Optical Absorption of Semiconductors

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Abstract

The aim of this experiment was to determine values for the direct and indirect band gaps of the semiconductors Gallium Arsenide and Gallium Phosphate respectively. This was done through shining monochromatic light through each semiconductor and measuring the light intensities at the detector. These values were then used to calculate absorption as a function of wavelength. This was done through utilising Lock-in detection. Data acquisition was automated using MATLAB. The value for the direct band gap for Gallium Arsenide was calculated to be $(1.4 \pm 0.1) \mathrm{eV}$ and the that for Gallium Phosphide was calculated to be $(2.1 \pm 0.2) \mathrm{eV}$. The empirical values agree with the known values.

1 Introduction

Semiconductors are present in all of our technology: from our phones to even our washing machines. Understanding how semiconductors work and how to maximise their efficiencies is vital in order to continue making advancements in technology. One way in which semiconductors have been utilised has been in the generation of solar energy through the use of photovoltaics. In 1839, a Edmond Becquerel discovered that when a wet silver cell is exposed to sunlight, it's voltage increases. This effect was labelled as the photovoltaic effect [1]. As the name implies, a photovoltaic device is a device which can undergo the photovoltaic effect and is therefore able to convert light to electricity. Semiconductors are also key components in Lasers and LEDs [2]. LEDs operate through the utilisation of excitation and de-excitation. [3] When light is shone onto a material, a photon can be absorbed by an electron in the material to cause it to excite. This means that it 'jumps' from it's current energy state to a higher one. To be more precise, it jumps from the valence band to the conduction band leaving a 'hole' in the valence band [4]. Excitation can also occur through the absorption of energy through other means for example: electrical excitation. The difference between the conduction and valence band is known as the band gap. Materials with large band gaps are better insulators; materials with lower band gaps are semiconductors and materials with little or no band gap are better conductors. In this report, I will venture deeper into the idea of excitation, and optical properties of semiconducters by explaining an experiment which was conducted to determine the values for the direct and indirect energy band gaps for Gallium Arsenide and Gallium Phosphide respectively.

2 Theory

The temperature of a solid is governed by vibration of the particles which make up the crystal. These vibrations are associated with a k-space vector called the angular wave vector which represents the spatial frequency of normal modes of vibrations. The relationship between momentum, \mathbf{P} can be expressed by the following equation:

$$\mathbf{P} = \hbar \mathbf{k} \tag{1}$$

Where \hbar is the reduced Planck's constant and ${\bf k}$ is the angular wave vector. Each angular wave vector has a corresponding energy value. These energy values are quantised and are known as phonons.

Electrons have discrete energy levels governed by the geometry and charge distribution of the overall atom, molecule or lattice. An electron is described as excited when it has absorbed a specific amount of energy and therefore exists in a higher state. One way in which electrons can gain energy to excite is through the absorption of photons. The energy of a photon , E, is dependent on it's wavelength λ and is related by the following equation:

$$E = \frac{hc}{\lambda} \tag{2}$$

where h is Planck's constant and c is the speed of light. When considering the electron orbitals, the outermost electron orbital of an atom can be described as the valence band. The conduction band is simply the range of orbitals in which the electrons can exist in, once excited. A band gap can be described as the energy difference between the valence and conduction bands of an electron. This represents the minimum energy required to excite an electron from its ground state to a higher energy state to allow for conduction. There are two basic types of band gaps - a direct band gap and an indirect band gap . A direct band gap is characterised by an electron's ability to directly emit a photon once jumping from its valence band to its conduction band. This can be done since the momentum of the electrons in the crystal and in the holes are the same in both the conduction and valence bands. On the other hand, an indirect band gap is characterised by an electron's inability to emit a photon directly since it must pass through an intermediary stage and transfer momentum to the crystal before emitting a photon [4]. This is because the momenta of the electrons in the crystal and the holes in the energy bands are not the same therefore a phonon needs to be absorbed or emitted in order for the excitation to occur. When light is shone through a semiconductor, electrons in the crystal lattice excite to a higher energy state. Only specific wavelengths of light can be absorbed by these electrons since there are discrete energy states in which the electrons can exist in. The absorption coefficient is a measurement of how much light has been absorbed by the semiconductor. Conversely, the transmission coefficient is the ratio of the intensity of light emanating from the source and of light shone through the semiconductor. By placing a semiconductor in the path of a monochromatic light beam, varying the wavelength of the source light, and measuring the intensity of light received by the detector, the transmitted intensity can be obtained as a function of wavelength. The intensity of detected light would decrease due to the excitation of electrons through the absorption of photons as discussed previously and due to the reflection of light at the air semiconductor boundary. The transmission coefficient, T, is given by the following equation [5]:

$$T = \frac{[(1-R)^2 e^{-\alpha x}]}{[1-R^2 e^{-2\alpha x}]}$$
 (3)

where α is the absorption coefficient, R is the reflection coefficient and x is the thickness of the semiconductor. The reflection coefficient is given as [5]:

$$R = \left[\frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \right]^2 \tag{4}$$

where n is the real component and k is the imaginary component of the refractive index of the semiconducting material. However, because near the band edge the imaginary component of the refractive index is negligible, the reflection coefficient can be approximated as [5]:

$$R \approx \left\lceil \frac{(n-1)}{(n+1)} \right\rceil^2 \tag{5}$$

For a direct band gap semiconductor, the absorption coefficient, α is given by the following equation [5]:

$$\alpha = A(E - E_g)^{1/2} \tag{6}$$

where E is the energy of the photon and E_g is the energy of the band gap. As mentioned previously, in order for excitation for an electron to occur for materials with indirect band gaps, there must be an interaction with phonons. This means that when the semiconductor is absorbing light, it must also absorb a phonon. Due to factors such as impurities within the crystal and temperature variation, the absorption coefficient will exponentially increase near the absorption edge. This results in the following relationship [5]:

$$\alpha = Be^{E/E_0} \tag{7}$$

where E is the energy of the photon and E_0 is the Urbach slope. Equation 6 shows that the x intercept for a graph of α against E would result in the direct band gap energy value.

For an indirect band gap semiconductor, the absorption coefficient α is given by the following equation [5]:

$$\alpha = \alpha_a + \alpha_e \tag{8}$$

where α_a is the absorption coefficient due to the absorption of a phonon and α_e is the absorption coefficient due to the emission of a phonon. When the energy of the photon is greater than the difference between the gap and phonon energies, absorption of a phonon occurs whereas when the energy of the photon is greater than the sum of the gap and phonon energies, a phonon is emitted. Both of these values can be represented by the following equations [5]:

$$\alpha_a = C(E - E_g + E_p)^2 \tag{9}$$

$$\alpha_e = D(E - E_g - E_p)^2 \tag{10}$$

where the constants C and D are dependent on the properties of the material. Equation 9 shows that E_g-E_p would be the x intercept of the plot for the root of the absorption coefficient $(\alpha^{1/2})$ against photon energy (E) for low photon energies. Furthermore, equation 10 shows that E_g+E_p would be the x intercept of the plot for the root of the absorption coefficient $(\alpha_e^{1/2})$ against photon energy (E) for low photon energies.

3 Experimental method

In order to determine the value for the direct band gap for gallium arsenide and the indirect band gap for gallium phosphide, the absorption and transmission coefficients for each semiconductor needed to be determined for a range of wavelengths. This was done through the use of the experimental set up shown in Figure 1.

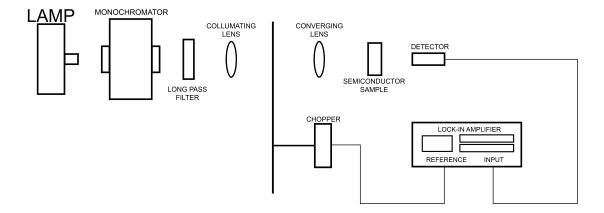


Figure 1: A diagram which shows the experimental setup for this experiment.

