Heterostructure Semiconductor Optical Device — GaAs & GaP

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Part 1

In this project the objective is to select a specific wavelength for absorption, the use a heterostructure semiconductor device which employs reduced dimensionality to absorb at that wavelength.

The wavelength chosen was $800\ nm$. This wavelength was chosen as it the wavelength for high energy infrared light (slightly lower energy than red light which is about $700\ nm$). This wavelength is in the range of the wavelengths used for night vision devices.

The materials chosen are:

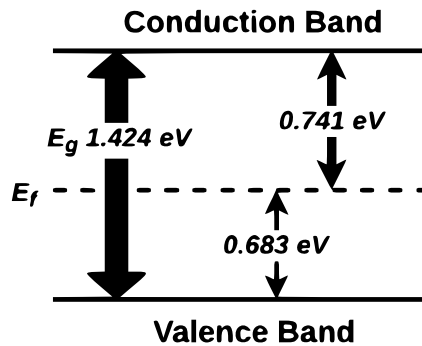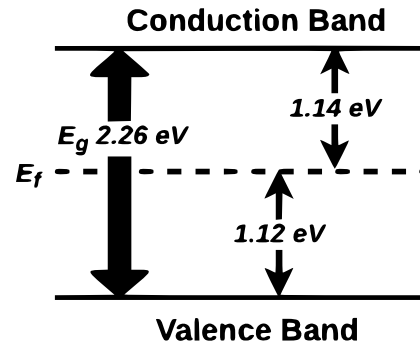|	
Material A (at 300K)	**Material B (at 300K)**
Gallium Arsenide (GaAs) [1]	**Gallium Phosphide (GaP) [2]**

Figure 1: Band Gap Diagram Of GaAs

Figure 2: Band Gap Diagram Of GaP

Material A

Type: N
Direct Band Gap: $1.424\ eV$
Longitudinal effective electron mass: $1.98\ m_e$
Heavy Hole effective mass: $0.45\ m_e$
Fermi Energy: $0.983\ eV$
Maximum Photon Wavelength (λ_{max}) for Band Gap Transition: $871\ nm$

Material B

Type: N
Direct Band Gap: $2.26\ eV$
Longitudinal effective electron mass: $1.12\ m_e$
Heavy Hole effective mass: $0.79\ m_e$
Fermi Energy: $1.12\ eV$
Maximum Photon Wavelength (λ_{max}) for Band Gap Transition: $549\ nm$
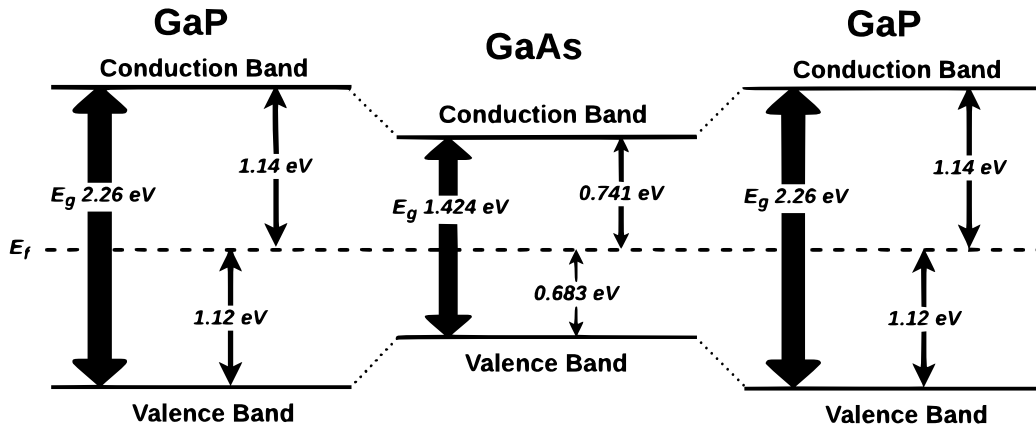
Heterostructure of GaAs And GaP

