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UNIVERSITY OF NOTTINGHAM

FORMAL REPORT

INVESTIGATION B

# Optical Absorption in Semiconductors

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# Contents

**Abstract**

*The electrical conductivity of a semiconductor is strongly dependent on its ability to absorb heat or light. This paper investigates optical absorption in semiconductors and describes an experiment to measure the band gap energy $(E_g)$ and the Urbach energy $(E_0)$ and slope of GaAs, a direct band gap semiconductor and the band gap energy and phonon energy $(E_p)$ of GaP, an indirect band gap semiconductor. In the experiment a lock-in amplifier was used in conjunction with MATLAB to automate the measuring of the transmission data for the respective wavelength around the semiconductors' band edge. The results for the band gap were found to be $1.38 \pm 0.05eV$ and $2.10 \pm 0.19eV$ for GaAs and GaP respectively. The phonon energy was found to be $0.05 \pm 0.01eV$ for GaP and the Urbach energy was $(6.9 \pm 0.03) \times 10^{-3} eV$ for GaAs. These results are consistent with published values.*

# 1   Introduction

The first mention of a semiconductor was by Alexandro Volta (1745 - 1827), the Italian scientist famous for the invention of the electric battery.[1] He observed that "the surface of these bodies does not contract any electricity, or if any electricity adheres to them, it vanishes soon, on account of their semi-conducting nature".[2] However, it was Michael Faraday (1791 - 1867) who in 1833 first documented a material which is now known as a semiconductor, when he found that the conductivity of silver sulphide increased with increasing temperature.[3]

Neither of these scientists had the conceptual understanding to know the real reasons behind these phenomena. Now, with modern physics, we know that increasing the temperature of semiconductors leads to the generation of free carriers, both electrons and holes, which leads to an increase in electrical conductivity. This increase in electrical conductivity is triggered by the movement of electrons from a lower energy level (the valence band) to a higher energy level (the conduction band). This difference in energy levels $(E_g)$ is known as the band gap. The band gap varies between materials, but there is a common pattern. Metals have little to no band gap, or even an overlap of bands. Insulators have an exceptionally large gap, typically greater than 3eV, meaning they do not conduct electricity. Semi-conductors sit in the middle ground, with a gap of $0 < E_g < 3eV$ and do not conduct well under normal conditions. However, a little energy (whether heat or light) is enough for electrons to start to be promoted and therefore for electrical conductivity to increase.[4] This dictates the thermal and electrical properties of the material. Analysing the absorption spectrum therefore tells us about key properties of the semiconductor.

A semiconductor diode was first used in a primitive radio receiver in 1904.[5] Now the use of semiconductors is synonymous with electronics and the importance of semiconductors and the effect that they have had upon on our society cannot be understated. The first transistor made from semiconducting material was demonstrated on December 23, 1947 at Bell Laboratories.[6] The transistor was a much more elegant solution for use in electronics compared to the vacuum tube it replaced, which was larger and used more power. Individually, the elements germanium and silicon played a crucial role in the making of transistors, but silicon has become the preferred choice because it can be used at higher temperatures. Indeed, silicon has played such a fundamental role that it gave its name to Silicon Valley.[7] Semiconductors now play a key role in everyday life from LEDs in televisions, to solar cells and most importantly to integrated circuits where billions of transistors are bundled together for use in computers. Such is their prevalence that the semiconductor industry is reportedly worth more than $480,000,000,000.[8]

## 2   Theory

In free space, electrons can have an almost continuous spectrum of energies. When confined in an atom, however, as a result of quantum mechanics, they can have only a discrete set of energies. Because atoms in a solid are packed closely together, these energy levels get smeared out into bands, as shown in Figure 1.[9]
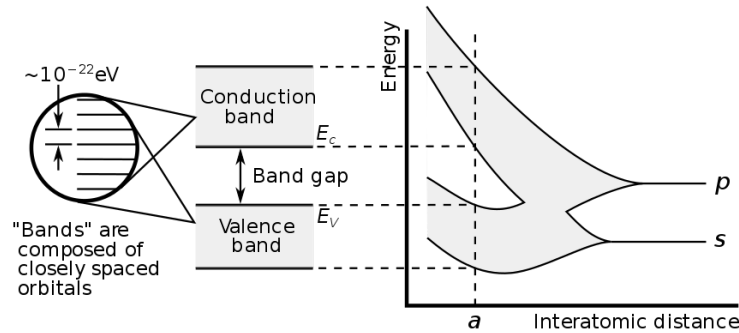


**Figure 1:** Illustration of the smearing of the energy levels into bands within a solid[21]

The band structure is unique to the material; different materials will have a different set of band structures as the electrons will have a different set of allowed energies. There are also regions in which no electrons can reside, as they are forbidden to have the corresponding energy.[10] These forbidden energy bands, of which there are many, exist because only certain values are allowed solutions to the wave equations.[11] The two highest energy bands within a material, which are the bands of interest in this experiment, are the valence band and the conduction band. The valence band is where the electrons with the highest energy within the orbital reside while still being bound to the atom. The conduction band in semiconductors contains electrons which have gained enough energy to allow them to escape from the valence band. These electrons have been stripped from the atom and are therefore allowed to flow freely through the lattice of the material.[9] Whilst semiconductors have a forbidden region between the highest level of the valence band and the lowest level of the conduction band (the band gap) it is small enough that excitations from a thermal or other energy source can enable electrons to bridge it.

The Fermi level, $E_F$, describes the highest energy level which can be reached by an electron, at absolute zero, 0K. At this temperature, no electron has enough energy to be promoted above it. The Fermi level lies in various places depending on the material. The Fermi level of a perfect semiconductor will lie close to the middle of the band gap between the valence and the conduction bands, as illustrated in Figure 2. However, as is normally the case, impurities within the semiconducting material cause the Fermi level to be shifted. This is especially prominent in doped semiconductors.

The Fermi level is closely related to the Fermi function, which gives the probability that a given available electron energy state will be occupied at a given temperature;[12]
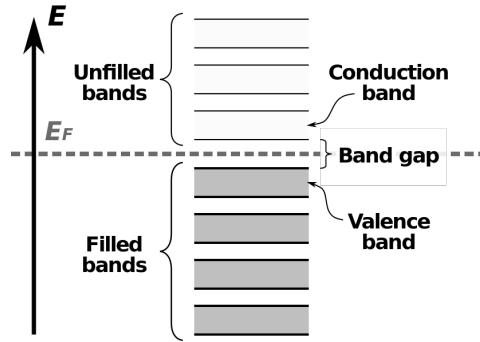
**Figure 2:** Illustration showing the relationship between bands and the Fermi level, $E_F$ [20]

$$\frac{1}{e^{\frac{\epsilon_i - \mu}{k_B T}} + 1} \tag{1}$$

where $\epsilon_i$ is the energy of a single state $i$, $\mu$ is the total chemical potential, $k_B$ is Boltzmann's constant and $T$ is the absolute temperature.

