Criteria for the Use of Approximations for Full Band Structures of Compound III–V Semiconductor Quantum Wells

Zoe C. M. Davidson and Judy M. Rorison

The calculation of material gain and performance characteristics of compound III–V semiconductor quantum well (QW) lasers has been developed, incorporating various approximations for the band structure. As the accuracy and sophistication of the band structure are increased, the computational time and mathematical complexity rise accordingly. The modeling of QW lasers is examined to determine the criteria for the accurate use of a parabolic approximation for the full band structure in the calculation of the material gain and performance characteristics of a conventional III–V QW. A comparison of the cosine approximation of band structure in highly mismatched alloys is also presented.

1. Introduction

To understand the electronic and optical properties of a quantum well (QW) laser, we must know the band structure of the active region. Several methods, codes, and softwares have been developed to model the optical and electronic properties of a QW laser; however, some methods and open-source softwares use a parabolic approximation of the band structure to save time and computational cost. However, the use of the parabolic approximation may be inaccurate depending on the material parameters of the QW laser. We offer a criterion for which QW lasers can be accurately modeled using approximations of the band structure by investigating the QW material and width, barrier material, strain, and cladding.

There are several methods for approximating the band structure of a semiconductor material which vary in accuracy, with this variation dependent upon the level of mathematical complexity and computational effort. The most popular methods for approximating the band structure are density functional theory, the effective mass approach, and the parabolic approximation. While approximations to the band structure have low computational needs, their accuracy is not consistent across a variety of materials. To counter many of these difficulties, we aim to show when the parabolic or cosine approximation is in good agreement with the full band structure solution. Doing so will be attractive to optical designers wanting to include more physical effects, such as carrier dynamics, transport, and interaction within the band structure, and to those wanting to design using software employing parabolic approximations knowing the likely accuracy of the model based on material parameters.

In this article, we compare prototype QW systems to demonstrate when an approximation of the band structure is appropriate, when it is not, and why. These prototype QW systems include an unstrained QW, compressive and tensile strained QW, and highly mismatched QWs. We will examine the impacts of composition, barrier height, and strain to give criteria for using the parabolic or cosine approximation. We focus on separate confinement heterostructure (SCH) lasers where a wide bandgap cladding region Al\(_x\)Ga\(_{1-x}\)As sandwiches a smaller bandgap optical confinement layer Al\(_x\)Ga\(_{1-x}\)As, where \(x < x_c\), within which are grown the smaller bandgap QW material for carrier confinement and recombination. We shall designate the SCH laser structures as QW material/optical confinement layer material/cladding layer and will consider one QW in the structure. The material compositions determine the bandgap and strain.
2. Theoretical Model

2.1. Bulk

We begin by examining the description of the electronic states in the conduction and valence bands of a semiconductor crystal lattice. The wavefunctions of the conduction and valence bands are found by solving the Schrödinger equation, which relates the Hamiltonian of the system, \( H \), to the kinetic and potential energy, the first and second terms, respectively

\[
H \Psi = \left[ \frac{p^2}{2m_0} + V_0 \right] \Psi = E \Psi
\]  

(1)

where \( p \) is the momentum operator, \( r \) is the position vector, \( m_0 \) is the free electron mass, \( \Psi \) is the wavefunction, and \( V_0 \) is the potential created by the crystal lattice. Translational symmetry in the crystal lattice dictates that the energy eigenfunctions (\( \Psi \)) obey Bloch’s theorem. Due to the periodicity of \( V_0 \), the energy eigenfunctions are given by Bloch waves.

\[
\Psi_{n,k} = e^{ik \cdot r} u_{n,k}(r)
\]  

(2)

where \( k \) is the wave-vector of the particle, \( u_{n,k} \) is a function with the same periodicity as the crystal lattice, and \( n \) is the band label. \( k \cdot p \) perturbation theory can provide analytical solutions to the relationship between the wave-vector and the energy of the state. The periodic function \( u_{n,k} \) satisfies the following Schrödinger-type equation.

\[
H_k u_{n,k} = E_{n,k} u_{n,k}
\]  

(3)

We find the eigenvalue equation for the wave-function is

\[
\left[ \frac{p^2}{2m_0} + V_0 + \frac{\hbar^2 k^2}{2m_0} \right] u_{n,k} = E_{n,k} u_{n,k}
\]  

(4)

where \( E_{n,k} \) is the energy of the \( n \)-th state of the \( n \)-th band containing dispersion in \( k \).

The Hamiltonian shown earlier combines both the unperturbed Hamiltonian, \( H_0 \), and the perturbed Hamiltonian, \( H_k \), which we can express as

\[
H = H_0 + H_k
\]

\[
H_0 = \sum_{n} \left[ \frac{p^2}{2m_0} + V_0 \right] + \sum_{n} \frac{\hbar^2 k^2}{2m_0}
\]

\[
H_k = \sum_{n} \frac{\hbar^2 k^2}{2m_0} + V_k
\]  

(5)

For a nondegenerate energy band, a band with no spin and a derivative of zero at the band edge, such as the conduction band, we can express the energy across the reciprocal lattice as

\[
E_{n,k} = E_{n,0} + \frac{\hbar^2 k^2}{2m_0} \sum_{n'} \frac{\langle u_{n,k} | k | u_{n',k} \rangle^2}{E_{n',0} - E_{n,0}}
\]  

(6)

where \( E_{n,0} \) is the energy of the state at the band edge.