Figure 3: Band Gap Diagram Of Heterostructure At Equilibrium

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 Note:  In this figure Anderson's rule was foregone and simple dotted
lines are used to represent the connection of the heterostructure,
but not the energy at the heterojunction.
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The heterostructure of GaAs and GaP forms a straddling gap hetero-junction. Where the conduction and valence band of GaAs have less of a difference in absolute energy with respect to the Fermi energy then GaP. This can be shown by a quantum well:
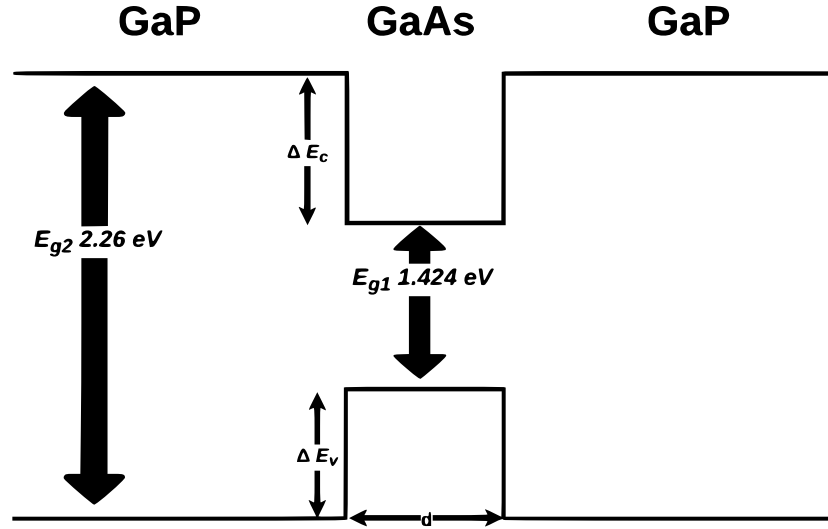
Figure 4: Quantum Well Of Heterostructure [GaAs & GaP]

Were:
$$\Delta E_c \approx 0.7(E_{g2} - E_{g1}) \ \& \ \Delta E_v \approx 0.3(E_{g2} - E_{g1})$$
$$\Delta E_c \approx 0.585 \ eV \ \& \ \Delta E_v \approx 0.251 \ eV$$

Let the effective mass of the heterostructure in energy regions in E_{g2} for electrons/holes be an approximation. Where the electrons/holes effective mass is equal to the electrons/holes effective mass for GaAs:
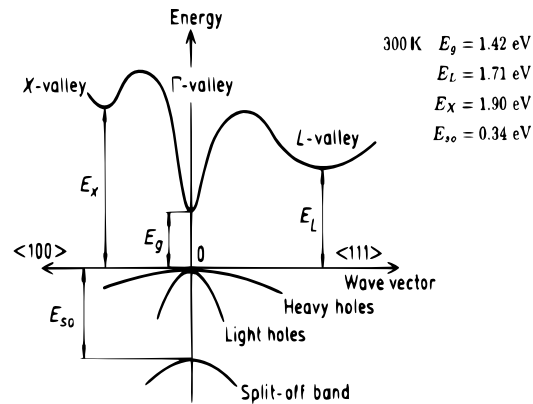$m_h^* = 0.45 \ m_e \ \& \ m_e^* = 1.98 \ m_e$

Figure 5: Band Structure Of Gallium Arsenide[GaAs]

Part 2

A material can be modelled as a box well with infinite potential. The solution to the time independent schrodinger wave equation leads to energy states described by the following equation:

$$E = \frac{n_x^2 \hbar^2 \pi^2}{2mL_x^2} + \frac{n_y^2 \hbar^2 \pi^2}{2mL_y^2} + \frac{n_z^2 \hbar^2 \pi^2}{2mL_z^2}$$

This equation can be rewritten into k-space such that $k_i = \frac{\pi n_i}{L}$.

$$E = \frac{k_x^2 \hbar^2}{2m} + \frac{k_y^2 \hbar^2}{2m} + \frac{k_z^2 \hbar^2}{2m}$$

In the case of reduced dimensionality, one of these dimensions is much smaller than the other two. Say for example $L_x << L_y \approx L_z$; in this case one may visualize the coordinates in k-space. Each state in k-space has a spacing of $\frac{\pi n_i}{L}$, where n is an integer, so in k-space there will be a large spacing between each x-level, resulting in planes of points in the y-z dimensions separated by a large K value in the x-direction.