The Fermi equation dictates that at normal temperatures, most of the levels up to the Fermi level are filled, with only a few electrons having energies above that level. The higher the temperature, the greater the number of electrons which exist above the Fermi level, as shown in Figure 3. While the Fermi function has a finite value within band gaps, there are no electrons populating these regions. This is because the population is dependent not only on the Fermi function but also the density of states (which is zero in forbidden regions). At high temperatures, both the Fermi function and density of states have discrete values in the conduction band and therefore there is a finite population of electrons in that band. In contrast, at absolute zero, there are many available states but the Fermi function is zero for the conduction band which therefore has no population of electrons. [13]
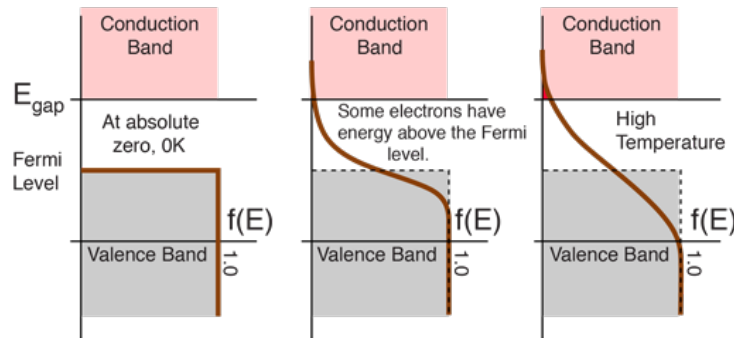


**Figure 3:** Illustration of Fermi probabilities at different temperatures [12]

Absorption is expressed in terms of a coefficient $\alpha$ which is defined as the relative rate of decrease in light intensity L(hv) along its propagation path, [19] and can be represented by

$$\alpha = \frac{1}{L(hv)} \frac{dL(hv)}{dx} \tag{2}$$

In its simplest form, absorption occurs when a photon is absorbed by an electron which causes the excitation of that electron from the valence to the conduction band as shown in Figure 4.
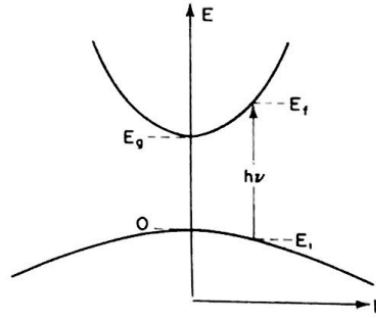


**Figure 4:** Illustrates a transition from $E_i$ to $E_f$ across the band gap triggered by the absorption by an electron of a photon of energy $hv$[19]

The initial and final states of the electrons can therefore be linked by the equation

$$E_f = hv - |E_i| \tag{3}$$

where $E_f$ is the energy of the final state, $hv$ is the energy of a photon and $E_i$ is the energy of the initial state. In order for the photon to excite the electron sufficiently, the minimum energy required is equal to the band gap $(E_g)$ of the semiconductor. It follows that optical absorption will have a threshold, above which there is a near continuous range of transitions.

It is important to note that not all photons are absorbed. This will be dependent on the photon's energy, the thickness of the material and the type of semiconductor. When the photon reaches the semiconducting material, it may be reflected by the surface, pass right throough the material or be absorbed by it. Its fate is dependent upon its energy. If $E_{photon} < E_g$, (the band gap energy), the photon does not have enough energy to promote the electron into the conduction band and if it is not reflected the photon passes through the material, meaning it is transparent in that region. When $E_{photon} \geqslant E_g$, the photon may have enough energy to be absorbed by and promote an electron to create an electron hole pair. When the photon's energy is greater than the band gap and the photon gets absorbed it may have extra energy beyond that needed to promote the electron to the conduction level.[14] This extra energy is initially absorbed by the electron, and then emitted back in the form of phonons into the lattice of the material. Such a process is called thermalisation and, as the name suggests, produces heat.[15]

Band gaps are of two basic types: direct band gaps and indirect band gaps. In both types, the promotion of an electron must obey the fundamental laws of conservation of momentum and energy.[19] The momentum $(p)$ of sub-atomic particles is given by

$$p = \frac{hc}{\lambda} \tag{4}$$

where $h$ is Planck's constant, $c$ is the speed of light and $\lambda$ is the wavelength. The wavelength of electrons in a crystal lattice is of the same order of magnitude as the distance between atoms, whereas the wavelength of visible light is about three orders of magnitude greater.[17] It follows from equation (4) that the momentum of a photon is about three orders of magnitude less than that of an electron and therefore that the absorption of a photon by an electron has no appreciable effect on the momentum of the electron. Where the absorption of such a photon is sufficient, by itself, to promote the electron to the conduction band, the energy gap is a direct band gap. In an indirect band gap semiconductor, a change in energy is not sufficient to promote an electron to the conduction band. That also requires a change in momentum. Such changes in momentum are caused by the absorption or emission of a phonon as illustrated in Figure 5.
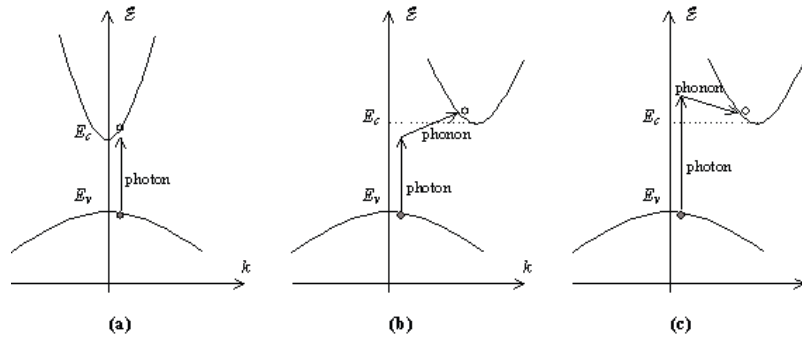


**Figure 5:** Illustrates transition mechanisms for (a) photon only – direct (b) phonon absorption – indirect (c) phonon emission – indirect[16]

It is well known that the probability of a process involving a number of particles decreases with the increasing number of particles taking part in it. A direct band gap transition is an efficient process involving only two particles; an electron and a photon, and the absorption coefficient is typically high; $\alpha \approx 10^4 - 10^5 \ cm^{-1}$. For indirect band gaps, there is a three-particle process involving an extra phonon. The process is therefore less likely to occur within a given time period and the absorption coefficient is around $10^3 \ cm^{-1}$.[18] Accordingly, light absorption in indirect semiconductors near the absorption edge occurs less intensely compared to direct band gap semiconductors.[19]