However, when we encounter degenerate bands, such as the valence bands, our solution becomes nontrivial, and we introduce an effective Hamiltonian \( (H_{\text{eff}})_{n,n'} \) given by

\[
H_{\text{eff}} \Psi_{n,n'} = \left\langle u_{n,0} | H_0 | u_{n',0} \right\rangle + k \cdot \left\langle u_{n,0} | \nabla_k H_k | u_{n',0} \right\rangle
\]  

(7)

For a conventional III–V semiconductor compound, we obtain \( H_{\text{eff}} \) by performing multiband \( k \cdot p \) calculations using the eight-band Hamiltonian derived by Luttinger and Kohn, which includes in the off-diagonal terms the crystal potential symmetry.\(^{[3]}\) Equation (8) is the matrix representation in the four-band model taking the bandgap as \( E_g = E_c - E_v \), taking the asymmetry parameter of the magnetic field set to zero, assuming weak mixing between the conduction band and valence band, and taking the spin-orbit splitting, \( \Delta_m \), to be arbitrarily large.\(^{[11]}\)

\[
H_{\text{eff}} = \begin{pmatrix}
P + Q & -S & R & 0 \\
-S & P - Q & 0 & R \\
R & 0 & P - Q & S \\
0 & R & S & P + Q
\end{pmatrix}
\]  

(8)

The diagonal terms are the eigenstates of the 3D bulk semiconductor representing heavy hole \( (E_{hh} = P + Q) \) and light hole \( (E_{lh} = P - Q) \), and exhibiting the two-fold degeneracy. The off-diagonal terms \((R, S)\) represent the interaction terms introduced by the crystal potential. These are defined as\(^{[12]}\)

\[
P = P_x + P_z
\]

\[
Q = Q_x + Q_z
\]

\[
P_k = \frac{2m_0}{\hbar^2} \gamma_1 (k_x^2 + k_y^2 + k_z^2)
\]

\[
Q_k = \frac{2m_0}{\hbar^2} \gamma_2 (k_x^2 + k_y^2 + 2k_z^2)
\]

\[
S = \frac{\hbar}{m_0} 2\sqrt{3} \gamma_3 (k_x - i k_y)
\]

\[
R = 2\sqrt{3} \frac{\hbar}{m_0} [(\gamma_2 + \gamma_3) (k_x - ik_y)^2 - (\gamma_1 + \gamma_2) (k_x + ik_y)^2]
\]

\[
P_x = -\alpha_x (\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})
\]

\[
Q_x = -\frac{1}{2} (\epsilon_{xx} + \epsilon_{yy} - 2\epsilon_{zz})
\]

where \( \gamma_1, \gamma_2, \gamma_3 \) are the Luttinger parameters. Strain is included in two parts. The hydrostatic component strain, represented by \( P_x \), caused by the lattice mismatch uniformly raises or lowers the bandgap. For our calculations, we have accounted for the hydrostatic strain by including it in the calculation of bandgap energy. The axial component of the strain, represented by \( Q_x \), which affects the heavy and light holes oppositely, is included in the Hamiltonian.\(^{[11-13]}\) The strain tensors \( \epsilon_{xx}, \epsilon_{yy}, \) and \( \epsilon_{zz} \) are calculated as shown by Krijn.\(^{[16]}\) Common representations of the effective Hamiltonians neglect to show the below diagonals as the Hamiltonians are Hermitian matrices.\(^{[17]}\)

2.2. Confinement

In bulk, the crystal symmetry and strain perturbations are minor corrections to the band structure and alter the dispersion only qualitatively. However, it is known in a QW that the confinement of the states in the growth direction \( z \) alters the band structure, causing dispersion to have a more significant effect. This is what we shall investigate. As the particle in a QW is confined only
along the growth direction of the crystal, it is still free in the plane of the well and acquires in-plane momentum and dispersion, defined as $k^2_{\parallel} = k_x^2 + k_y^2$.

$$H = H_k + V(z)$$  \hspace{1cm} (10)

where $V(z)$ is the energy of the confined state of the QW at the band edge ($k_z = 0$) found using a transcendental approach, and $H_k$ is solved using different approaches for dispersion within the free direction. To transform the effective Hamiltonian, we quantize and symmetrize the set of equations, shown in Equation (9), along the z axis by replacing $k_z$ with $-i \partial / \partial z$. We also take the axial approximation, so set the warping effect, $(\gamma_3 - \gamma_z)$, seen in the $R$ interaction term to zero.