Density of states refers to the rate of change of states with respect to energy. An equation for the density of states can be derived from the volume in k-space. If the lengths/K value in some particular dimensions are equal the states are uniformly distributed in those directions, therefore there is a relationship between volume in k-space and the number of states in that space (although states are discrete, since k-space is very large at higher energy values the number of states is directly proportional to the volume in k-space). The volume is connected to the energy of the system; $E = \frac{k^2 \hbar^2}{2m}$, where k is the radius of k-space since $k = \sqrt{k_x^2 + k_y^2 + k_z^2}$.

In the case described above where $L_x << L_y \approx L_z$, this proportionality between volume in number of states is still true, however there is a sparsity of states per volume in the x-direction. One can consider that the density of states doesnt change very much as a function of energy is the x direction but does in the two others. Note that each point in k-space corresponds to two states, since for that k-value there are spin-up and spin-down states. As such the number of states as a function of energy becomes a function of two dimensions:

$$N(E) = 2 \cdot \frac{\text{area in k-space}}{volume\,in\,area} = 2 \cdot \frac{\pi k^2 (L_x L_y)}{4\pi} = \frac{(L_x L_y) m^* E}{\pi \hbar}$$

Density of states is:

$$\frac{\delta}{\delta E} N(E) = Z(E) = \frac{(L_x L_y) m^*}{\pi \hbar}$$

Density of states per unit area(most commonly used version):

$$Z(E) = \frac{m^*}{\pi \hbar^2}$$

This means that the density of states is in fact independent of energy. Although k-space is continuous in the y-z direction at higher energies, due to the large spacing in the x-direction k-space is still discrete in that dimension. Note the equation $Z(E) = \frac{m^*}{\pi \hbar}$ is only valid for the $n_x = 1$. When $n_x = 2$, another plane of states is available in k-space; when this second plane (y-z plane) of states becomes available, the density of states will precisely double, since the rate of change of states with respect to increasing energy in the y and z dimension will double due to the second plane of states being available, this logic can be extended for all nx values where $Z(E) = N_x \frac{m^*}{\pi \hbar}$. The density of states can be represented by the following diagram:
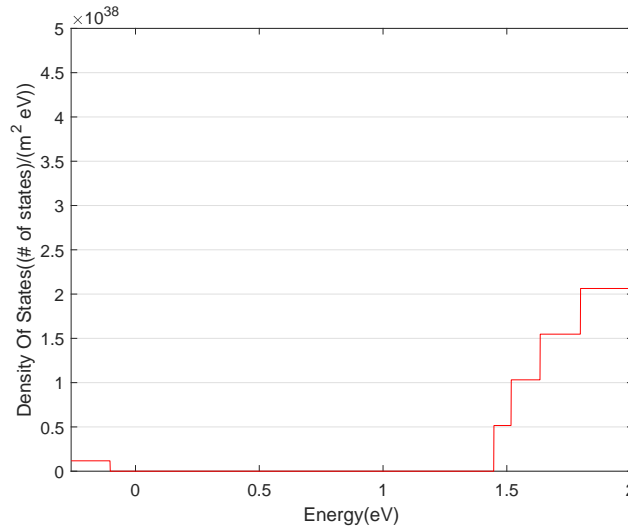

Figure 6: Density Of States For Heterostructure In 2D

In the above sketch, the momentum (k-values) are in the x-direction. The density of states is zero immediately above the band gap. There is another gap between the end of the band gap and where density of states begin. This is due to the fact that the first energy state above the valence band is at energy $E = \frac{\hbar^2 \pi^2}{2m^* L_x^2}$. In fact this is true in all dimensions, however $L_x << L_y \approx L_z$ so it is only significant in the x-direction. The density of states double at an energy of $E = \frac{2\hbar^2 \pi^2}{L_x^2}$ corresponding to the second energy state in the x-direction. In fact the density of states will increase by a factor of $\frac{m^*}{\pi\hbar^2}$ at $E = \frac{n_x^2 \hbar^2 \pi^2}{2L_x^2}$, where nx is an integer. A similar phenomenon occurs for the valence band, where the density of states for holes will obey the same trend. In fact these two densities of states would be identical and symmetric about the band gap had they the same effective mass. In practise their effective masses will cause asymmetry about the band gap as holes will have effective density of states $Z(E) = \frac{m^*}{\pi\hbar^2}$ at energies $E = \frac{n_x^2 \hbar^2 \pi^2}{2m^* L_x^2}$

To create this material such that $L_x << L_y \approx L_z$, a thin piece of GaAs is placed between GaP (Figure 3,4).