The momentum of a free charge carrier is given by the equation $p = mv = \hbar k$ and its kinetic energy $E = \frac{1}{2}mv^2$. Substituting $p$ yields

$$E = \frac{p^2}{2m^*} = \frac{\hbar^2 k^2}{2m^*} \tag{5}$$

where $m^*$ is the effective mass, in this case of an electron, $m_e^*$ or a hole, $m_h^*$ and $k$ is the wave vector. To simplify the mathematics, the assumption is made that the shape of the valence and conduction bands is parabolic. For direct promotions equations (3) and (5) can be combined to relate the momentum to the band gap giving,

$$E_f - E_g = \frac{\hbar^2 k^2}{2m_e^*} \tag{6}$$

and

$$E_i = \frac{\hbar^2 k^2}{2m_h^*} \tag{7}$$

Combining equations (3), (6) and (7) yields

$$hv - E_g = \frac{\hbar^2 k^2}{2}\left[\frac{1}{m_e^*} + \frac{1}{m_h^*}\right] = \frac{\hbar^2 k^2}{2}\left[\frac{1}{m_r^*}\right] \tag{8}$$

where $m_r$ is the reduced mass. When combined with the density of states (the derivation of which is given in [20]) this gives

$$N(hv)d(hv) = \frac{8\pi k^2 dk}{(2\pi)^3} = \frac{(2m_r)^{\frac{3}{2}}}{2\pi^2\hbar^3}(hv - E_g)^{\frac{1}{2}}d(hv) \tag{9}$$

The absorption coefficient for direct allowed transitions can then be expressed as (where $A^*$ is a constant);

$$\alpha(hv) = A^*(hv - E_g)^{\frac{1}{2}} \tag{10}$$

Momentum conserving transitions between parabolic bands should result in an absorption edge which obeys (10), ie the absorption coefficient increases with the square root of the photon energy in excess of the gap energy. For direct transitions (10) predicts no absorption below the energy gap and then a steeply rising absorption edge. In practice, as shown in Figure 6, experimental results show an exponentially increasing absorption edge. This is because the valence and conduction bands are not actually parabolic but have a tail which extends into the energy gap as shown in Figure 7. In this region the absorption coefficient does not adhere to the absorption coefficient relationship as shown in (10). Instead it is given by Urbach's rule.[26]

$$\alpha = \alpha_0 e^{\frac{hv}{E_0}} \tag{11}$$

where $\alpha_0$ is a constant and $E_0$ is the Urbach energy. Put simply this equation tells us the structural disorder of the material at its band edges which interferes with the absorption in the material, the differences of which are shown in Figure 6. Equation (11) is equivalent to

$$\ln(\alpha) = \ln(\alpha_0) + \frac{hv}{E_0} \tag{12}$$

from which it is apparent that a plot of $\ln(\alpha)$ vs $hv$ yields a straight line, in which the reciprocal of the gradient is the Urbach slope.

When a transition requires both a change in energy and momentum, a two-step process is required as a photon cannot provide the change in momentum. A phonon is needed to conserve momentum, which is a quantum vibration of the lattice. Although a broad range of values are available, only a select few phonons have the correct momentum to make them usable. To complete a transition in an indirect band gap a phonon has to be either emitted or absorbed. As such the respective processes are given by

$$hv_e = E_f - E_i \pm E_p \tag{13}$$
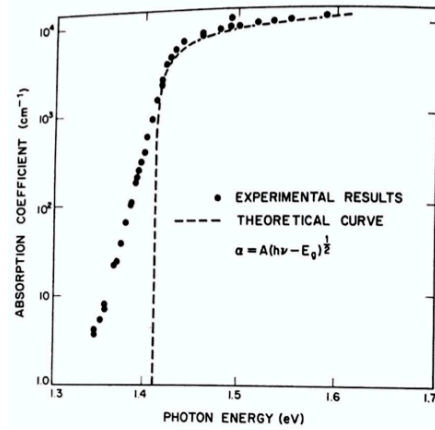
**Figure 6:** Shows experimental vs theoretical model for $\alpha$ against energy
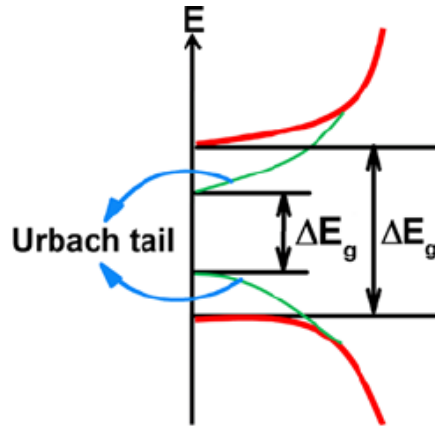


**Figure 7:** Shows how the Urbach tail affects the band structure

where $E_p$ is the energy of the phonon. In indirect transitions, all occupied states of the valence band can be connected to all the empty states of the conduction band. The density of initial states at an energy $E_i$ is[19]

$$N(E_i) = \frac{(2m_h)^{\frac{3}{2}}}{2\pi^2\hbar^3}|E_i|^{\frac{1}{2}} \tag{14}$$

The density of the final state is[19]

$$N(E_f) = \frac{(2m_h)^{\frac{3}{2}}}{2\pi^2\hbar^3}(E_f - E_g)^{\frac{1}{2}} \tag{15}$$

Substitution yields

$$N(E_f) = \frac{(2m_h)^{\frac{3}{2}}}{2\pi^2\hbar^3}(hv - E_g + E_i \pm E_p)^{\frac{1}{2}} \tag{16}$$

The absorption coefficient is proportional to the product of the densities of the initial state given by $N(E_i)$ and the final state given by $N(E_f)$ integrated over all the possible combinations

of states separated by $hv \pm E_p$. $\alpha$ is also proportional to the probability of interacting with phonons, which is itself a function which is given by Bose-Einstein statistics.[27] After some integration, the mathematics of which are not relevant but are shown in [20], the absorption co-efficient for a transition with phonon absorption for $hv > E_g - E_p$ can be shown to be
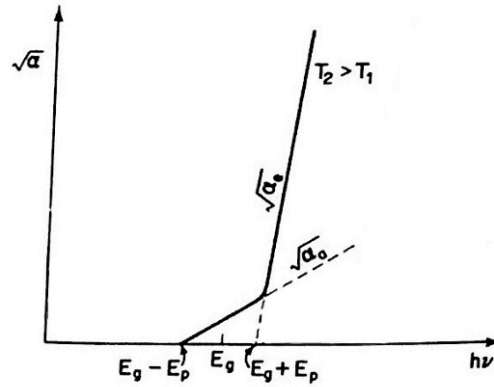
$$\alpha_a(hv) = \frac{A(hv - E_g + E_p)^2}{e^{\frac{E_p}{kT}} - 1} \tag{17}$$

And the absorption coefficient for a transition with phonon emission for $hv > E_g + E_p$ as

$$\alpha_e(hv) = \frac{A(hv - E_g - E_p)^2}{1 - e^{-\frac{E_p}{kT}}} \tag{18}$$

Since both phonon absorption and emission are possible when $hv > E_g + E_p$, the absorption coefficient is

$$\alpha(hv) = \alpha_a(hv) + \alpha_e(hv) \tag{19}$$



**Figure 8:** Shows the dependence of $\alpha_a$ and $\alpha_e$ on energy and the intercepts of the respective plots[19]

At low energies ($hv > Eg - Ep$) the absorption of phonons is solely responsible for the absorption coefficient. It follows that at such energies a graph of $\alpha^{\frac{1}{2}}$ vs energy should yield a straight line, the x intercept of which is $E_g - E_p$.