There are three approaches that we will examine for solving the $k_z$ dispersion of the crystal: the parabolic approximation, the cosine approximation, and a free particle method which uses a Newtonian FDT. The Newtonian FDT $k \cdot p$ solution finds the unique solutions of $E_{n_k}^k$, where $n$ is the confined state of the QW, by using a Newtonian approach. Due to the degeneracy of the valence band effective mass equations, there is a coupling effect on the sub-bands, which must be considered. Therefore, to obtain a full solution of the band structure, we must solve the effective Hamiltonian. To solve the band structure using an FDT $k \cdot p$ solution, we apply the boundary conditions at the QW interfaces between the active region and the barriers. These consist of the wave-function continuity and continuity of its first derivative divided by the effective mass: in the form of current continuity given below:[14,18]

$$F_{z,w} = F_{z,b}$$ \hspace{1cm} (11)

$$\frac{1}{m_w} \frac{dF_{z}}{dz} = \frac{1}{m_b} \frac{dF_{z}}{dz}$$ \hspace{1cm} (12)

where $F_{z,w/b}$ is the envelope function and $dF_{z,w/b}/dz$ is the derivative of the envelope function with respect to $z$, of the well ($w$) and barrier ($b$), respectively. The effective masses of the well and barrier are represented by $m_w$ and $m_b$, and are calculated using the Luttinger parameters for light and heavy holes for zinc blende materials, as described by Vurgaftman et al.[19] The boundary conditions applied to the four-band Hamiltonian enable us to reduce the calculation of eigenstates to a set of four coupled equations. Full derivations of these coupled equations have been outlined by Coldren et al.[20] The QW eigenstates calculated from Equation (8) using the Newtonian FDT method show good agreement with those calculated by Andreani et al.[14]

The parabolic approximation simplifies the nondegenerate $k \cdot p$ effective mass equation (Equation (6)) to enable us to find simple solutions for $E_{n_k}^k$. Using Equation (6) for the energy dispersion relationship, a simplified expression for the effective mass of a semiconductor can be found.

$$E_{n_k} = E_{n,0} + \frac{\hbar^2 k_z^2}{2m_{\text{eff}}} + \frac{\hbar^2}{E_{g}} \sum \frac{|\langle \mu_n | k \cdot p | \mu_0 \rangle|^2}{m_{\text{eff}}^2}$$ \hspace{1cm} (13)

where $m_{\text{eff}}$ is the effective mass of the band and is calculated using the Luttinger parameters for zinc blende materials.[19] $E_{n,0}$ is the energy of the confined state at the band edge, and $E_g$ is the energy gap of the QW. By assuming weak mixing between sub-bands, we can omit the final term of the above-mentioned equation and give the parabolic approximation

$$E_{n_k} = E_{n,0} + \frac{\hbar^2 k_z^2}{2m_{\text{eff}}}$$ \hspace{1cm} (14)

The cosine approximation will be discussed in more detail in Section 3.3.

The obtained QW eigenstates are used directly to compute material gain for each laser structure.[21] The material gain spectra are calculated following the procedure outlined by Chang and Chuang with the homogeneous linewidth broadening described using a hyperbolic secant lineshape corresponding to a relaxation time of $\tau_{\text{in}} = 100$ fs.[22,23] The laser gain is given by

$$G(\omega \alpha) \propto \left[ \frac{1}{\omega \alpha} \right] \int |M_{\alpha}^2| \rho^{2D}(k_z) \left| f(E_{g,k_z}) - f(E_{n_k}) \right| \frac{S(\omega \alpha)}{d k_z}$$ \hspace{1cm} (15)

where $|M_{\alpha}^2|$ is the $k_z$ and sub-band dependent inter-band optical transition strength for allowed and forbidden transitions, $\rho^{2D}$ is the QW 2D density of states (DOS), $f(E_{g,k_z})$ is the Fermi function for electrons(holes), and $S$ is the spontaneous emission rate. As outlined by Corzine, the polarization of our QW laser is determined by the strain of the QW.[10] Transverse electric (TE) polarization is dominant in compressively strained QWs, and transverse magnetic (TM) polarization is dominant in tensile strained QWs. If we assume that the polarization states are isotropically distributed over the two polarizations (TE and TM), we can give the total transition matrix element strength as

$$|M_{\alpha}^2| = \frac{1}{2} |M_{\alpha}^2| + |M_{\alpha}^2|$$ \hspace{1cm} (16)

We compute the inter-band optical transition matrix elements using the general formalism of Szmulowicz.[24] To compare threshold characteristics calculated by the FDT $k \cdot p$ solution and the approximations, we take threshold material gain as

$$g_{\text{th}} = \frac{1}{L} \left( \frac{\alpha}{1 + \frac{1}{L} \ln \frac{1}{R}} \right)$$ \hspace{1cm} (17)

where we have assumed internal losses of $\alpha = 4.0 \text{ cm}^{-1}$ for a single QW with a cavity length of $L = 0.1 \text{ cm}$ with cleaved facets. For highly mismatched alloys, both the internal losses and the line shape broadening will be higher; however, for the purpose of comparison of models, we set these parameters to those mentioned earlier.