Part 3

Optical absorption requires that the energy of the incident photon is greater or equal to the energy gap magnitude between the conduction and valence band. Additionally, the absorption will have a proportionality to density of states. Density of states in a semiconductor that isn't subject to reduced dimensionality will have a quadratic form of valence and conduction band density of states:
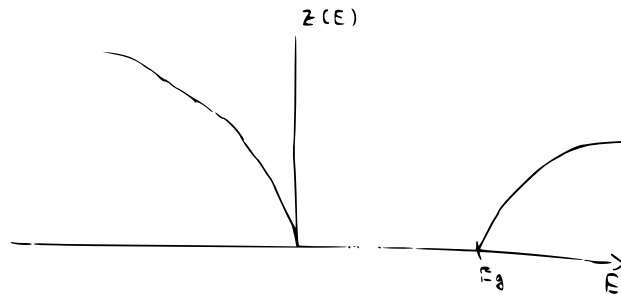

Figure 7: Density Of States In 3D

Optical absorption demands that the energy of a photon is absorbed by promoting an electron from the valence to the conduction band. The rate of absorption will depend on the electrons available to be promoted. Since density of states (in plot above) is low for both the conduction and valence band near the band gap and increases while moving away from the band gap, incident photons of greater energy would cause a higher rate of absorption since there are more states from which to excite the electrons from and more states to excite the electrons to (since density of states increases with increasing energy). Note that this means that technically right at the band gap there is zero absorption since no states from which to excite from and to.

In the case of the design, due to reduced dimensionality the density of states is zero at the band gap but increases as a step function instead of a smooth continuous function. By the same logic as above absorption will increase at a level of greater density of states. Therefore due to the step function nature of the density of states, the absorption will greatly increase at the desired photon wavelength since the density increases from zero to $\frac{m_h^*}{\pi\hbar^2}$ at that specific energy. Better yet, the absorption will be constant for energies slightly greater than that value since density of states is constant until the next step up (which occurs at each $E = \frac{n_x^2\hbar^2\pi^2}{2m^*L_x^2}$, n being an integer).

To get absorption at the desired wavelength (800 nm), the total energy gap must equal the energy of the photon. The total energy gap is the sum of the GaAs energy gap, the gap between the top of the band gap and the beginning of the conduction density of states and the distance between the bottom of the band gap and the beginning of the density of states for the valence band: $E_T = E_v + E_c + E_g$

Hole Energy   Electrons Energy   Gap Energy

$$E_v = \frac{n^2\hbar^2\pi^2}{2m_h^*d^2} \qquad\qquad E_c = \frac{n^2\hbar^2\pi^2}{2m_e^*d^2} \qquad\qquad E_g = E_{g1} = 1.424 \ eV$$

Find the relationship between the number of states n_e and the width of the band d in the conduction band:

$$d = \frac{\hbar\pi}{\sqrt{2m_e^*\Delta E_c}}n_e$$

$$d = 0.570 \ nm \ n_e$$

Find minimum width for ΔE_c at a state minimum $n_h = 1$:

$$d = 0.570 \ nm$$

Therefore, the minimum width the band can be while still having a viable energy state is $0.570 \ nm$ for the conduction band.

Find the relationship between the number of states n_h and the width of the band d in the valence band:

$$d = \frac{\hbar\pi}{\sqrt{2m_h^*\Delta E_v}}n_h$$

$$d = 0.570 \ nm \ n_h$$

Find minimum width for ΔE_V at a state minimum $n_h = 1$:

$$d = 0.570 \ nm$$

Therefore, the minimum width of the band were GaAs can have viable energy state is $1.83 \ nm$ for the valence band.

The minimum width is the valence band minimum width; being the greater of the two minimum widths. Where the limiting width is: $d > 1.83 \ nm$ for the heterostructure to have viable energy states in the conduction and valence bands of GaAs.