In order to determine these values, the intensity of light at varying wavelengths needed to be measured first. The light emitted from the tungsten-halogen lamp was shone through a monochromator allowing for the variation of its wavelength. The emerging light beam was then shone through a long pass filter to reduce noise, then through a collimating lens to ensure that only the beams travelling in parallel were allowed through. The resulting beam was passed through a chopper operating at 1109Hz to further reduce the noise and thus improve the signal-to-noise ratio. The light beam was then shone through a converging lens to focus the beam and into the detector. This process was repeated but with the semiconducting sample in between the converging lens and detector. Through utilising lock-in detection, the intensity of light received at the detector was converted into corresponding voltages. Lock-in amplifiers operate by comparing the input signal to a reference signal. A specific component of the input signal at a specific frequency and phase is 'focused on' and essentially rejects noise signals at other frequencies [6]. Data acquisition and processing was automated through the use of MATLAB. 3 programs were used: the first one functioned as shown by figure 2 and was used to collect detector readings.

This program firstly asked for an initial and final wavelength to inputted. It then cleared the session to erase any DAQ data from preliminary tests. It then created a new session with one analog input channel. The sampling rate was set to 2 with a duration dependent on the difference in the initial and final wavelengths. For Gallium Arsenide, a wavelength range of 800nm to 1000nm was used. For Gallium Phosphide, a wavelength range of 400 to 600nm was used. The program utilises a callback function to control the monochromator which operated as shown in figure 3. The program would then record wavelengths and voltage values which corresponded to specific light intensities. The second and third programs functioned as shown by figure 4 and was used to process and manipulate the data in order to determine the required

results.

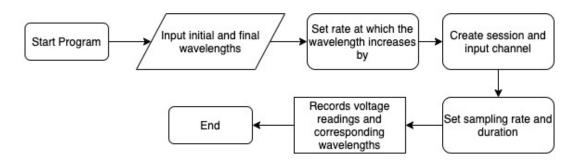


Figure 2: A flow chart which represents the functionality of the data acquisition program.

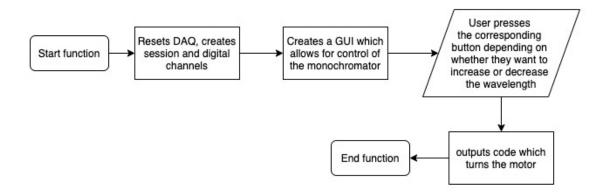


Figure 3: A flow chart which represents the functionality of the callback function.

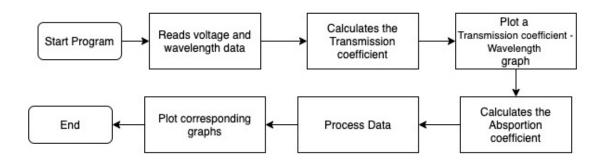


Figure 4: A flow chart which represents the functionality of the data processing programs.

The program calculated the transmission coefficient, T, using the following equation:

$$T = \frac{|V|}{|V_0|} \tag{11}$$

where V is the voltage detected when the sample is present and V_0 is the voltage detected when the sample is not present. The values for reflection, R, were calculated using equation 5 and was approximated to be constant since the range of wavelengths used was small. For values for R calculated for Gallium Arsenide and Gallium Phosphide were 0.25 and 0.32 respectively. The program used these values to calculate the absorption coefficient, α , using a rearranged version of equation 3.

The way in which the data processing programs processed the information depended on what semiconductor was used. In order to acquire the value for the direct band gap for Gallium Arsenide, a graph of Absorption squared against Photon Energy was plotted. The linear section of the graph was extrapolated and the value for the direct band gap was determined by finding the value of E when $\alpha^2=0$, i.e. the x intercept. In order to acquire the value for the indirect band gap for Gallium Phosphide, a graph of $\alpha^{1/2}$ against Photon Energy was plotted. The linear region located at the low energy values was then extrapolated and the x intercept and therefore the difference between the energy of the band gap and energy of the phonon (E_g-E_p) was determined. This is because at low energy values, $\alpha^{1/2}=\alpha_a^{1/2}$. This value was then subtracted from all values of alpha and was plotted against energy. This resulted in α_e values. A graph of $\alpha_e^{1/2}$ was plotted against Photon Energy and the linear region located at high energy values was extrapolated. The x intercept of this graph was determined. This value is equal to the sum of the energy of the band gap and the energy of the phonon (E_g+E_p) . The value for the indirect band gap was calculated by averaging both x intercepts.