The calculated QW band structure and eigenstates, and laser optical properties calculated from them, can now be compared to determine the level of accuracy of the parabolic approximation in comparison with the full solution.

3. Results

Due to the nondegenerate nature of the conduction band of a conventional III–V semiconductor compound, the parabolic
approximation and the FDT $k \cdot p$ solution give the same result. This article, therefore, focuses on the band structure calculation of the degenerate valence bands. We begin by focusing on our analysis on two 8 nm QWs: (i) unstrained GaAs/$Al_{0.2}Ga_{0.8}As$/$Al_{0.4}Ga_{0.6}As$ and (ii) compressively strained In$_{0.2}Ga_{0.8}As$/GaAs/$Al_{0.2}Ga_{0.8}As$.

A key parameter that determines the performance of a QW laser is the valence band density of states (VB DOS). The VB DOS can be predicted by the valence band structure. The less perturbed the band structure, the smaller the VB DOS. Thus, the accuracy of using a parabolic approximation of the band structure for calculating the performance of a QW laser can be predicted in the agreement of the parabolic approximation to an FDT $k \cdot p$ calculated band structure. In Figure 1 (unstrained GaAs/$Al_{0.2}Ga_{0.8}As$/$Al_{0.4}Ga_{0.6}As$) and Figure 2 (compressively strained In$_{0.2}Ga_{0.8}As$/GaAs/$Al_{0.2}Ga_{0.8}As$), we can see confined levels of the valence band using the parabolic approximation (dashed lines) and FDT $k \cdot p$ solution (solid lines). In the case of the unstrained QW, we can see clearly that the parabolic approximation does not account for sub-band mixing and valence band anti-crossing (VBAC). This results in a less perturbed band structure than the solution provided by the FDT solution. In the case of the compressively strained QW, the strain ($ε_{xx}$) is pushing the light holes down within the well and thus decreasing VBAC. Due to the decreased VBAC in the compressively strained QW, the parabolic approximation has increased accuracy in comparison with the unstrained QW. It is worth noting that while the first confined state of the unstrained QW shows good agreement to the parabolic approximation, the closeness of a nearby warped state alters the population of the first confined level, which is reflected in characteristics such as material gain, transition inter-band optical transition matrix elements, and performance characteristics are calculated using all confined states of the well.

In addition to VB DOS, the performance of a QW laser can also be predicted by the inter-band optical transition strength. The inter-band optical transition strengths ($|M_{ij}|$) calculated by the parabolic approximation is ten times greater than that calculated by the FDT $k \cdot p$ solution as we reach values of $k_{||} > 0.1$. At high values of $k_{||}$, the valence band structure predicted by the parabolic approximation is closer to symmetry with the conduction band than what is calculated by the FDT solution. This, in turn, leads to an increased predicted wave-function overlap, and thus increased $|M_{ij}|$. This is true for both the unstrained and the compressively strained QWs. Thus, as the material gain rises above the threshold, becoming more dependent on the inter-band optical transition strengths, we find that the parabolic approximation becomes less accurate in nature for both the unstrained and the compressively strained QWs. As the width of the well is varied, there is, in turn, an impact on the accuracy of the parabolic approximation. We find that as our active region becomes thinner, our accuracy of the parabolic model increases for the unstrained QW, and the compressively strained QW. While both QWs have greater accuracy at thinner well widths, it is more dramatic for the unstrained QW due to the increasing sub-band separation with decreasing well width.

### 3.1. Varying Strain

In addition to the impact of well width on the accuracy of the parabolic approximation, there is also an impact of QW material and barrier material composition. We find that as our barrier height decreases, the accuracy of the parabolic model increases due to fewer confined states, leading to smaller VBAC interactions (Figure 3 and 4). It is natural to assume that by increasing the In composition of the compressively strained QW, the corresponding increase in compressive strain would lead to greater accuracy of the parabolic approximation due to increased sub-band separation. However, the increased composition leads to
increased barrier height, which in turn increases the number of confined levels, thus an increasing band mixing through VBAC leading to decreased accuracy (as seen in Figure 4). The barrier height for the valence band ($V_B$) for both the unstrained and the compressively strained QWs, assuming a standard 40:60 ratio of the barrier height to the valence:conduction band, is 1) $x = 0.1$ (red), $V_B = 50 \text{ meV}$, 2) $x = 0.2$ (blue), $V_B = 100 \text{ meV}$, and 3) $x = 0.3$ (purple), $V_B = 150 \text{ meV}$. The strain ($\varepsilon_{xx}$) for the compressively strained In$_{0.1}$Ga$_{0.9}$As/GaAs/Al$_{0.2}$Ga$_{0.8}$As is 1) $x = 0.1$ (red), $\varepsilon_{xx} = -2.3\%$, 2) $x = 0.2$ (blue), $\varepsilon_{xx} = -4.7\%$, and 3) $x = 0.3$ (purple), $\varepsilon_{xx} = -7.1\%$. While $\varepsilon_{xx} = -4.7\%$ is a very high strain, we are performing a theoretical calculation to show the trend.