The value of $\alpha_e$ can be obtained from equation (19). By plotting $\alpha_e^{\frac{1}{2}}$ vs energy, the straight line section for high energies ($hv > Eg + Ep$) yields the value of $E_g + E_p$.

A semiconductor's optical absorption coefficient $\alpha$ can be calculated from its optical transmission data. The transmission coefficient $T$ is defined as the ratio of transmitted to incident power,

$$T \equiv \frac{I}{I_0} \tag{20}$$

If the specimen has thickness x, an absorption $\alpha$ and a reflectivity R, the radiation passing through the first boundary is $(1-R)I_0$ and the radiation reaching the second boundary is $(1-R)I_0e^{-\alpha x}$. It follows that $(1-R)^2 I_0 e^{-\alpha x}$ emerges on the other side of the material. Accounting

for further multiple internal reflections, it can be shown that the overall transmission is then given by the fraction

$$T = \frac{(1-R)^2 e^{-\alpha x}}{1 - R^2 e^{-2\alpha x}} \tag{21}$$

The refractive index is complex and may be expressed as

$$\bar{n} = n + ik \tag{22}$$

In the case of non-absorbing media, the expressions for R and T are real and, for the normal incidence of an interface between media of indices $n_1$ and $n_2$ can be expressed as:

$$R = \frac{(n_2 - n_1)^2}{(n_2 + n_1)^2} \tag{23}$$

For a case which is a reflection normal to the conducting surface, as in our experiment, where the first medium with air is $n = 1$ , and the second medium $\bar{n} = n + ik$, the equation for the reflectivity coefficient above is valid and according to the equations (22) and (23) gives:

$$R = \frac{(n - ik - 1)^2}{(n - ik + 1)^2} = \frac{(n - 1)^2 + k^2}{(n + 1)^2 + k^2} \tag{24}$$

The extinction coefficient k, is defined as

$$k = \frac{\lambda \alpha}{4\pi} \tag{25}$$

Where $\alpha$ is the absorption coefficient, and $\lambda$ is the wavelength. This gives a value for k of $k \leqslant \frac{10^{-2}}{4\pi}$ in the range of $\lambda$ and $\alpha$ used in this experiment. As k is therefore very small compared to n $\approx$ 3.0 for GaAs and GaP, (24) can be simplified to

$$R = \left(\frac{n-1}{n+1}\right)^2 \tag{26}$$

The optical reflection coefficient R can be determined from the transparent region of the sample where $\alpha = 0$. Therefore in this region equation (21) becomes

$$T = \frac{1-R}{1+R} \tag{27}$$

which can be simplified to make R the subject so that

$$R = \frac{1-T}{1+T} \tag{28}$$

It can be shown that rearranging (21) for $\alpha$ yields

$$\alpha = -\frac{\ln\left(\frac{((1-R)^4 + 4T^2 R^2)^{\frac{1}{2}} - (1-R)^2}{2TR^2}\right)}{x} \tag{29}$$

Hence if R and T can be determined experimentally, $\alpha$ can be found.

# 3  Experimental method

The experimental setup to determine the band gaps of GaAs and GaP is illustrated in Figure 9. A tungsten light source was used in conjunction with a monochromator to supply a light source of a single known wavelength. The monochromator was connected to a computer via an LED card. The computer ran a MATLAB m-file which, when connected with the step motor on the monochromator, allowed the wavelength to be changed automatically at specified steps. This was then passed through a long-pass filter, to ensure that ultraviolet and blue light was blocked from getting through. A chopper was also used in tandem which was connected to a lock-amplifier. The frequency of the chopper was set to a four-digit prime number, and in this case to 1109Hz. The chopper is used to improve the signal to noise ratio by preventing harmonics from forming which could affect the experiment. The chopper must be placed correctly to ensure that its blades obstruct the beam. A silicon photo-detector circuit, which received the light and produced a voltage, was placed at the end, and was also connected to the computer so that the results could be automated. The positions of the apparatus were recorded and maintained throughout the whole experiment to avoid fluctuations which could result in unwanted error.
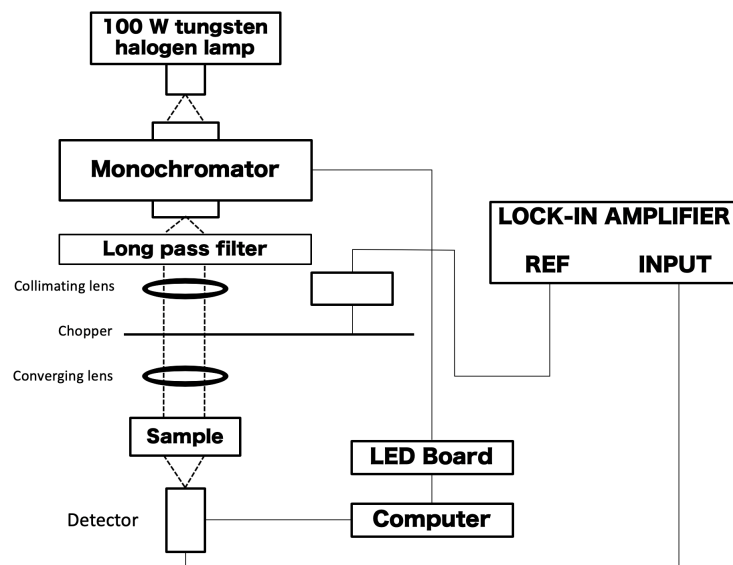


**Figure 9:** Shows experimental set-up for measuring the band gap

Although similar, there were some significant differences between the two experimental setups for GaAs and GaP. For the GaAs system, a 1200-line grating blazed at 800nm was used. This design enhanced the infrared around that wavelength. The monochromator had a resolution of 1nm, on which there was a long pass filter which blocked wavelength less than 560nm which ensured that ultraviolet and blue light from the 2nd order did not overlap with the infrared part of the first order diffraction. The reason for this setup is because the working range for this system is 800-1000 nm with an expected slope at around 890nm. In the GaP system, a lower grade monochromator was used with a resolution of about 5nm and a 300 or 600 line grating. A less intense and cooler lamp was also used so that little to no ultraviolet was produced. This was because this system was designed to operate in the visible range of

around 400-750nm, the data range in this experiment being in the 450-600 nm range, with a slope expected at around 560nm. Prior to starting the experiment, the apparatus was aligned by centring the light beam on the photodiode surface; this ensured that the highest intensity achievable reached the detector.