Error was propagated using known propagation rules such as adding error in quadrature. Furthermore, since I had utilised MATLAB for my data acquisition, through the use of the 'cftool' function, error on figures were outputted and were used to calculate errors on the values for the direct and indirect band gaps for Gallium Arsenide and Gallium Phosphide respectively. The errors outputted by MATLAB where to a 95% confidence but these values were manipulated to calculate one standard deviation.

4 Results

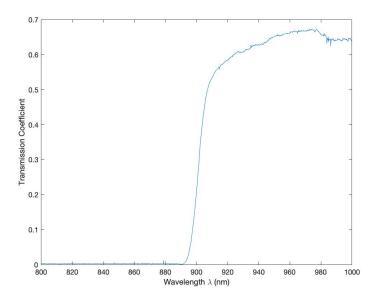


Figure 5: Transmission Coefficient against Wavelength for Gallium Arsenide.

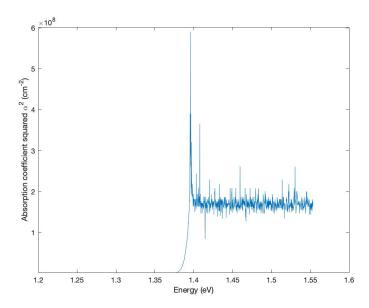


Figure 6: Absorption Coefficient squared (α^2) against Photon Energy for Gallium Arsenide.

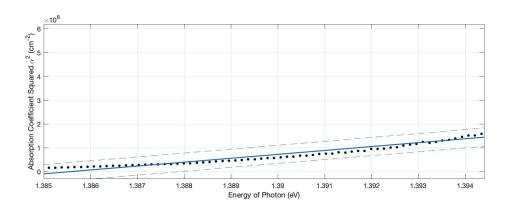


Figure 7: Absorption Coefficient squared (α^2) against Photon Energy for Gallium Arsenide for low photon energies.

Using figure 7, the x intercept and therefore the direct band gap energy for Gallium Arsenide was determined to be $(1.4\pm0.1)~\rm eV$

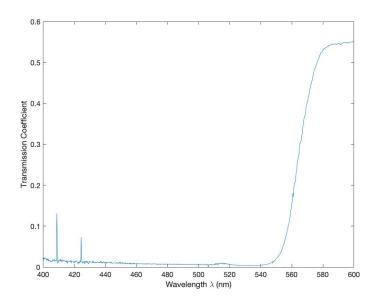


Figure 8: Transmission Coefficient against Wavelength for Gallium Phosphide.

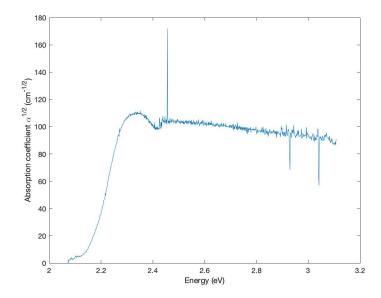


Figure 9: The square root of the Absorption Coefficient ($\alpha^{1/2}$) against Photon Energy for Gallium Phosphide.

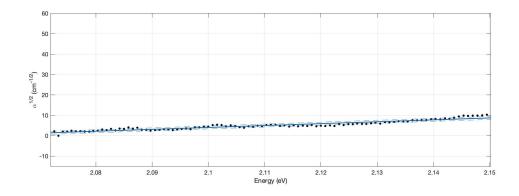


Figure 10: The square root of the Absorption Coefficient ($\alpha^{1/2}$) against Photon Energy for Gallium Phosphide for low photon energies.

Using figure 10, the x intercept and therefore the value for E_g-E_p was determined to be (2.1 ± 0.1) eV. This value was subtracted from all Absorption coefficient values resulting in α_e values. This was then square rooted and plotted against Photon Energy to produce the following figure:

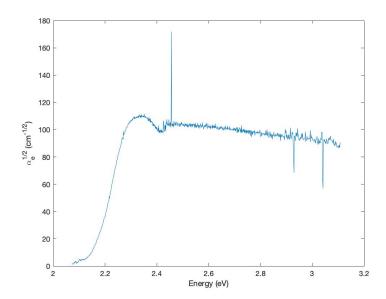


Figure 11: The square root of the Absorption Coefficient due to the emission of a phonon $(\alpha_e^{1/2})$ against Photon Energy for Gallium Phosphide.