When considering the accuracy of the parabolic approximation at threshold carrier density, \(2 < 2 \times 10^{12} \text{ cm}^{-2}\) for most materials with the parameters given in Section 2, we compare the parabolic approximation (dashed lines) to the full FDT $k \cdot p$ solution (solid lines) in Figure 5 for varying compositions ($x = 0.1$, $x = 0.2$, and $x = 0.3$) against varying well widths for unstrained GaAs/Al$_{0.2}$Ga$_{0.8}$As/Al$_{0.2}$Ga$_{0.8}$As (left) and strained In$_{0.2}$Ga$_{0.8}$As/ GaAs/Al$_{0.2}$Ga$_{0.8}$As (right). For $x = 0.1$ and $x = 0.2$, we can see that the parabolic approximation for the unstrained QW shows accuracy only at smaller well widths. Therefore, we can predict that calculating threshold characteristics using a parabolic approximation will give good accuracy for unstrained QWs with an active region width of 5 nm or less. When $x = 0.3$, we find that the parabolic approximation offers a decreased level of accuracy, even at lower well widths. Meanwhile, the parabolic approximation for the compressively strained QW has good accuracy at threshold across a range of well widths for $x = 0.1$ and $x = 0.2$. For $x = 0.3$, we find that the compressively strained QW can only be accurately modeled at well widths 4 nm and less. It is important to note that when considering the abovementioned threshold characteristic, the accuracy of parabolic approximation for both strained and unstrained QWs, the level of accuracy will decrease. This can be seen in Figure 3 and 4.

We summarize the agreement of predicted performance of threshold carrier density calculated by both the parabolic approximation and the full FDT $k \cdot p$ solution of the band structure in Table 1. We see that as the barrier height and well width increase, there is a decreasing agreement between the predicted threshold carrier density calculated by the two solutions of the band structure. There is $< 10\%$ difference between the predicted threshold carrier density calculated by the two solutions of the band structure when $x = 0.1$. However, when $x = 0.3$ and the well width $> 4$ nm, there is an $\approx 30\%$ difference in the predicted threshold carrier density calculated by the two solutions of the band structure. This variation in accuracy corresponds to the number of confined states in the valence band. If there are no more than two heavy-hole sub-bands and one light-hole sub-band confined in either an unstrained or a compressively strained QW, then the agreement between the threshold carrier density predicted by the parabolic approximation and that predicted by the FDT $k \cdot p$ solution is $> 90\%$.

As the well gets wider, we have an increased VB DOS at the band edge caused by a more perturbed band structure of the FDT $k \cdot p$ solution that extends into larger $k_f$ space regimes, leading to a decreased peak material gain, and in turn increased threshold carrier density in comparison with the parabolic approximation, as shown in Figure 5. The valence band structure predicted by the parabolic approximation will be less perturbed due to a lack of VBAC, resulting in a decreased VB DOS at the band edge. As we rise above the threshold, the peak material gain becomes a function dominated by the transition matrix element. As the parabolic approximation has an increased transition matrix element with respect to the FDT $k \cdot p$ solution, we see a larger peak material gain above the threshold, as shown in Figure 3 and 4.

It should be stated that the parabolic approximation is only applicable to simple unstrained or compressively strained

---

**Figure 3.** Calculated peak TE material gain for the 3 nm unstrained GaAs/ Al$_{0.2}$Ga$_{0.8}$As/Al$_{0.2}$Ga$_{0.8}$As for $x = 0.1$ (red), $x = 0.2$ (blue), and $x = 0.3$ (purple). The dashed lines represent the parabolic approximation, and the solid lines represent the FDT $k \cdot p$ solution of the band structure.

**Figure 4.** Calculated peak TE material gain for the 3 nm compressively strained In$_{0.2}$Ga$_{0.8}$As/GaAs/Al$_{0.2}$Ga$_{0.8}$As for $x = 0.1$ (red), $x = 0.2$ (blue), and $x = 0.3$ (purple). The dashed lines represent the parabolic approximation, and the solid lines represent the FDT $k \cdot p$ solution of the band structure.

---

**Table 1.** Comparison of threshold carrier density for 3 nm unstrained and strained QWs.
eight-band Hamiltonian QWs. For tensile strained materials, the extreme VBAC caused by the light-holes lifting above the heavy-holes in the well nullifies the use of a parabolic approximation. In the case of more complex materials, such as the highly mismatched alloys of dilute nitrides and dilute bismides, the added band anti-crossings introduced by the resonant bands of the materials make the parabolic approximation completely inaccurate.