Chosen λ is $800 \ nm$
$E_{800nm} = 1.55 \ eV$
To choose a width for GaAs to absorb the chosen wavelength of 800 nanometers we consider the energy of GaAs band gap and valence/conduction band of the heterostructure. Substitute equations from above and solve for d explicitly:

$$E_{light} = E_v + E_c + E_g$$

Sub, equations and values for the energy's:

$$E_{light} = \frac{n^2\hbar^2\pi^2}{2m_h^*d^2} + \frac{n^2\hbar^2\pi^2}{2m_e^*d^2} + E_{g1}$$

$$d = \frac{\hbar\pi}{\sqrt{2}}\sqrt{\frac{n_h^2}{m_h^*} + \frac{n_e^2}{m_e^*}}\frac{1}{\sqrt{E_{light} - E_{g1}}}$$

Now, to find a particular width for the device test the values of the lowest energy states in both the conduction and Valence band. If the width is greater than the minimum width derived above then; the width can be used for the heterostructure to detect the target wavelength. It is important to find a width at the lowest energy state possible, because this will allow for the minimum width of GaAs. The thinner the GaAs lair, the less energy states and the more sparse those energy states are. This precaution will help isolate the target wavelength from uninteresting wavelengths.

Try, for 800 nm wavelength at $n_e = 1$ and $n_h = 1$:

$$d = 2.854 \; nm$$

Therefore, this Is a valid width for the quantum well because it doesn't violate the minimum thickness. This is the minimum width of GaAs with the most discrete energy levels.

\# Energy states conduction band

$$d = 0.570 \ nm \ n_e$$

Sub, d and find n_e:

$$2.854 \ nm = 0.570 \ nm \ n_e$$

$$n_e \approx 5.01 = 5$$

\# Energy stats valence band

$$d = 1.83 \ nm \ n_h$$

Sub, d and find n_h:

$$2.854 \ nm = 1.83 \ nm \ n_h$$
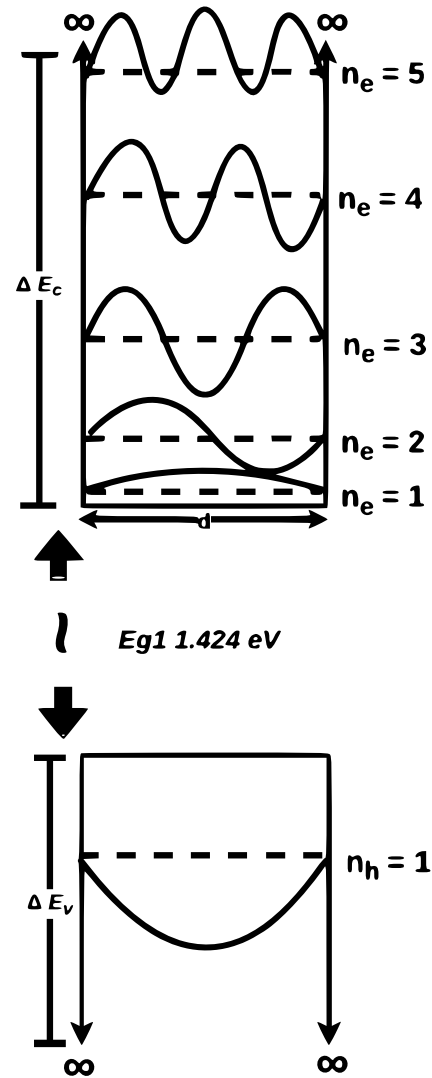
$$n_h \approx 5.01 = 5$$

Figure 8: Density Of States In 3D

Part 4

In practise, the quantum wells created by the heterostructure are not of infinite potential; their potential is clearly finite as outlined by the quantum well representation of the heterostructure as seen in figure 4. To get an estimate of the error associated with this assumption the energy levels of the finite potential well are calculated for the actual potential wells (see figure from part 1 on the quantum well representation of the heterostructure).

The time-independent schrodinger equation is therefore solved inside and outside of the quantum well. The boundary conditions is that the waveform must approach 0 at $x = \infty$ for a bound state. Additionally the waveform inside and outside the well must be equal and have equal derivatives at each side of the well:

$$\Psi_{in}(0) = \Psi_{out}(0)$$

$$\frac{\delta}{\delta x}\Psi_{in}(0) = \frac{\delta}{\delta x}\Psi_{out}(0)$$

$$\Psi_{in}(d) = \Psi_{out}(d)$$

$$\frac{\delta}{\delta x}\Psi_{in}(d) = \frac{\delta}{\delta x}\Psi_{out}(d)$$

This allows for a smooth continuous solution.