A key piece of equipment was the lock-in amplifier, which was locked to the chopper. To set up the equipment correctly, at the start of every equipment change, the phase was adjusted to yield zero signal when then the $90°$ button was pressed in, which yielded the maximum signal. The use of a lock-in amplifier in conjunction with a chopper is of paramount importance. This setup reduces the signal to noise ratio dramatically by ensuring that the desired signal is acquired from a myriad of noise from sources such as dark current and stray (ambient) light, which reduced the need for completely dark conditions. The signal wanted was often several orders of magnitude smaller than the noise. The lock-in amplifier overcomes the problem of the signal to noise ratio "by modulating the input signal by a reference signal omega r (created by a light chopper and a laser, in our case), and upon signal detection, measuring only the voltage input modulated by omega r".[22] The LED and photodetector were positioned on the bottom of the chopper, which converted the square wave into sinusoidal form. The signal was then multiplied by the reference signal and integrated over time as any discrepancy between the signal frequency and the reference frequency will result in a net value of zero once integrated. This is because the noise produced by the detector is a broad spectrum and spread, meaning the noise at the frequency of the measurement is low. Therefore, the detector noise is reduced drastically, as the measurement is confined to a single frequency. The result is that the noise can be reduced by three magnitudes or more.[23]

This explanation does not do justice to the intricacies of the lock-in amplifier nor the mathematics, further details of which can be found at [24]. Other than the phase, the time constant (associated with the low-pass filter) was the only other parameter that was adjusted. Choosing the correct time constant is imperative for reliable and accurate results. Having the time constant too low will result in the lock-in amplifier responding very quickly to real changes in the voltage of the input signal; however, the reading is not sufficiently stable to acquire a proper measurement. Conversely, if too high a time constant is used, the lock-in amplifier may take many times the time constant to respond to real changes in the input signal. If there are regions of interest, such as in this experiment, if the time constant is too long, the regions of interest could be missed or identified too late resulting in incorrect values. Therefore, it is important to have a balance between these two extremes. By running some preliminary tests we found that a time constant of 300 ms struck a good balance.[22]

A key aspect of the experiment was the MATLAB code, the flow chart of which is shown on page 14. This was written so that the wavelength of the stepper motor could be incrementally changed automatically. The script also automated the measurement of light transmission. The user inputted an initial starting value for the wavelength. Then a UI window prompted the user to start the motor for the wavelength. Once the desired wavelength is reached the user must stop the motor and record the wavelength reached when prompted on MATLAB. The wavelength can then be plotted against the light intensity in MATLAB, the variable was automatically saved for data analysis to obtain a value for $\alpha$. Generally, three time constants should be allowed between moving and measuring, so given a time constant the speed of the motor should be correspondingly adjusted in the MATLAB m-file.

The experiment was set up in such a way that in conjunction with the MATLAB m-file, the ratio of the incident and transmitted light intensity $\frac{I_0}{I}$ ws obtained. This is equivalent to the ratio $\frac{V}{V_0}$ being the voltages with and without the sample. For a given wavelength $\lambda$, there is a given $V_0$ which was measured when the sample was removed. The sample was then placed in front of the photo-diode detector and the intensity transmitted through it measured. As only a rough range of wavelengths is needed to start off with, the motor is run at a higher speed, to check the range. The ranges were found to be 800-1000 nm and 400-600 nm for GaAs and GaP respectively, which was the expected range. Once the rough range is known the motor speed can be decreased. Although this takes far longer, the range is much narrower and enables more accurate results to be obtained. Values of $V$ and $V_0$ were then obtained over the specified ranges. Only one set of data was recorded each for the direct and indirect band gap samples. From the values of $V$ and $V_0$ obtained, the transmission coefficient $T$ was calculated by using equation (20). This allowed a graph of transmission coefficient against wavelength to be plotted for both the GaAs and GaP samples.

The values for T within the transparent region, around 980nm for GaAs and 580 for GaP, were averaged out. These were inserted into equation (28) to obtain values of R. These values were compared with the approximate theoretical values for R, using equation (26).

With both the values for T, R and x obtained a value of $\alpha$ could now be calculated using equation (29), which yielded a value for $\alpha$ at each wavelength in the range of T. The optical energy, E, was then plotted against $\alpha$ using
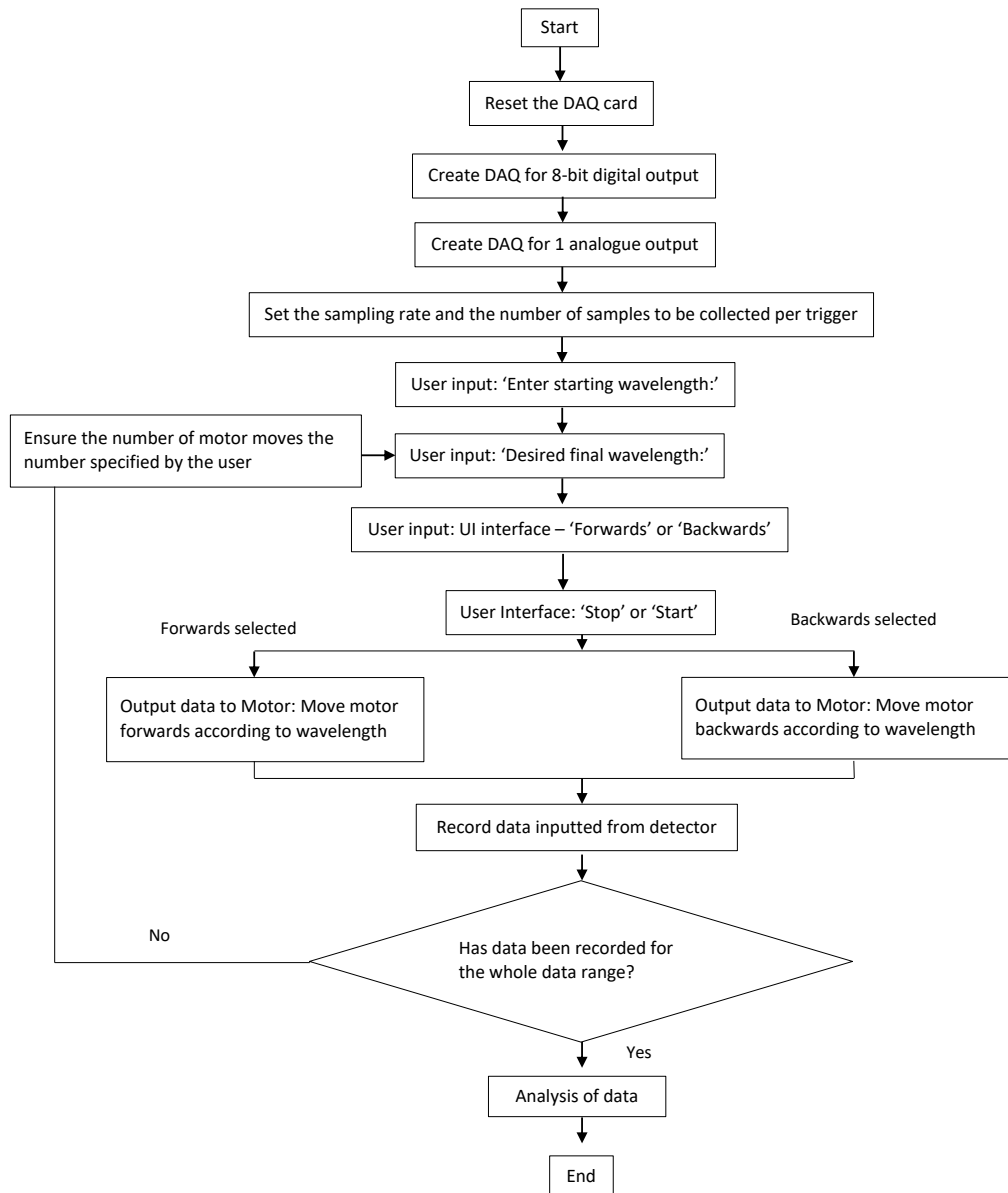
$$E = \frac{hc}{\lambda} \tag{30}$$