3.2. Tensile Strained QWs

The introduction of tensile strained in conventional III–V QWs nullifies the use of a parabolic approximation due to the extreme VBAC caused by the light-holes lifting above the heavy-holes in the well, in contrast to the compressively strained QW, where the movement of the sub-bands results in decreased VBAC. If we examine a tensile strained In$_{0.4}$Ga$_{0.6}$As/In$_{0.66}$Ga$_{0.34}$As/Al$_{0.25}$Ga$_{0.75}$P/InP QW, we see the impact on the band structure of the VBAC caused by tensile strain in Figure 6. Due to the VBAC interaction between the light-hole and heavy-hole, we see a band structure extending into larger $k$ space regime than what is predicted by the parabolic approximation. As the parabolic approximation does not consider the VBAC of the band structure, the result is a less perturbed band structure than the solution provided by the FDT $k \cdot p$ solution.

We further see the impact of the increased VBAC of the tensile strained QW in Figure 7, where the peak TM material gain is calculated from the parabolic approximation (red dashed lines) compared to the peak material gain calculated from the FDT $k \cdot p$ solution (solid blue lines). As we have a tensile strained QW laser, the dominant polarization shifts to the TM polarization. We can see that the peak TM material gain calculated by the parabolic approximation is almost threefold larger than that calculated from the FDT $k \cdot p$ solution. Our decreased accuracy is explained by the extreme VBAC effects caused by the low effective mass light-hole interaction with the higher effective mass heavy-hole below it, in turn causing a much smaller VB DOS.
at the band edge predicted by the parabolic approximation. Even as we decrease well width, or decrease barrier height, the accuracy of the parabolic approximation does not improve. In the case of the tensile strained QW, the accuracy of the QW decreases with decreasing well width.

3.3. Highly Mismatched QWs

In highly mismatch alloys, we move from an eight-band $k \cdot p$ calculations for conventional III–V to 10-band (dilute nitride) and 12-band (dilute bismide) due to the introduction of defect resonant levels, or basis states, into the band structure.\[^{26,27}\] We obtain the dilute nitride 10-band model by augmenting the eight-band basis of host matrix band edge Bloch states through the inclusion of a set of two-fold degenerate N-related basis states at an energy $E_N$ above the conduction band edge.\[^{28}\] Using the same procedure, we also obtain the dilute bismide 12-band model by augmenting the eight-band basis of host matrix band edge Bloch states through the inclusion of a set of four-fold degenerate Bi-related basis states at an energy $E_B$ below the valence band edge.\[^{29}\] These resonant defect levels cause increased band anti-crossing and lead to increased perturbations in the band structures of highly mismatched alloys, as shown in Figure 8, where we can see the impact of the nitrogen resonant band on the conduction band of the dilute nitride QW (left-hand side) and the impact of the bismuth resonant band on the valence band of the dilute bismide QW (right-hand side). Due to the complexity of the Hamiltonians for the highly mismatched alloys, a plane wave approach is often used.\[^{30}\]

Due to the resonant defect levels introduced by bismuth (below the valence band edge) and nitrogen (above the conduction band edge), a cosine approximation should be used, if an approximation is desired, when calculating the band structure of a highly mismatched III–V semiconductor alloy QW.\[^{26,27,31}\] The cosine approximation of a conduction band can be given by Equation (18) and (19) for the conduction and valence band, respectively.

$$E_{cn}(k_{||}) = E_{cn0} + \frac{E_{CB}}{2} (1 - \cos(2k_{||}a)) \quad (18)$$

$$E_{vm}(k_{||}) = E_{vm0} + \frac{E_{VB}}{2} (1 - \cos(k_{||}a)) \quad (19)$$
where $a$ is the lattice constant, $E_{n0}$ is the energy of the confined level at $k_{\parallel} = 0$, and $E_{CB,VB}$ is the height of the conduction band and valence band, respectively. We have adjusted the equation of the cosine approximation of the conduction band from that given by Dyson to account for the increasing effective mass of the conduction band structure of a QW compared to bulk band structure. We do not see the inflexion of the parabolic approximation due to the $k$ values used in an examination of material gain of a QW laser. An inflexion would be seen at a value of $k_{\parallel} = 0.54$ for the valence band, and $k_{\parallel} = 0.27$ for the conduction band, values far higher than what is required in the calculation of material gain.

We demonstrate the comparison of three solutions to the band structure in a 3 nm dilute bismide:

GaAs$_{0.86}$Bi$_{0.14}$/GaAs/Al$_{0.4}$Ga$_{0.6}$As QW with a compressive strain of $\varepsilon_{xx} = -1.6\%$, and a 3 nm dilute nitride In$_{0.34}$Ga$_{0.65}$As$_{0.92}$N/GaAs/Al$_{0.4}$Ga$_{0.6}$As QW with a compressive strain of $\varepsilon_{xx} = -1.0\%$.

We begin by examining the band structure. In the dilute bismide QW, the impact of the resonant defect level below the valence band edge causes an extreme band bending. Thus, by plotting the first three confined valence band levels in the right-hand side of Figure 9, we see that in comparison, the cosine approximation (purple dotted lines) of the conduction band is in better agreement with the FDT $k \cdot p$ solution (solid blue lines) than the parabolic approximation (red dotted lines). When examining the valence band of the dilute nitride, shown in the right-hand side of Figure 10, we find that a parabolic approximation (red dashed lines) can be used with good accuracy for calculating the valence band of the dilute nitride provided that only a small number of holes are confined within the wells. However, if comparing the cosine approximation (purple dotted lines) to the full solution to the band structure (solid blue lines), there is poor agreement.