Inside the well:

$$\Psi_{in} = A\cos(k_{in}x) + B\sin(k_{in}x)$$

$$\frac{\delta^2\Psi_{in}}{\delta x^2} = -k_{in}^2\Psi_{in}$$

$$k_{in} = \frac{\sqrt{2m_{in}^*E}}{\hbar} = \frac{n\pi}{d}$$

$$E\Psi_{in} = -\frac{\hbar^2}{2m_{in}^*}\frac{\delta^2\Psi_{in}}{\delta x^2}$$

Outside the well:

$$\Psi_{out} = Ce^{-k_{out}x}$$

$$E_{g2}\Psi_{out} - E\Psi_{out} = -\frac{\hbar^2}{2m_{out}^*}\frac{\delta^2\Psi_{out}}{\delta x^2}$$

$$k_{out} = \frac{\sqrt{2m_{out}^*(E_{g2} - E)}}{\hbar}$$

Continuity Conditions for well boundaries where $x = 0$ or $x = d$

$$\Psi_{out}(x) = \Psi_{in}(x) \text{ and } \Psi'_{out}(x) = \Psi'_{in}(x)$$

Substituting corresponding equations into Ψ_{out} and Ψ_{in}:

$$Ce^{-k_{out}x} = A\cos(k_{in}x) + B\sin(k_{in}x)$$

The above equation can be split into 2 different equations. One for even cosine wave functions, and a second for odd sinusoidal wave functions:

$$Ce^{-k_{out}x} = A\cos(k_{in}x) \tag{1}$$

$$Ce^{-k_{out}x} = B\sin(k_{in}x) \tag{2}$$

And their first derivatives:

$$-k_{out}Ce^{-k_{out}x} = Ak_{in}\sin(k_{in}x) \tag{3}$$

$$-k_{out}Ce^{-k_{out}x} = Bk_{in}\cos(k_{in}x) \tag{4}$$

Substituting, (1) into (3) and rearranging gives:

$$k_{out} = \frac{k_{in}\sin(k_{in}x)}{\cos(k_{in}x)} = k_{in}\tan(k_{in}x)$$

Similarly for (2) and (4):

$$k_{out} = \frac{-k_{in}\cos(k_{in}x)}{\sin(k_{in}x)} = -k_{in}\cot(k_{in}x \cdot d)$$

For an even wave function such as the $n = 1$ state,

$$k_{out} = k_{in}\tan(k_{in}x)$$

$$\frac{\sqrt{m^*_{out}(E_{g2} - E)}}{\sqrt{m^*_{in}E}} = \tan\left(\frac{\sqrt{m^*_{in}E}}{\hbar}\right)$$

In part 3, due to the infinite well barrier assumption it was said that the spacing between the edge of the band gaps and non-zero density of states is calculated as $E = \frac{\hbar^2\pi^2}{2L_x^2}$. . In practise this is not the case and due to finite barriers one would expect lower energy for the first energy state (in the x-direction) due to the fact that the particle penetrates outside the well. This would in turn lower the total gap defined as $E_{light} = E_v + E_c + E_{g1}$, affecting the absorption wavelength. To determine the magnitude of this effect on the absorption wavelength, E_v and E_c are re-calculated using the a finite potential well solution and the results are contrasted.

The figure below shows a plot of the lowest energy finite well solution for the conduction band
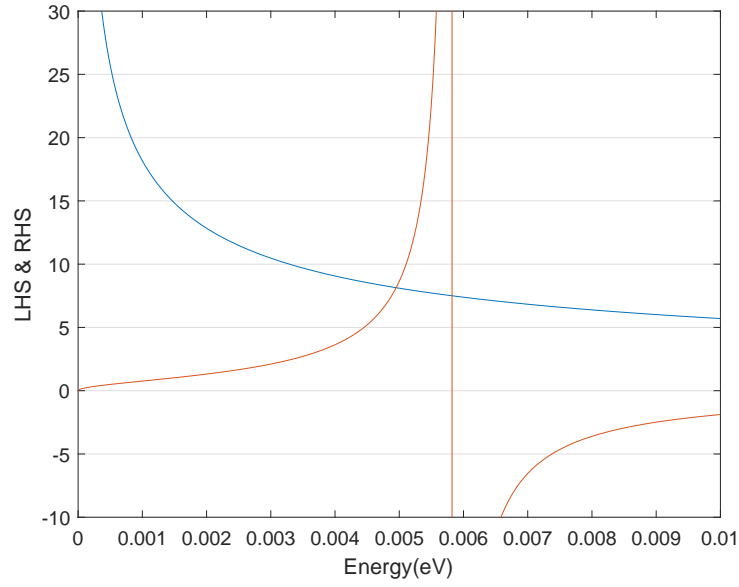

