Simulation and comparison of GaAs, AlGaAs and GaInP barriers in InGaAs quantum well lasers

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Abstract. InGaAs quantum wells with GaAs, AlGaAs and GaInP barriers have been simulated, respectively. The InGaAs/GaInP structure reveals a high material gain which could be nearly 1.4 times of that of InGaAs/GaAs. Threshold current of InGaAs/GaInP structure is less than half of InGaAs/AlGaAs. A high slope efficiency of 1.57 W/A from InGaAs/GaInP structure is observed with indium content as high as 0.35. InGaAs/GaInP structure will be the most appropriate candidate to fabricate a laser diode with high slope efficiency and low threshold current.

1. Introduction
Strained InGaAs/GaAs quantum well (QW) structure has been widely used in optoelectronic devices such as semiconductor lasers and fiber amplifiers. With lattice mismatches accumulating when the indium (In) content in the quantum well increases, the bandgap becomes wider and the light and heavy holes depart because of the tension strain. The lattice mismatch makes it hard to grow quantum wells with high In content, resulting in a negative influence on device behaviors[1]. AlGaAs has been used as the barrier in quantum well structures for it matches well with GaAs substrates and wider bandgap than GaAs. Though the epitaxial technique of AlGaAs is pretty mature, the Al is easy to get oxidized at high temperature, which has a strong impact on lasers properties[2]. GaInP is used as the barrier for fabrication of devices with strain effect. Devices with GaInP has been studied a lot since Yoshino et al for the first time managed to grow GaInP on GaAs substrates with MOCVD in 1981. It’s reported that GaInP can effectively improve the performance of light diodes. Since the absence of Al, donor complex centers which may cause ineffective donor activation are avoided[3]. Compared with GaAs and AlGaAs, GaInP is more easily to grow high purity wafers, stable surface[4]. Now GaInP has always been used for quantum well lasers, quantum dot lasers and solar cells for its large bandgap and decent lattice constant[5-11]. It’s been demonstrated that the recombination rate in the interface between GaInP and GaAs is much slower than that of AlGaAs and GaAs[12]. Besides, the lattice constant of GaInP can be bigger than GaAs and smaller than InGaAs at the same time which makes a GaInP barrier also a strain buffer layer(SBL). A single mode InGaAs/GaInP ridge waveguide laser is fabricated with threshold current of 24 mA and slope efficiency of 0.9 W/A[13]. A InGaAsP/GaInP/AlGaInP semiconductor laser is obtained with slope efficiency of 1.2 W/A and
internal quantum efficiency of 0.87 before coating[14]. A slope efficiency of 1.31 W/A is observed when GaInP is the barrier layer which is tested on a AlGaInP/GaInP quantum well with asymmetric cladding structure[15]. For reasons such as noted above, GaInP is a strong candidate to substitute AlGaAs in the manufacture of optoelectronic devices[16].

To investigate the impact of GaInP on lasers material gain, wavelength and P-I character, we present three InGaAs quantum well structures with GaAs, AlGaAs and GaInP as barriers, respectively. The effect of different barriers on designed structure performance are studied based on simulation results.

2. Physical model

A laser structure with InGaAs QW is designed as shown in Fig. 1 briefly. GaAs, AlGaAs, GaInP are used as barriers, respectively.

![Figure 1. InGaAs QW laser structures with GaAs, AlGaAs and GaInP as barriers, respectively.](image)

The lattice constant and strain effect must be taken into account in order to obtain a high property laser structure [17]. When the x\textsubscript{Ga} of GaInP barrier is 0.37, the lattice constant is 5.712 Å and the lattice constant of InGaAs is 5.792 Å with the x\textsubscript{In} of 0.35 based on Eq. (2.1).

\[
a_{\text{GaInP}} = a_{\text{GaAs}} - x_{\text{Ga}} \cdot \Delta a = 5.8696 - 0.4184 x + 0.1894 y + 0.013 xy
\]  

