

EEE3037 Nanotechnology Coursework

6420013

Part I

Quantum Engineering Design

1 Structure Design

In order to design a quantum well which emits light of wavelength $1.55\mu\text{m}$, a well material must be chosen such that an interband electron transition emits photons of this wavelength.

This band gap energy can be found from the equation

$$E = hf$$

When considering photons, f can be substituted with

$$f = \frac{c}{\lambda}$$

Therefore in order to find the E in terms of wavelength

$$E = \frac{hc}{\lambda}$$

Returning to the specifications, this allows $1.55\mu\text{m}$ to be expressed as 1.28×10^{-19} J or approximately 0.800 eV.

This energy value will be the same as the total interband transition for the well from the first confined hole energy level to the first confined electron energy level,

$$E_{g,transition} = E_{1h} + E_g + E_{1e} \approx 0.800\text{eV} \quad (1)$$

see figure 1.

E_g should be the dominant term in this equation and as such when investigating suitable materials the bulk band gap should be close to but lower than 0.8eV.

Ternary alloys were investigated in order to allow precise control over the lattice constants and band gap by varying the composition ratio.

Indium gallium arsenide ($\text{In}_x\text{Ga}_{(1-x)}\text{As}$) as a well material with indium phosphide (InP) as a barrier material would provide a suitable combination assuming that a composition ratio x could be found that satisfied the two conditions of having the required bulk band gap and being lattice matched. A common ratio in industry is $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ and as such this was tested first.

1.1 Lattice Match

Lattice matching is the process of ensuring that two crystalline structures are of similar dimensions in order to decrease strain at the interface between the two materials. This is particularly important for quantum wells formed through epitaxial growth as strain introduced between such thin layers can cause defects which ultimately negatively affect its electronic properties.

The lattice constants between the barrier and well materials should be as close as is deemed acceptable for the application. The lattice constants for the prospective materials are shown in table 1.

In order to compute a compound lattice constant for InGaAs, Vegard's law can be applied. Vegard's law provides an approximation for the lattice constant of a solid solution by finding the weighted average of the individual lattice constants by composition ratio and is given by:

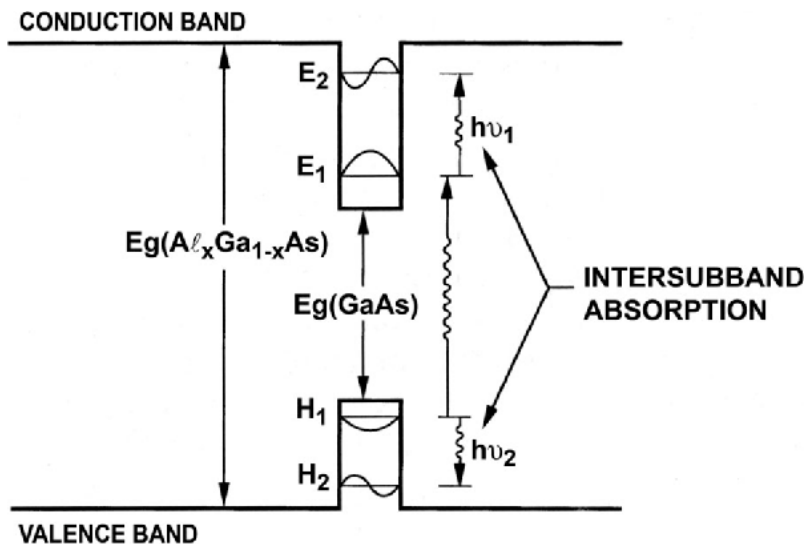


Figure 1: Band structure of an AlGaAs/GaAs/AlGaAs quantum well including discrete confined energy levels [1]

Material	Lattice Constant, α (\AA)
InAs	6.0583
GaAs	5.6532
InP	5.8687

Table 1: Lattice constants for prospective well and barrier materials [2]

$$\alpha_{A(1-x)B_x} = (1-x)\alpha_A + x\alpha_B$$

Applying this to the prospective well material gives the following,

$$\alpha_{In_{0.53}Ga_{0.47}As} = 0.53 \cdot 6.0583 + 0.47 \cdot 5.6532 = 5.8679$$

This shows that to 4 significant figures the composition of InGaAs is lattice matched to InP to within 0.001\AA which is sufficient for this application.

1.2 Band Gap

Vegard's law can also be used to approximate the band gap of a ternary alloy, such as InGaAs. The band gaps at 300K for each alloy can be seen in table 2.