Figure 9: F.P.W Solutions For Heterostructure [Conduction Stats]

For the conduction band, the lowest energy state was therefore calculated as being
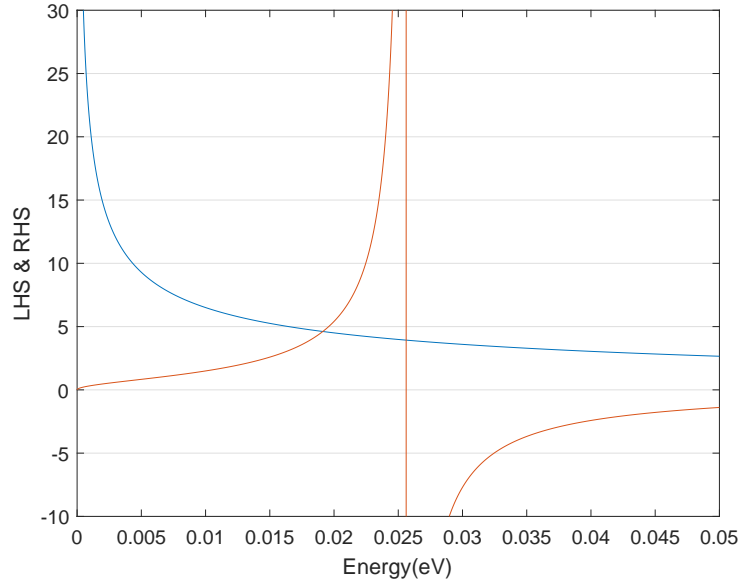
$$E_c = 0.00495 \ eV$$

Similarly, for the valence band:

Figure 10: F.P.W Solutions For Heterostructure [Valence Stats]

The first energy level solution for the valence band is:

$$E_v = 0.0191 \ eV$$

The effect that this has on the absorption wavelength can now be recalculated:

$$E_{light} = E_v + E_c + E_{g1}$$
$$h\frac{c}{\lambda} = 1.448 \ eV$$
$$\lambda = 856 \ nm$$

And,

$$\Delta\lambda = 56 \ nm$$

Therefore, since in practise the heterostructure has a finite barrier form instead of an infinite barrier form this results in an absorption starting at 856 nm instead of 800 nm. The infinite barrier approximation therefore yielded an absorption wavelength uncertainty of 56 nm.