Comparing the accuracy of the models in calculating the peak material gain of the dilute bismide (Figure 11) and dilute nitride (Figure 12) QWs, we find that the cosine approximation (purple dotted lines) shows far better agreement to the full solution of the band structure (solid blue lines) when calculating the peak material gain of the QW in comparison with the parabolic approximation (red dashed lines). For the dilute bismuth QW, the cosine

---

**Figure 8.** Schematic of the band structure of the dilute nitride and dilute bismide highly mismatched alloy QW. The left-hand figure shows the impact of the nitrogen resonant band (dashed black line) on the host matrix conduction band (dot dashed green line), resulting in the first confined conduction band, $E_{\text{CB}}$ (blue solid line). We do not show $E_{\text{VB}}$ as we focus on the QW state. The valence band is represented by the solid red line. The right-hand figure shows the impact of the bismuth resonant band (dashed black line) on the host matrix valence band (dot dashed green line), resulting in the first confined valence band, $E_{\text{VB}}$ (red solid line). We do not show $E_{\text{CB}}$ as we focus on the QW state. The conduction band is represented by the solid blue line.
approximation of the peak material gain takes the “cosine” approximation of the “valence” band but the “parabolic” approximation of the “conduction” band. For the dilute nitride QW, the cosine approximation of the peak material gain takes the “cosine” approximation of the “conduction” band but the “parabolic” approximation of the “valence” band. As we can see in both figures, the parabolic approximation of the band structure results in extremely large, and extremely inaccurate, predictions of the

Figure 9. Calculated band structure for a 3 nm dilute bismide GaAs$_{0.86}$Bi$_{0.14}$/GaAs/Al$_{0.4}$Ga$_{0.6}$As QW using parabolic approximation (red dashed lines), cosine approximation (purple dotted lines), and FDT k·p solution (blue solid lines) for the confined levels of the conduction band (left-hand side) and valence band (right-hand side).

Figure 10. Calculated band structure for a 3 nm dilute nitride In$_{0.35}$Ga$_{0.65}$As$_{0.92}$N$_{0.08}$/GaAs/Al$_{0.4}$Ga$_{0.6}$As QW using parabolic approximation (red dashed lines), cosine approximation (purple dotted lines), and FDT k·p solution (blue solid lines) for the confined levels of the conduction band (left-hand side) and valence band (right-hand side).
As the approximation of the highly mismatched alloys does not provide complete agreement with the full solution, such a model could be used with accuracy in the following situations: Tensile requirements will vary greatly with material, strain, width, and barrier height. Second, that the parabolic approximation cannot be used with accuracy in the following situations: Tensile strained QWs, highly mismatched QWs such as dilute bismides and nitrides, and for calculations above the threshold. Third, and final, we conclude that the cosine approximation has a good level of accuracy in highly mismatched alloy QWs to account for the defect resonant levels, and can be used to give an indication of performance for a given structure.

4. Conclusions

The parabolic approximation offers increased accuracy across a range of structures when we have QWs with increased compressive strain. This is due to the separation of the light and heavy holes caused by the introduction of compressive strain, resulting in a decreased VBAC that more closely matches a parabolic approximation. In contrast, unstrained QWs have increased VBAC, resulting in varying accuracy of the parabolic approximation. A reduced VBAC will then result in a decreased predicted VB DOS at the band edge, in turn, decreasing threshold carrier density \( n_{th} \) and increasing differential gain with respect to carrier density \( (dg/dn) \) at the threshold. An inaccurate band structure will result in an inaccurate prediction of the performance of the QW.

The parabolic approximation also shows a larger inter-band optical transition strength than the FDT \( k \cdot p \) solution. As the peak gain rises above transparency, it becomes a function of carrier density and is strongly influenced by the inter-band optical transition strengths. Thus, an inaccurate inter-band optical transition strength will result in an inaccurate prediction of the performance of the QW at high carrier densities.

The use of the cosine approximation in highly mismatched alloys offers increased accuracy in comparison with the parabolic approximation of the band structure due to the large band anticrossing interactions present due to the resonant defect states in such materials. In a dilute bismide, we take a “parabolic” approximation of the “conduction” band, and a “cosine” approximation of the “valence” band. In a dilute nitride, we take a “cosine” approximation of the “conduction” band, and a “parabolic” approximation of the “valence” band. The use of a parabolic approximation of the valence band in the dilute nitride only remains accurate if the valence band is compressively strained with no more than three confined levels.