In this case the band gap approximates to,

$$E_{g,In_{0.53}Ga_{0.47}As} \approx 0.53 \cdot 0.35 + 0.47 \cdot 1.42 \approx 0.85\text{eV}$$

However the band gap has been experimentally found to be 0.75eV [3]. This implies that the linear relationship provided by Vegard's law is not accurate enough and in this case a modified version including a bowing parameter b should be used,

Material	Band Gap at 300K, E_g (eV)
InAs	0.35
GaAs	1.42
InP	1.34

Table 2: Band gaps for prospective well and barrier materials [2]

Charge Carrier	Effective mass ratio in $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ ($\frac{m^*}{m_0}$)
Electron	0.041 [4]
Light Hole	0.051 [5]
Heavy Hole	0.2 [6]

Table 3: Effective masses of charge carriers in

$$E_{g,total} = xE_{g,a} + (1-x)E_{g,b} - bx(1-x)$$

For this application, however, the experimentally determined value will be used. This value is ideal for this application as it is comparable to and slightly lower than the required 0.8eV energy value.

1.3 Width Calculation

Having found two materials that are lattice matched with a suitable band gap value, the final calculation is that of the quantum well width. In order to calculate this value, the equation for confined energy levels within an infinite quantum well will be used,

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad (2)$$

Referring back to equation 1, the terms for the first electron and hole energy levels can each be replaced with equation 2 as seen below,

$$E_{g,transition} = 0.8\text{eV} = E_{1h} + E_{g,\text{InGaAs}} + E_{1e} = \frac{1^2\pi^2\hbar^2}{2m_h^*L^2} + E_{g,\text{InGaAs}} + \frac{1^2\pi^2\hbar^2}{2m_e^*L^2}$$

With the experimentally determined value for $E_{g,\text{InGaAs}}$ this equation becomes

$$0.8\text{eV} = \frac{\pi^2\hbar^2}{2m_h^*L^2} + 0.75\text{eV} + \frac{\pi^2\hbar^2}{2m_e^*L^2}$$

$$0.05\text{eV} = \frac{\pi^2\hbar^2}{2L^2} \left(\frac{1}{m_h^*} + \frac{1}{m_e^*} \right)$$

$$L = \sqrt{\frac{\pi^2\hbar^2}{2 \cdot (0.05\text{eV})} \cdot \left(\frac{1}{m_h^*} + \frac{1}{m_e^*} \right)}$$

As a frequently studied composition due to its favourable structural parameters with InP, The charge carrier effective masses of $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ have been found experimentally to be as shown in table 3.

As the electrical and optical properties of the valence band are governed by the heavy hole interactions, this effective mass ration will be used.

Substituting these ratios into the above provides,

$$L = \sqrt{\frac{\pi^2\hbar^2}{2 \cdot (0.05\text{eV}) \cdot m_e} \cdot \left(\frac{1}{0.2} + \frac{1}{0.041} \right)}$$

which reduces to a well length of 14.87nm.

1.4 Confined Energy Level Calculations

With all the parameters of the well ascertained the first and second confined electron and hole energy levels can be found by utilising equation 2.

For confined electron states:

$$E_{1e} = \frac{1^2 \pi^2 \hbar^2}{2 \cdot m_e^* \cdot (14.87\text{nm})^2}$$

$$E_{1e} = 6.65 \times 10^{-21} \text{J} = 0.041\text{eV}$$

This equation shows that confined energy level values are proportional to the square of n , the principal quantum number or energy level. As such:

$$E_{2e} = 2^2 \cdot E_{1e}$$

$$E_{2e} = 2.66 \times 10^{-20} \text{J} = 0.17\text{eV}$$

For confined hole states:

$$E_{1h} = \frac{1^2 \pi^2 \hbar^2}{2 \cdot m_h^* \cdot (14.87\text{nm})^2}$$

$$E_{1h} = 1.36 \times 10^{-21} \text{J} = 0.0085\text{eV}$$

$$E_{2h} = 2^2 \cdot E_{1h}$$

$$E_{2h} = 5.45 \times 10^{-21} \text{J} = 0.034\text{eV}$$

With the dimensions and first confined energy levels calculated, the final design for the quantum well can be seen in figure 2.