to obtain the desired results.

Armed with the values of $\alpha$, graphs of $\alpha^2$, $\alpha^{\frac{1}{2}}$ and $\alpha_e^{\frac{1}{2}}$ against optical energy were plotted and analysed to find values for the band gap. A graph of $\ln(\alpha)$ against $E$ was also plotted and analysed to find the Urbach slope for GaAs.

The analysis for the GaAs sample is simplest as it has a direct band gap. As $\alpha^{\frac{1}{2}}$ is proportional to E a graph of $\alpha^2$ vs energy should yield a straight-line graph for the energy region of interest. The band gap Eg can then be determined as the x intercept of this line. A graph of $\ln(\alpha)$ against $E$ was also plotted for the GaAs sample and using the inverse of the gradient, the Urbach slope $E_0$ can be calculated by virtue of equation (12).

In the case of GaP, the analysis is more complex as it is an indirect band gap semiconductor. Two lines of best fit are required in the relevant portions of a graph of $\alpha^{\frac{1}{2}}$ against optical energy to obtain values for $E_g \pm E_p$. The dependence on $\alpha^{\frac{1}{2}}$ is plotted because in an indirect band gap semiconductor $\alpha$ is dependent on the square of the optical energy. From the low energy region of interest of $\alpha^{\frac{1}{2}}$ vs optical energy, the line of best fit yields $E_g - E_p$. From the straight line section of a graph of $(\alpha - \alpha_a)^{\frac{1}{2}}$ against optical enegy, the line of best fit yields $E_g + E_p$. These two simultaneous equations can then be solved to found both the band gap, $E_g$, and the energy of the phonon, $E_p$.