We have successfully identified the trends for which the performance of a separate confined heterostructure can be accurately calculated using a parabolic approximation or cosine approximation of the band structure. We reach three conclusions. First, that the parabolic approximation has a good level of accuracy in conventional III–V semiconductor QWs if there are no more than two heavy-hole sub-bands and one light-hole sub-band confined in either an unstrained or a compressively strained QW. The exact design of a structure that fits these requirements will vary greatly with material, strain, width, and barrier height. Second, that the parabolic approximation cannot be used with accuracy in the following situations: Tensile strained QWs, highly mismatched QWs such as dilute bismides and nitrides, and for calculations above the threshold. Third, and final, we conclude that the cosine approximation has a good level of accuracy in highly mismatched alloy QWs to account for the defect resonant levels, and can be used to give an indication of performance for a given structure.

Acknowledgements

This work was supported by the University of Bristol (via a Doctoral Studentship, held by Z.C.M.D.) and the EPSRC. Special thanks go to Dr Scott Corzine.

Conflict of Interest

The authors declare no conflict of interest.
Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

band structure, k·p, nonparabolicity, parabolic approximation

Received: October 19, 2021
Revised: December 21, 2021
Published online: February 11, 2022

[1] H. Hebal, Z. Koziol, S. Lisesivdin, R. Steed, Comput. Mater. Sci. 2021, 186, 110015.
[2] R. A. Jabr, M. Harnad, Y. M. Mohanna, Int. J. Electr. Eng. Educ. 2007, 44, 23.
[3] L. Nevou, https://github.com/LaurantNevou/Q_SchrodingerPoisson1D, 2020 (accessed: April 2021).
[4] S. Balle, Physical Review A 1998, 57, 1304.
[5] T. Makino, IEEE J. Quantum Electron. 1996, 32, 493.
[6] M. Oloumi, C. C. Matthai, J. Phys.: Condens. Matter 1991, 3, 9981.
[7] P. Vogl, in Predictions of Deep-Impurity-Level Energies in Semiconductors, Vol. 62 (Ed.: P. W. Hawkes), Academic Press, Cambridge, Massachusetts, United States 1984, p. 101.
[8] E. O. Kane, J. Phys. Chem. Solids 1956, 1, 82.
[9] J. M. Luttinger, W. Kohn, Physical Review 1955, 97, 869.
[10] S. W. Corzine, R. H. Yan, L. A. Coldren, Appl. Phys. Lett. 1990, 57, 2835.
[11] D. A. Broido, I. J. Sham, Phys. Rev. B 1988, 8, 2.
[12] J. C. Yong, J. M. Rorison, I. H. White, IEEE J. Quantum Electron. 2002, 38, 1553.
[13] D. Ahn, S. L. Chuang, IEEE J. Quantum Electron. 1988, 24, 2400.
[14] L. C. Andreani, A. Pasquarello, F. Bassani, Phys. Rev. B 1987, 36, 5887.
[15] B. Gonul, A. T. Meney, E. P. O’Reilly, Phys. Rev. B 1994, 50, 10893.
[16] M. P. Krijn, Semicond. Sci. Technol. 1991, 6, 27.
[17] T. B. Bahder, Phys. Rev. B 1990, 41, 11992.
[18] J. Faist, Quantum Cascade Lasers 2013, QE-22, 26.
[19] I. Vurgaftman, J. R. Meyer, L. R. Ram-Mohan, J. Appl. Phys. 2001, 89, 5815.
[20] S. Corzine, R.-H. Yan, L. Coldren, Quantum Well Lasers, 1 ed., Academic Press, London 1993.
[21] C. A. Broderick, P. E. Harnedy, E. P. O’Reilly, IEEE J. Sel. Top. Quant. Electron. 2015, 21, 1503313.
[22] C.-S. Chang, S. L. Chuang, J. R. Minch, W.-C. W. Fang, Y. K. Chen, T. Tanbun-Ek, IEEE J. Sel. Top. Quant. Electron. 1995, 1, 1107.
[23] S. L. Chuang, J. O’Gorman, A. F. J. Levi, IEEE J. Quantum Electron. 1993, 29, 1631.
[24] F. Szmulowicz, Phys. Rev. B 1995, 51, 1613.
[25] A. R. Adams, IEEE J. Sel. Top. Quant. Electron. 2011, 17, 1364.
[26] E. P. O’Reilly, A. Lindsay, S. Tomic, M. Kamal-Saadi, Semicond. Sci. Technol. 2002, 17, 870.
[27] C. A. Broderick, M. Usman, E. P. O’Reilly, Phys. Status Solidi (B) Basic Res. 2013, 250, 773.
[28] A. Lindsay, S. Tomić, E. P. O’Reilly, Solid-State Electron. 2003, 47, 443.
[29] C. A. Broderick, M. Usman, E. P. O’Reilly, Semicond. Sci. Technol. 2013, 28, 12.
[30] E. P. O’Reilly, O. Marquardt, S. Schulz, A. D. Andreev, Plane-Wave Approaches to the Electronic Structure of Semiconductor Nanostructures, Springer International Publishing, Cham 2014, pp. 155–189.
[31] A. Dyson, B. K. Ridley, J. Appl. Phys. 2008, 104, 113709.