ln[1 + e^{(E_{\mathbf{m}} - E_0) / k_b T}] \]  

(3.27)

\[ P = \frac{m^*_{\mathbf{m}} kT}{\pi \hbar^2 W} \sum_{\mathbf{m}} \ln[1 + e^{(E_{\mathbf{m}} - E_0) / k_b T}] + \frac{m^*_{\mathbf{m}} kT}{\pi \hbar^2 W} \sum_{\mathbf{m}} \ln[1 + e^{(E_{\mathbf{m}} - E_0) / k_b T}] \]  

(3.28)
where \( m_{hh}^* \) and \( m_{lh}^* \) are the effective masses of the heavy and light holes respectively and the effective mass of electrons is given by \( m_e^* \).

### 3.3 Mode Gain

The product of the material (or optical) gain of single quantum well along with the optical confinement factor associated with it provides the modal (or mode) gain. Hence the modal gain as a function of current density is given as;

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

(3.29)

In equation (3.29), \( G_m(J) \) is the modal gain, \( G(J) \) is the material gain, \( G_o(J) \) is optimum gain and \( J_o \) is the current density at \( G_o(J) \). Now refer to equation (3.29), the appearance of +1 in right hand side parentheses ensures existence of optimum gain at \( J = J_o \). The modal gain as given in [11, 12] in terms of the transparency current density \( J_{tr} \) is represented as

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

(3.30)

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

\[
\Gamma = \frac{\int_{-\infty}^{\infty} |\epsilon(z)|^2 \, dz}{\int_{-\infty}^{\infty} |\epsilon(z)|^4 \, dz}
\]  

(3.31)

where the intensity of radiation of the electric field (in z-direction) is denoted as \( \epsilon(z) \). The geometry of the quantum well or active layer, the emission wavelength, the refractive indices, are the parameters on which the confinement factor of the lasing heterostructure depends.

The transparency current density \( J_{tr} \) is related with threshold current density \( J_{th} \) as [13];

\[
J_{th} = J_{tr} + \frac{eW}{G\Gamma \tau} \left( \alpha_i + \frac{1}{2L} \ln \frac{1}{R_1R_2} \right)
\]  

(3.32)

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

For Multiple Quantum Wells, the modal gain in terms of transparency current density is;

\[
n\Gamma G(J) = n\Gamma G_o(J) \ln \left( \frac{nJ}{nJ_{tr}} \right)
\]  

(3.33)

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

For lasing, the condition for finding out the threshold modal gain is given as;
\[ R_i R_e \exp \left[ 2L \left( n \Gamma G(J) - \alpha_e \right) \right] = 1 \]  

(3.34)

Therefore, threshold modal gain \( G_{th} \) can be given as;

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

(3.35)

where \( \alpha_m \) represents the mirror loss.

Similarly, for lasing action, the threshold current density is given as;

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

(3.36)

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

\[
J_{th} = \left( \frac{n J_0}{\eta} \right) \exp \left[ \frac{1}{n \Gamma G_0(J)} \right] \times \left( \alpha_i + \frac{1}{2L} \ln \frac{1}{R_i R_e} \right) - 1
\]  

(3.37)

where \( \eta \) is the quantum efficiency.

3.4 Differential Gain

Differentiating the optical gain with respect to carrier density yields the differential gain. It plays crucial role in determining the characteristics of a quantum well based lasing heterostructure. The differential gain coefficient in terms of energy of photon is given as;

\[
G'(E) = \frac{dG(E)}{dN} = \frac{8\pi^2 m_e E}{cc \hbar^3 W} \int_E^\infty \left| M_{\beta} \right|^2 \left( \frac{df_\gamma^E}{dN} - \frac{df_\gamma^E}{dN} \right) L(E) dE
\]  

(3.38)
3.5 Gain Compression

The gain compression factor (also known as gain suppression or gain saturation or non linear gain coefficient) is substantial parameter to design QW lasing structures properly. This factor can also be used in influencing the phase (amplitude and frequency) modulation of the lasing diodes. In general, the change in material gain with respect to density of photon is termed as gain compression. In other words, the variation in differential gain with respect to optical gain can be defined as 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 occurs, this type of saturation mechanism is called gain compression and it can be given in terms of carrier density as;

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

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 enactment of opto-electronic equipments at nano-scale. For heterostructure, the crucial alterations 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 valence and conduction bands. The variations in index of refraction can be utilized to develop the optical waveguides, hence, it has essential role to find the variation of refractive index with respect to the density of carriers in the quantum region of the nano-scale heterostructure. The coefficient of refractive change (which is a function of energy of photon) with respect to carrier density is given as

\[
n'(E) = \frac{dn(E)}{dN} = \frac{4\pi^2 m_e E \lambda\tau}{c e h^2 W} \int \frac{dE}{E} \left( \frac{df_e(E)}{dN} - \frac{df_s(E)}{dN} \right) \cdot (E - E)L(E')dE'
\]

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 is yet another important parameter in determining the optical gain of lasing heterostructure. It is dependent on refractive index change and the differential gain as;

\[ \alpha = \frac{4\pi(-n')}{\lambda G} \quad (3.41) \]

where \( \lambda \) is the lasing wavelength, the differential gain is denoted as \( G' \) and \( n' \) is the differential refractive index change with respect to carrier concentration.

References