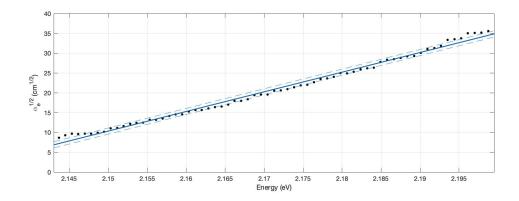


Figure 12: The square root of the Absorption Coefficient due to the emission of a phonon $(\alpha_e^{1/2})$ against Photon Energy for Gallium Phosphide for low energies.

Using figure 12, the x intercept and therefore the value of E_g+E_p was determined to be (2.1 ± 0.1) eV. This value and the value determined in figure 10 were averaged resulting in a value of (2.1 ± 0.2) eV which is the value for the indirect band gap for Gallium Phosphide.

5 Discussion of Results

The known value for the direct band gap of Gallium Arsenide is known to be $1.4~{\rm eV}$ and that for the indirect band gap of Gallium Phosphide is known to be $2.3~{\rm eV}$ [7]. I determined these values to be $(1.4\pm0.1)~{\rm eV}$ and $(2.1\pm0.2)~{\rm eV}$ respectively. Since the expected values fall within the uncertainty range of my empirical values, it's fair to assume that my obtained values are

accurate. The calculated errors for each value are small in comparison to their corresponding values meaning that they are somewhat precise.

There was random error on the transmission (T) values which was dependent on the error on the voltage values V and V_0 . The error on these voltage values were dependent on the precision of the detector and lock-in amplifier set up. Error also could've arose due to insufficiently aligning the apparatus. Furthermore, another possible source of random error could be due to background light interfering with the results. The apparatus used for this experiment was very sensitive so if not done in a dark room, results can be rendered inaccurate. This was controlled by ensuring that the lights for the room were off for the entirety of the experiment. The error on the transmission values were propagated through into absorption values.

As seen in figures 6 and 9, there are peaks at approximately $1.4~{\rm eV}$ and $2.5~{\rm eV}$ respectively. This was due to interference in the room as a desk lamp was turned on during the experiment. Luckily, the lamp was turned on after the point at which the absorption coefficients started to exponentially increase so this did not affect our results negatively.

There was systematic error in the voltage readings for Gallium Phosphide since some of the calculated values for the absorption coefficient were negative. This was accounted for by adding the absolute value for the lowest value absorption coefficient to each absorption coefficient value.

In order to determine the direct and indirect band gaps for Gallium Arsenide and Gallium Phosphide respectively, I determined the x intercepts for each corresponding absorption vs energy graph. The error on the x intercept was determined through the use of the 'cftool' function. Through utilising this function, I was able to focus on the low energy regions where the results are linear, and use a y = mx + c' fitting model to create an equation. The 'cftool' function outputted the 2 standard deviation error on the gradient, m, and the y intercept, 'c' and these were used to calculate the 1 standard deviation errors and therefore the error on the x intercept.

For this experiment, it was assumed that the refractive index was constant and that the imaginary component was negligible for the entirety of the experiment. In reality, as the experiment was conducted, the refractive index would change due to temperature changes. Another issue with the way in which I conducted my experiment was that I used manually selected the linear region to extrapolate to determine the x intercepts. This adds a degree of ambiguity to my results due to human error since I chose the region to use. If this experiment were to be repeated, it may be favourable to design some kind of program to automate this process and provide a more accurate and possibly a more precise result.

6 Conclusions

To conclude, after conducting this experiment, I deduced the direct band gap energy value of Gallium Arsenide to be (1.4 ± 0.1) eV and the indirect band gap energy value of Gallium Phosphide to be (2.1 ± 0.2) eV. I expected these values to be 1.4eV and 2.3eV [7]. Since my expected values fall within the uncertainty range of my empirical values, it's fair to say that my results were accurate. Furthermore, since the error on each value is small in comparison

to the actual value, my empirical values are precise.