2 Probability Plot

The probability of finding an electron in a quantum well is given by

$$P = \int_0^L \psi^* \psi dx \quad (3)$$

with ψ in the case of an infinite quantum well being given by,

$$\psi(x) = A \sin(kx) = A \sin\left(\frac{n\pi}{L}x\right)$$

Here A acts as a normalisation constant to satisfy the conditions

$$\int_{\text{allspace}} \psi^* \psi dV = 1$$

in this case providing the wave function ψ as

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \quad (4)$$

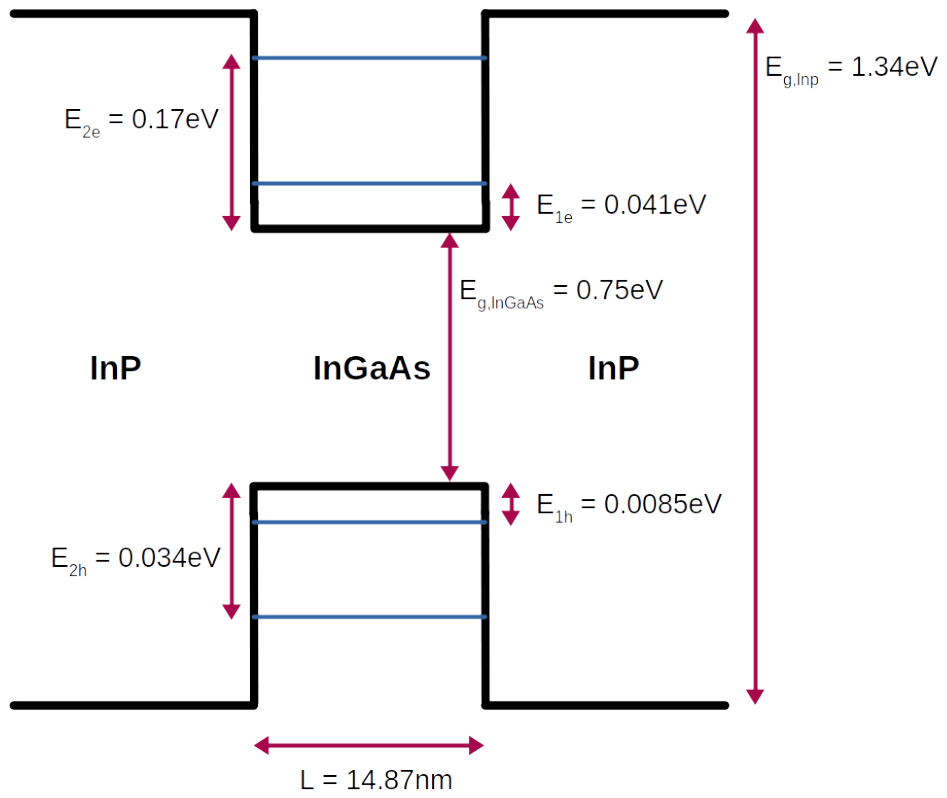


Figure 2: InP/InGaAs/InP quantum well design

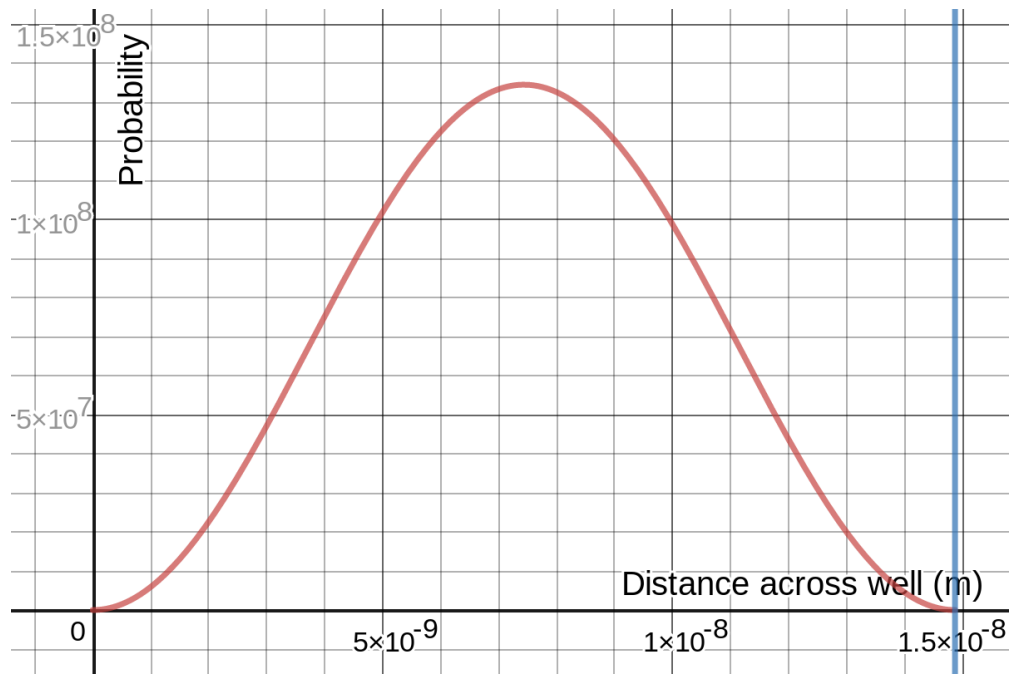


Figure 3: Probability plot for electron in ground state

Importantly, the above conditions are for an infinite quantum well where an assumption is made that the well has a barrier region of infinite potential such that the wavefunction is confined to the well. A real quantum well is unable to satisfy this leading to the wavefunction “spilling” into the barrier region. For the purposes of plotting the probability density, however, it is a reasonable assumption to make.

Considering equation 3, if the probability can be found by integrating $\psi^*\psi$, or in this situation ψ^2 then the probability can be shown by plotting ψ^2 , see figure 3. Here the well stretches from 0 to the blue line along the x axis and n has been set to 1 for the ground state. This function for the first excited state can be seen in figure 4.