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                                         ▼
                          ┌──────────────────────────────┐
                          │ Create DAQ for 1 analogue output │
                          └──────────────────────────────┘
                                         │
                                         ▼
             ┌───────────────────────────────────────────────────────┐
             │ Set the sampling rate and the number of samples to be  │
             │                collected per trigger                   │
             └───────────────────────────────────────────────────────┘
                                         │
                                         ▼
                       ┌──────────────────────────────────┐
                       │ User input: 'Enter starting wavelength:' │
                       └──────────────────────────────────┘
                                         │
  ┌─────────────────────────────┐        ▼
  │ Ensure the number of motor moves the │──▶┌──────────────────────────────────┐
  │ number specified by the user │        │ User input: 'Desired final wavelength:' │
  └─────────────────────────────┘        └──────────────────────────────────┘
                                         │
                                         ▼
                  ┌──────────────────────────────────────────┐
                  │ User input: UI interface – 'Forwards' or 'Backwards' │
                  └──────────────────────────────────────────┘
                                         │
                                         ▼
                       ┌──────────────────────────────────┐
   Forwards selected   │ User Interface: 'Stop' or 'Start' │   Backwards selected
                       └──────────────────────────────────┘
```

Output data to Motor: Move motor forwards according to wavelength

Output data to Motor: Move motor backwards according to wavelength

Record data inputted from detector

No

Has data been recorded for the whole data range?

Yes

Analysis of data

End

## 4    Results

The transmission coefficient for each wavelength was calculated from the values of $V_0$ and $V_1$ using equation [20]. Figures 10 and 11 graph the transmission coefficients against wavelength for GaAs and GaP respectively. From these graphs a value of the transmission coefficient was determined from the long wavelength (low energy) portion of the graph as shown in red using MATLAB. Then using equation (28) and the average values of T calculated, experimental values for R were found. The theoretical values for R were also found from equation (26) using known values of the refractive index, n.[25] The results are shown in table 1

| Sample | Experimental R | Theoretical R | Refractive index |
|--------|----------------|---------------|------------------|
| GaAs | $0.21 \pm 0.03$ | 0.31 | 3.52 |
| GaP | $0.29 \pm 0.04$ | 0.32 | 3.59 |

**Table 1:** Displays the experimental and theoretical values of the reflection coefficient for the different samples
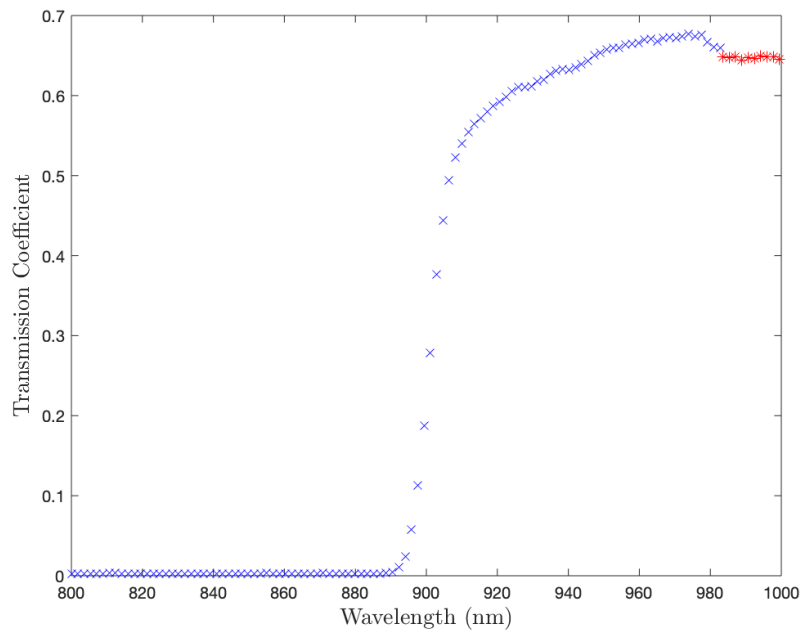


**Figure 10:** Transmission coefficient vs optical wavelength for GaAs sample

With the transmission and reflection coefficients now obtained and the thickness x of the sample being known, $\alpha$ was calculated using equation (29). Figure 12 plots $\alpha^2$ against energy in electron volts for the GaAs sample and shows a linear dependence in the region of interest. For this purpose, the theoretical value of R was used as the experimental result was not consistent with published values. A line of best fit was plotted in MATLAB which produced a value for the band gap, being the x intercept.

For the GaP sample, which is an indirect band gap semiconductor, two graphs were plotted to obtain the values of $E_g + E_p$ and $E_g - E_p$. Figure 13 plots $\alpha^{\frac{1}{2}}$ against optical energy in
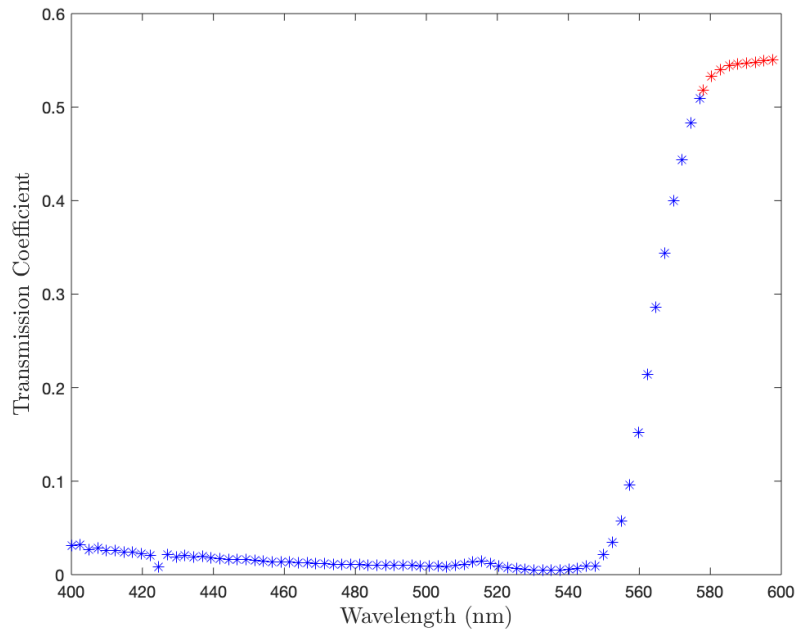
**Figure 11:** Transmission coefficient vs optical wavelength for GaP sample

| Sample | $E_g$ value | $E_p$ value |
|--------|-------------|-------------|
| GaAs | $1.38 \pm 0.05$ | $n/a$ |
| GaP | $2.10 \pm 0.19$ | $0.05 \pm 0.01$ |