According to Eq.(2.1), the lattice constant of GaInP could be right between GaAs and InGaAs, which makes the GaInP layer a SBL. The strain induced by lattice mismatch could be buffered by the SBL, resulting in an improvement of wafer quality. The equation of AlGaAs lattice constant is not shown because it’s so close to the GaAs lattice constant that the biggest lattice mismatch is 0.13%. For AlGaAs(0<x\textsubscript{Al}<0.45), the bandgap at 300 K without any strain can be described as Eq.(2.2):

\[
E_g (x, y) = 1.424 + 1.247 x + 0.03 xy - 0.069 xy - 0.322 x^2 y^2 - 0.17 y^2
\]  

Eq.(2.3) is the expression of Ga\textsubscript{x}In\textsubscript{1-x}As\textsubscript{y}P\textsubscript{1-y} bandgap. Based on Eq.(2.2) and Eq.(2.3), the bandgap of Al\textsubscript{0.2}Ga\textsubscript{0.8}As and Ga\textsubscript{0.37}In\textsubscript{0.63}P are 1.698 eV and 1.701 eV, respectively. As it’s calculated, the bandgap of Ga\textsubscript{0.37}In\textsubscript{0.63}P is even bigger than Al\textsubscript{0.2}Ga\textsubscript{0.8}As, which provides a better confinement effect to electrons.

2.1. Formatting the title

The title is set 17 point Times Bold, flush left, unjustified. The first letter of the title should be capitalized with the rest in lower case. It should not be indented. Leave 28 mm of space above the title and 10 mm after the title.
3. Result and discussion

3.1. Material gain

For semiconductor lasers with a single QW, the material gain can be expressed with an equation:

\[ g(E) = \frac{\hbar^2 c^2}{8 m^2 E_{21}^2} r_{st}(E_{21}) \]  

(3.1)

The \( n_R \) in the equation is the refractive index, \( r_{st}(E_{21}) \) is stimulated emission rate. A refractive index equation is proposed by Sellmeyer, which is known as:

\[ n^2_R(\lambda) = (A + \frac{B}{\lambda^2 - C \lambda^4}) \]  

(3.2)

where, \( \lambda \) is wavelength. The parameter \( A, B \) and \( C \) can be calculated by:

\[ A(x_1,x_2,y_1,y_2) = A_{11} x_1 y_1 + A_{21} x_2 y_1 + A_{22} x_2 y_2 \]  

(3.3)

\[ B(x_1,x_2,y_1,y_2) = B_{11} x_1 y_1 + B_{12} x_1 y_2 + B_{21} x_2 y_1 + B_{22} x_2 y_2 \]  

(3.4)

\[ C(x_1,x_2,y_1,y_2) = C_{11} x_1 y_1 + C_{12} x_1 y_2 + C_{21} x_2 y_1 + C_{22} x_2 y_2 \]  

(3.5)

The \( x_1 \) and \( x_2 \) in the equation above are content of two elements from elements III in InGaAsP. The \( y_1 \) and \( y_2 \) are content of two elements among elements V in InGaAsP. \( A_{ij}, B_{ij} \) and \( C_{ij} \) are the sellmeyer coefficient which are shown in Table 1.

|   | Compound | \( A_{ij} \) | \( B_{ij} \) | \( C_{ij} \) |
|---|----------|--------------|--------------|--------------|
| 1 | GaAs     | 8.95         | 2.054        | 0.39         |
| 2 | GaP      | 4.54         | 4.31         | 0.22         |
| 3 | InAs     | 7.79         | 4.0          | 0.25         |
| 4 | InP      | 7.255        | 2.316        | 0.392        |

Based on Eq. (3.2), Eq. (3.3), Eq. (3.4), Eq. (3.5) and Table 1, the refractive index of InGaAsP decreases with In content increasing when the content of phosphorus (P) is zero. According to Eq. (3.1), the material gain is improved with refractive index diminishing. In other way, the material gain is improved with In content of QW increasing.

All the projects are simulated with the injection current of 1000 mA, cavity length of 1000 μm and stripe width of 100 μm.