MatLab Code

```matlab
close all;

%Constance and values of physical properties...
%related to the material

hbar = 1.055E-34;
me = 9.109E-31;
ev_j = 1.602E-19;

Elight = 1.55;
Eg1 = 1.424;

Elight_j = Elight .* ev_j;
Eg1_j = Eg1 .* ev_j;

mh = 0.45;
mel = 1.98;

ne = 1;
nh = 1;

mh_kg = mh.*me;
mel_kg = mel.*me;

Ec = 0.585
Ev = 0.251

Ec_j = Ec.*ev_j;
Ev_j = Ev.*ev_j;

%Finding the minimum width the conduction...
%band can have while still having viable energy states
dminc = (hbar.* pi)./sqrt(2.*Ec_j.*mel_kg)

%Finding the minimum width the valence...
```

```matlab
36  %band can have while still having viable energy states
37
38  dminv =  (hbar.* pi)./sqrt(2.*Ev_j.*mh_kg)
39
40  %Finding the width for the chosen wavelength...
41  %at nc = nv =1 states
42
43  d = (hbar.* pi)./sqrt(2) .* sqrt( (ne.^2./mel_kg) +...
44      (nh.^2./mh_kg)).*(Elight_j - Eg1_j )^(-1./2)
45
46  %Defining energy steps for chosen width conduction band
47   stepEc = (hbar.^2.* pi.^2)./(2.*d.^2.*mel_kg)./ev_j
48
49  stepEc2 = 4 .*   stepEc
50  stepEc3 = 9 .* stepEc
51  stepEc4 = 4.^2 .* stepEc
52  stepEc5 = 5.^2 .* stepEc
53
54  %Defining energy steps for chosen width valence band
55
56   stepEv  = (hbar.^2.* pi.^2)./(2.*d.^2.*mh_kg)./ev_j
57
58  stepEv2 = 4 .*   stepEv
59  stepEv3 = 9 .* stepEv
60  stepEv4 = 16 .* stepEv
61
62
63  %Defining density of states in both conduction...
64  %and valence bands
65
66  Zh = mh_kg./( pi .*hbar.^2);
67  Ze = mel_kg./( pi .*hbar.^2);
68
69  E = -0.260:0.001:2.01;
70  z = 1:2270;
71  for ind = 1:2271
72      if (E(ind) <= -stepEv3)
73      z(ind) = 3.*Zh;
```

```matlab
74      elseif E(ind) <= -stepEv2
75      z(ind) = 2.*Zh;
76      elseif E(ind) <= -stepEv
77      z(ind) = Zh;
78      elseif E(ind) <= (stepEc + Eg1)
79      z(ind) = 0;
80      elseif E(ind) <= (stepEc2 + Eg1)
81      z(ind) = Ze;
82      elseif E(ind) <= (stepEc3 + Eg1)
83      z(ind) = Ze.*2;
84      elseif E(ind) <= (stepEc4 + Eg1)
85      z(ind) = Ze.*3;
86      elseif E(ind) <= (stepEc5+ Eg1)
87      z(ind) = Ze.*4;
88      else
89      z(ind) = Ze.*5;
90      end
91  end
92
93  %Plotting density of states
94
95  plot(E,z,'r')
96  axis([-0.260  2.01   0 50E37])
97  ax = gca;
98  ax.YGrid = 'on';
99  ax.GridLineStyle = '-';
100 %title('Density Of States For Heterostructure In 2D')
101 xlabel('Energy(eV)')
102 ylabel('Density Of States((# of states)/(m^2 eV))')
103
104
105 % defining desired energy's and wave numbers...
106 %in both regions of the heterostructure [Con Band]
107
108 ECON = 0:0.0000001:0.01;
109 kC0 = sqrt(2.*1.12.*9.109E-31.*1.60218e-19.*...
110     (0.585 - ECON))./(1.054E-34);
111 kC1 = sqrt(2.*1.98.*9.109E-31.*(1.60218e-19.*...
```

```matlab
112        ECON)).  / (1.054E−34);


115 %Plotting left and right hand side [Con Band]

117 figure
118 LHSC = kC0./kC1;
119 RHSC = tan(kC1.*d);
120 hold off
121 plot(ECON,LHSC)
122 hold on
123 plot(ECON,RHSC)
124 axis([0 0.01  −10 30])
125 ax = gca;
126 ax.YGrid = 'on';
127 ax.GridLineStyle = '−';

129 %title('Solutions For Heterostructure Of Finite
        Potential Well [Conduction    Stats]')
130 xlabel('Energy(eV)')
131 ylabel('LHS & RHS')

133 % defining desired energy's and wave numbers...
134 %in both regions of the heterostructure [Va Band]
135 Eva = 0:0.0000001:0.05;
136 kv0 = sqrt(2.*0.79.*9.109E−31.*1.60218e−19.*(0.251 −
        Eva))./(1.054E−34);
137 kv1 = sqrt(2.*0.45.*9.109E−31.*(1.60218e−19.*Eva))
        ./(1.054E−34);

139 %Plotting left and right hand side [VA Band]

141 figure
142 LHSV = kv0./kv1;
143 RHSV = tan(kv1.*d);
144 hold off
145 plot(Eva,LHSV)
146 hold on
```

```matlab
147  plot(Eva,RHSV)
148  axis([0  0.05   -10  30])
149
150  ax = gca;
151  ax.YGrid = 'on';
152  ax.GridLineStyle = '-';
153
154  %title('Solutions For Heterostructure Of Finite
          Potential Well [Valence  Stats]')
155  xlabel('Energy(eV)')
156  ylabel('LHS & RHS')
```

References

[1] https://ecee.colorado.edu/~bart/book/effmass.htm

[2] http://www.ioffe.ru/SVA/NSM/Semicond/GaP/bandstr.html#Masses

[3] http://www.ioffe.ru/SVA/NSM/Semicond/GaAs/bandstr.html

[4] https://people.rit.edu/vwlsps/314_w07/FiniteSquareWell.pdf