3 Probability Intervals

Combining equations 3 and 4 gives the final probability function for a distance across the well from $x = 0$ to $x = x_0$:

$$P(0 \leq x \leq x_0) = \frac{1}{L} \left(x_0 - \frac{L}{2n\pi} \sin\left(\frac{2n\pi x_0}{L}\right) \right)$$

For an arbitrary interval across the well, this becomes:

$$P(a \leq x \leq b) = \frac{1}{L} \left((b - a) - \frac{L}{2n\pi} \left(\sin\left(\frac{2n\pi b}{L}\right) - \sin\left(\frac{2n\pi a}{L}\right) \right) \right)$$

This equation can be utilised in order to find the probability of finding the electron between 2nm and 4nm and between 6nm and 8nm, the intervals for which can be seen plotted in figure 5.

3.1 2nm to 4nm

$$P(2\text{nm} \leq x \leq 4\text{nm}) = \frac{1}{L} \left(2\text{nm} - \frac{L}{2n\pi} \left(\sin\left(\frac{2n\pi \cdot (4\text{nm})}{L}\right) - \sin\left(\frac{2n\pi \cdot (2\text{nm})}{L}\right) \right) \right)$$

$$P(2\text{nm} \leq x \leq 4\text{nm}) = \frac{1}{14.87\text{nm}} \left(2\text{nm} - \frac{14.87\text{nm}}{2\pi} \left(\sin\left(\frac{2\pi \cdot (4\text{nm})}{14.87\text{nm}}\right) - \sin\left(\frac{2\pi \cdot (2\text{nm})}{14.87\text{nm}}\right) \right) \right)$$