![Figure 2. Material gain of In0.35Ga0.65As QW with Ga0.37In0.63P as barrier.](image-url)
The material gain of In$_{0.35}$Ga$_{0.65}$As is shown in Fig. 2 where Ga$_{0.37}$In$_{0.63}$P is applied as the barrier. With QW thickness of 5 nm, the specific material gain value is 6277 cm$^{-1}$. With the same QW thickness, the material gain of structure In$_{0.35}$Ga$_{0.65}$As/GaAs and In$_{0.35}$Ga$_{0.65}$As/Al$_{0.22}$Ga$_{0.78}$As are 4596 cm$^{-1}$ and 6764 cm$^{-1}$, respectively. All of the three structures’ material gain curve shapes are quite similar which is why not all of them are exhibited.

To further investigate the effect of QW thickness and In content of QW on laser property with GaAs, Al$_{0.22}$Ga$_{0.78}$As or Ga$_{0.37}$In$_{0.63}$P used as barrier, simulation are demonstrated. Fig. 3(a) shows the simulation results of material gain with In content of 0.35. Fig. 3(b) reveals the material gain property with QW width of 5 nm.

As it can be seen from Fig. 3(a) that QW thickness has a strong effect on material gain. For all of the three structures, the material gain enhance rapidly with QW thickness varying from 2 to 4 nm. The decreasing of material gain for all three structures is observed after QW thickness exceeding 5 nm. This is because the number of bound states increases as the QW thickness extending, which improves Auger recombination rate and decreases material gain. Fig. 3(b) reveals an increasing of material gain with In content ranging from 0.1 to 0.4, which is consistent with the theoretical analysis. The peak material gain of InGaAs/Ga$_{0.37}$In$_{0.63}$P structure is slightly less than InGaAs/Al$_{0.22}$Ga$_{0.78}$As structure and more than 1.4 times of InGaAs/GaAs at the same time.

3.2. Wavelength
Fig. 4(a) shows the relationship between quantum thickness and wavelength with In content of 0.35. Fig. 4(b) exhibits wavelength versus In content with the QW width of 5 nm. For InGaAs QW with GaAs barrier, there is no emission observed when the In content is smaller or equal to 0.5 since the Eg is too large to be restrictive based on Eq. (3).
Figure 4a. Wavelength of InGaAs QW with different QW thickness, when GaAs, Al$_{0.22}$Ga$_{0.38}$As and Ga$_{0.37}$In$_{0.63}$P are applied as barriers, respectively.

Figure 4b. Wavelength of InGaAs QW with different In content of QW, when GaAs, Al$_{0.22}$Ga$_{0.38}$As and Ga$_{0.37}$In$_{0.63}$P are applied as barriers, respectively.

The trends of wavelength versus QW thickness and In content can be seen from Fig. 4(a) and Fig. 4(b). The wavelength reveals a redshift with QW thickness and In content increasing. For a QW structure, because of the quantum size effect, the bandgap can be expressed as:

$$E_g^* = E_g + E_1 + E_{h1}$$

(3.6)

where $E_g$ is the bandgap under normal circumstance, $E_1$ and $E_{h1}$ are the sub energy levels of conduction band and valence band. Generally speaking, the $E_{h1}$ can be written as:

$$E_{h1} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L_w}\right)^2$$

(3.7)

where $L_w$ is the thickness of active region and $m^*$ stands for the effective mass. So $E_{h1}$ decreases when $L_w$ increases, resulting in a decreasing in $E_g^*$ according to Eq. (3.6). Based on the following equation where $\lambda$ is the wavelength:

$$\lambda = \frac{h \nu}{E_g^*}$$

(3.8)

the wavelength increases with the thickness of QW. Based on Eq. (2.2), the $E_g$ of InGaAs QW decreases with In content increasing, resulting in an wavelength redshift.