References

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A MATLAB code for Callback Function

```
function opticalthing
daq.reset
clear, close all
s = daq.createSession('ni'); % Creates the session object
s.addDigitalChannel('Dev1','Port0/Line0:7','OutputOnly');
% Adds 8 digital output channels (numbered 0:7) on the DAQ card
% create the uicontrols
onoff = uicontrol('Style','togglebutton','String','go',...
'Position',[20 200 70 40],'Callback',@move_buggy);
forwards = uicontrol('Style', 'pushbutton', 'String', 'forwards',...
'Position', [20 150 70 40], 'Callback', @go_forward);
backwards = uicontrol('Style', 'pushbutton', 'String', 'backwards',...
'Position', [20 100 70 40], 'Callback', @go_backward);
nout = [51 102 204 153]; % decimal sequence for forward motion
% This is the callback function for the toggle button.
% It moves the buggy when the toggle button is pressed.
% 'hObject' is the handle for the uicontrol calling the function.
```

```
function move_buggy(hObject,eventdata)
while hObject.Value == hObject.Max
for n=1:4
output_data=dec2binvec(nout(n),8);
% high state=1 low state=0
outputSingleScan(s,output_data);
\% outputs the data in output_data to the device
pause(1.6) % use this to change the speed of the motor
end
end
end
% These are the callbacks for the pushbuttons.
% They set the direction of travel for the motors.
function go_forward(hObject,eventdata)
nout = [51 102 204 153];
end
function go_backward(hObject,eventdata)
nout = [153 204 102 51];
end
end
```

B MATLAB code for Data acquisition

```
startw = input('Enter starting wavelength: ');
deend = input('Desired final wavelength: ');
r = 11/62; % this is the rate of wavelegth change with time for GaAs
% r = 29.5/66; this is the rate of wavelength change with time for GaP
opticalthing
% configure analog input channel AIO on the NI DAQ card
s1 = daq.createSession('ni');
s1.addAnalogInputChannel('Dev1',0,'Voltage');
% Set the sampling rate and the number of samples to be
% collected per trigger
s1.Rate = 2; s1.DurationInSeconds = (deend-startw)/r;
% get the data collected by channel AIO
pause(3);
disp('Ready!')
[Voltage,time] = startForeground(s1);
wavelength = (time .* r) + startw;
figure(2)
plot(wavelength ,Voltage)
title('Data sampled from signal generator')
xlabel('Wavelength(nm)')
```

```
ylabel('Voltage(volts)')
```

C MATLAB code for Data processing for Gallium Arsenide

```
R = 0.25; %refractive index of GaAs
x = 0.417e-3; %thickness of GaAs sample
T = abs(V1)./abs(V0);
figure(1);
plot(wavelength,T);
xlabel('Wavelength \lambda (nm)')
ylabel('Transmission Coefficient')
alpha = -(x.^{(-1)}).*log(((sqrt((1 - R).^4 + 4.*(T.^2).*(R.^2)) - ...
    (1 - R).^2))./(2.*T.*(R.^2)));
h = 6.63e-34; %plancks constant
c = 3.0e8; %speed of light
E = (h.*c./(wavelength.*10.^-9))./1.6e-19;
E = E.;
alphasqr = alpha.^2;
figure(2);
plot(E,alphasqr);
xlabel('Energy (eV)')
ylabel('Absorption coefficient squared \alpha^{2} (cm^{-2})')
```

D MATLAB code for Data processing for Gallium Phosphide

```
E = E.';

xlabel('Wavelength \lambda (nm)')
ylabel('Transmission Coefficient')

alphasqrt = sqrt(alpha);
figure(2);
plot(E,alphasqrt);
xlabel('Energy (eV)')
ylabel('Absorption coefficient \alpha^{1/2} (cm^{-1/2})')

alphae = abs(alpha - (191.5/93.11));
figure(3);
sqrtae = sqrt(alphae);
plot(E,sqrtae);
xlabel('Energy (eV)')
ylabel('\alpha_e^{1/2} (cm^{-1/2})')
```