$$P(2\text{nm} \leq x \leq 4\text{nm}) \approx 0.0955$$

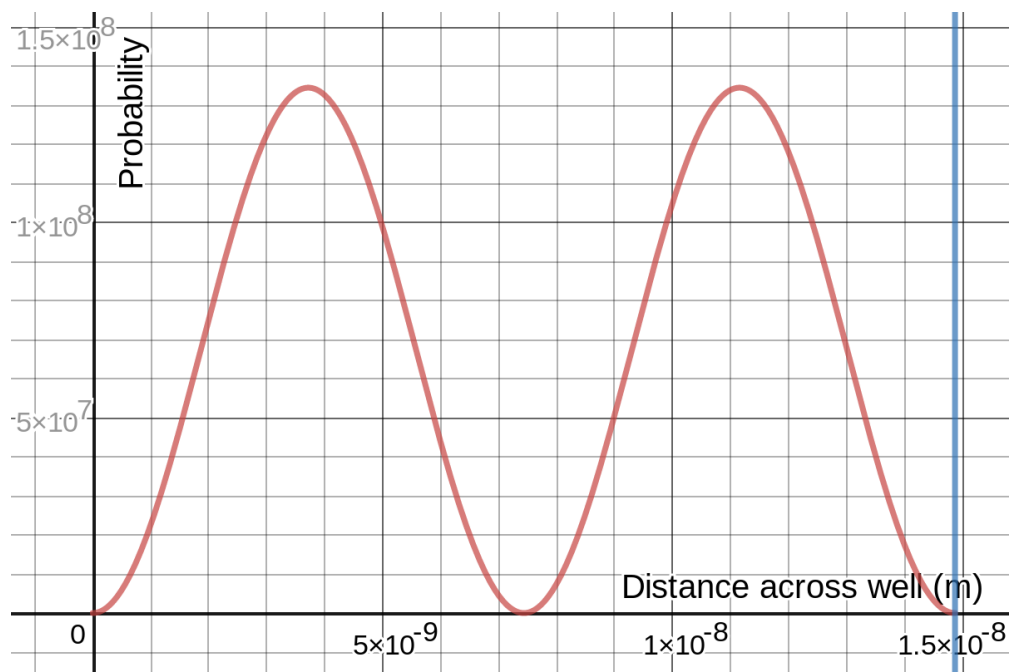


Figure 4: Probability plot for electron in 1st excited state

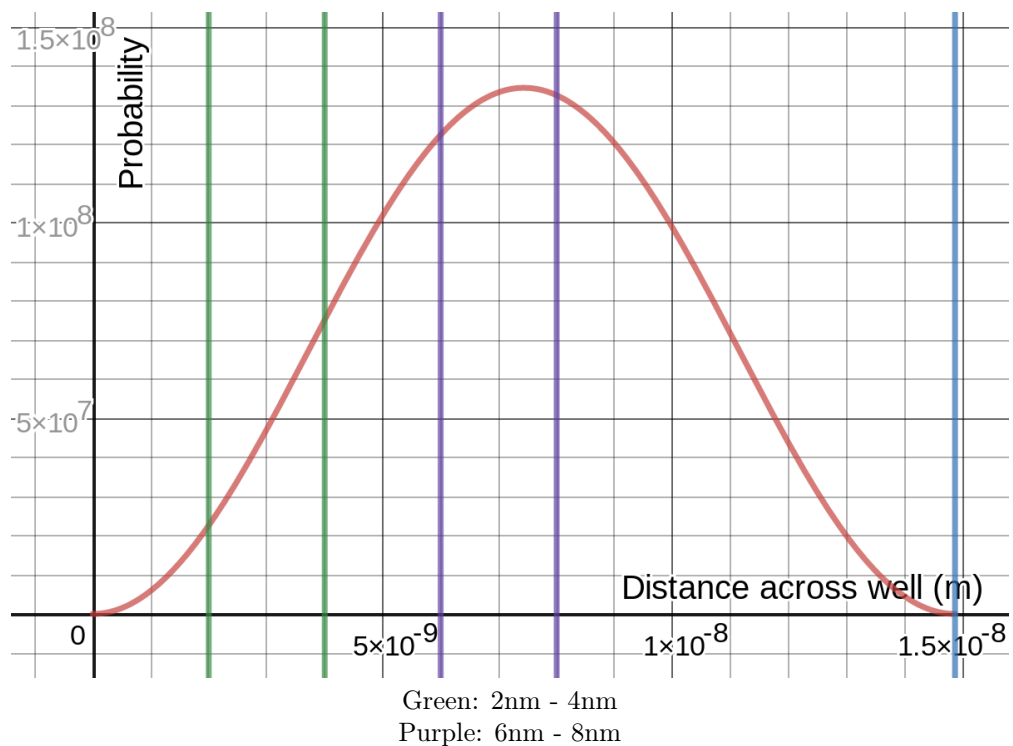


Figure 5: Probability plot for electron in ground state with distance intervals

3.2 6nm to 8nm

$$P(6\text{nm} \leq x \leq 8\text{nm}) = \frac{1}{L} \left(2\text{nm} - \frac{L}{2n\pi} \left(\sin \left(\frac{2n\pi \cdot (8\text{nm})}{L} \right) - \sin \left(\frac{2n\pi \cdot (6\text{nm})}{L} \right) \right) \right)$$

$$P(6\text{nm} \leq x \leq 8\text{nm}) = \frac{1}{14.87\text{nm}} \left(2\text{nm} - \frac{14.87\text{nm}}{2\pi} \left(\sin \left(\frac{2\pi \cdot (8\text{nm})}{14.87\text{nm}} \right) - \sin \left(\frac{2\pi \cdot (6\text{nm})}{14.87\text{nm}} \right) \right) \right)$$

$$P(6\text{nm} \leq x \leq 8\text{nm}) \approx 0.263$$

3.3 Conclusions

Considering these two probabilities it is clear that it is more likely for the electron to be found between 6nm and 8nm than between 2nm and 4nm across the well. This is as expected as 6nm to 8nm places the interval towards the center of the well. As the probability density function is a \sin^2 function, the maximum area will be towards the center. Referring to figure 5 this can be seen graphically as the region created by the purple lines has a far greater area under the probability density function than the region between the green lines.

Part II
Application of Nanomaterials

References

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