3.3. P-I property

The simulation P-I character is shown in Fig. 5, where structure with Ga$_{0.37}$In$_{0.63}$P barrier exhibits the highest slope efficiency 1.57 W/A and the lowest threshold current 63 mA. When Al$_{0.22}$Ga$_{0.78}$As works as the barrier, the threshold current of 145 mA is observed which is more than twice of In$_{0.35}$Ga$_{0.65}$As/Ga$_{0.37}$In$_{0.63}$P structure. The slope efficiencies of structure In$_{0.35}$Ga$_{0.65}$As/GaAs and In$_{0.35}$Ga$_{0.65}$As/Al$_{0.22}$Ga$_{0.78}$As are 0.79 W/A and 0.75 W/A, respectively. The slope efficiency of In$_{0.35}$Ga$_{0.65}$As/Ga$_{0.37}$In$_{0.63}$P structure is nearly double times of that of In$_{0.35}$Ga$_{0.65}$As/Al$_{0.22}$Ga$_{0.78}$As and In$_{0.35}$Ga$_{0.65}$As/GaAs.
Simulation results of threshold current and slope efficiency versus QW thickness are shown in Fig. 6(a) and Fig. 7(a) with In content of 0.35. Fig. 6(b) and Fig. 7(b) reveal P-I character with QW thickness of 5 nm.

As it's shown in Fig. 6(a), the threshold current decreases remarkably with QW thickness increasing until 4 nm. After reaching 4 nm, the QW thickness barely affects the threshold current. The InGaAs/Ga0.37In0.63P structure exhibits the lowest threshold current range which is from 61 to 176 mA. It can be seen from Fig. 6(b) that the threshold current decreases remarkably with In content of QW increasing. The threshold current of InGaAs/GaAs structure in Fig. 6(b) is pretty high when In content is equal to or lower than 0.15. It can be seen from Fig. 6 that the threshold current of InGaAs/Ga0.37In0.63P structure is basically half of InGaAs/Al0.22Ga0.78As and two-thirds of InGaAs/GaAs structure. For the analysis as noted above, the In0.35Ga0.65As/Ga0.37In0.63P structure always exhibits the lowest threshold current which makes it a decent choice for laser structure with low threshold current.
The slope efficiency slightly decreases with both of QW thickness and In content increasing which is observed in Fig. 7(a) and Fig. 7(b). Even though, the slope efficiency of InGaAs/Ga$_{0.37}$In$_{0.63}$P structure can still reach as high as 1.57 W/A with In content of 0.35 and QW width of 5 nm. Under the same circumstance, the slope efficiencies of InGaAs/Al$_{0.22}$Ga$_{0.78}$As and InGaAs/GaAs structures are 0.825 and 0.788 W/A, respectively. It’s reported that with QW thickness increasing, carrier delocalization will occur, leading to decreasing to both of carrier recombination rate and efficiency. Besides, the enhancement of QW thickness will bring increasing to bound states and Auger recombination rate, resulting in a decreasing in quantum efficiency as reported[18]. Both of the conditions noted above could lead to a slope efficiency decreasing. According to Eq. (2.2), When In content in QW increases, the energy gap between QW and barriers diminishes, leading to a consistent increasing in threshold current. As observed from Fig. 7, with QW thickness and In content ranging, the slope efficiency of InGaAs/Ga$_{0.37}$In$_{0.63}$P structure is almost as high as twice as the other two structures. Hence the InGaAs/Ga$_{0.37}$In$_{0.63}$P structure would be an appropriate option for a laser structure with a high slope efficiency.

4. Conclusion
Simulation of InGaAs QW with GaAs, Al$_{0.22}$Ga$_{0.78}$As and Ga$_{0.37}$In$_{0.63}$P barriers are demonstrated to study the impact of QW thickness and In content on laser performance. The material gain of InGaAs/Ga$_{0.37}$In$_{0.63}$P structure could be as high as almost 1.4 times of that of InGaAs/GaAs. A threshold current is observed in InGaAs/GaInP structure, which is nearly half of that of InGaAs/Al$_{0.22}$Ga$_{0.78}$As and two-thirds of InGaAs/GaAs structure. With In content as high as 0.35, the slope efficiency of InGaAs/Ga$_{0.37}$In$_{0.63}$P structure is 1.57 W/A. The slope efficiency value of InGaAs/Ga$_{0.37}$In$_{0.63}$P structure is always nearly twice of the other two structures. In conclusion, the InGaAs/Ga$_{0.37}$In$_{0.63}$P structure will be the most appropriate candidate in order to obtain laser diodes with high material gain, slope efficiency and low threshold current.

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