**Table 2:** Displays the $E_g$ and $E_p$ value for the given sample

the low energy region and a line of best fit produced in MATLAB to yield a value for $E_g - E_p$, being the x intercept of this line. Figure 14 plots $\alpha_e^{\frac{1}{2}}$ against optical energy from which, in the high energy region, a line of best fit was produced in MATLAB to yield an x intercept to give the value $E_g + E_p$. These values were $2.0506eV$ and $2.1513eV$ respectively. These equations were solved to obtain values for $E_g$ and $E_p$, as shown in table 2.

In addition to calculating the band gap and phonon energy, for the GaAs sample only the value for the Urbach slope was calculated. The value for the Urbach curve was calculated from Figure 15, being the reciprocal of the gradient produced by MATLAB.

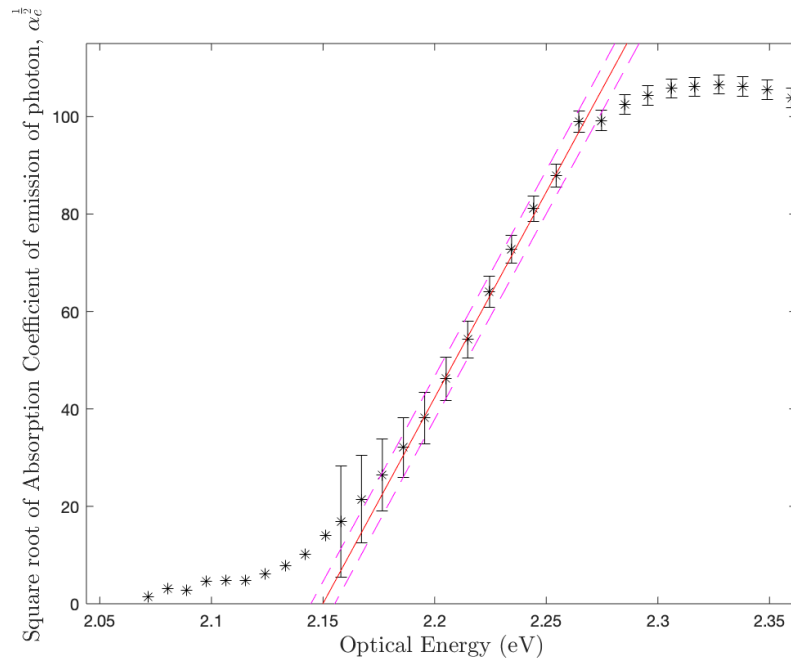| Sample | $E_0$ value |
|--------|-------------|
| GaAs | $(6.8 \pm 0.3) \times 10^{-3}$ |

**Table 3:** Displays the value for Urbach energy for GaAs
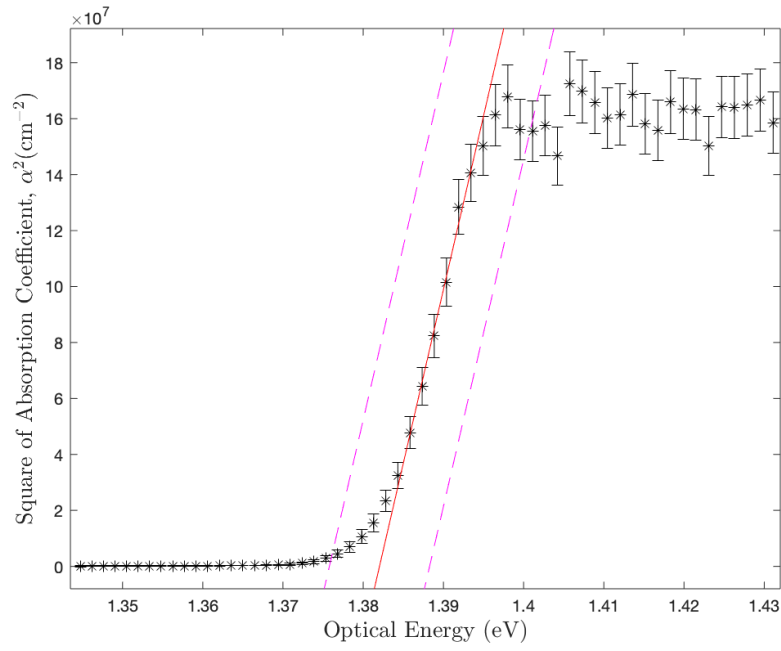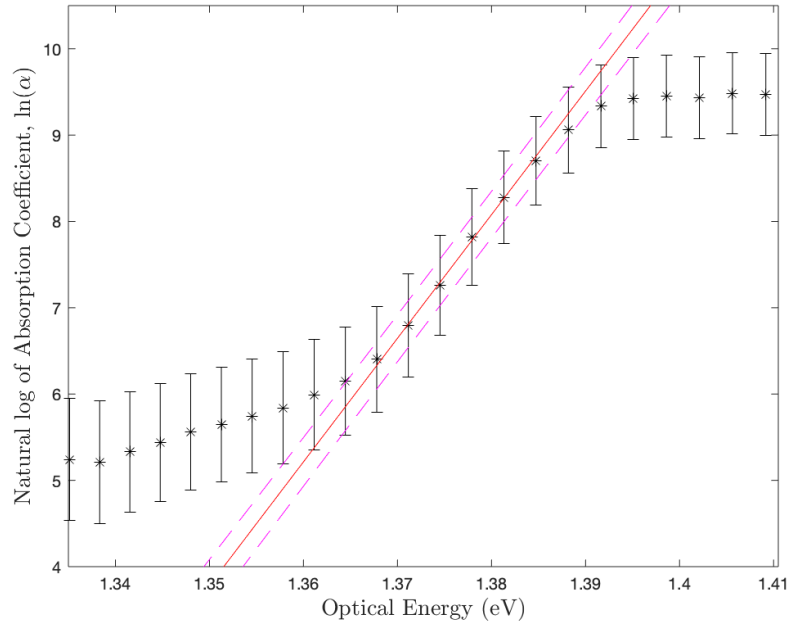
**Figure 12:** Shows the linear relation of $\alpha^2$ to optical energy for GaAs in the region of interest
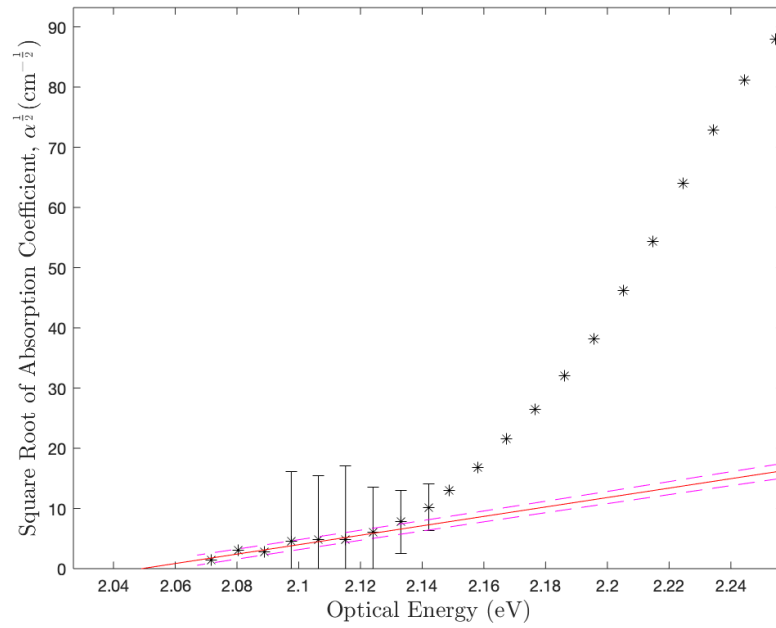


**Figure 13:** Shows the linear relation of $\alpha^{\frac{1}{2}}$ to energy in the low energy region for the GaP sample

**Figure 14:** Shows the linear relation of $(\alpha - \alpha_a)^{\frac{1}{2}}$ to energy in the region of interest for the GaP sample



**Figure 15:** Shows a plot of natural logarithm of absorption coefficient against optical energy for GaAs sample. The linear region yielding the reciprocal of the Urbach slope value

## 4.1   Analysis of uncertainties

To calculate the the error associated with the average value of $T$, which was needed to calculate the experimental value of R, the standard error was used. the standard error being given by

$$S = \frac{\sigma}{\sqrt{n}} \tag{31}$$

where S is the standard error, $\sigma$ the standard deviation (calculated by MATLAB) and n is the number of points. Where the function involves a number of variables together with their associated errors, as for $\alpha$, the individual errors need to be propagated. The error propagation equation is expressed in matrix form as:[28]

$$\sigma_f^2 = \mathbf{g}^T \mathbf{V} \mathbf{g} \tag{32}$$

in which $\sigma_f^2$ represents the variance of a function $f$ whose parameters are $\beta$, whose variance-covariance matrix is $\mathbf{V}$ with the $i$th element of the vector $\mathbf{g}$ being $\frac{\partial f}{\partial \beta_i}$. In this experiment, however, as the variables are uncorrelated, the matrix can be simplified by dropping the co-variances, simplifying the equation to

$$\sigma_f^2 = \sum \left( \frac{\partial f}{\partial \beta_i} \right)^2 \sigma_{\beta_i}^2 \tag{33}$$

which provides a simple but effective estimation of the error. Equation (33) was used for propagating the error for all elements of this experiment bar the error on T which used (31) and the error on the $x$ intercept. As T was just dependent on one variable (33) was not needed. Equation (33) is not appropriate to use to propagate the error on the $x$ intercept because any parameter $\beta$, which results from a least square fit analysis, as MATLAB did in this case with the gradient, make this equation redundant. This is because the equation (33) assumes independent, uncorrelated values. When the variables $\beta$ are correlated with each other the covariances are not negligible. As such a different error analysis needed to be done to find the error on the x-intercept.

All of the data in this experiment was fitted in MATLAB using cftool which involves using a least-square fit to find an approximate function. Note that all the graphs shown in this paper have more data points, only every 11th point was plotted to ensure the graph was easy to read. However, when conducting analysis the whole data set was used. In this experiment this produced a linear model fit to the data points in the regions of interest. The cftool produces a value for the gradient and the y intercept. It is important to note that the cftool also has a weighting and therefore takes into account the error on the measurements when calculating the gradient and other values. The coefficients produced by MATLABs cftool have 95% confidence bounds. However to find the standard error the lower ($B_{low}$) and upper ($B_{high}$) confidence bounds are used via

$$S = \frac{B_{high} - B_{low}}{2 \times 1.960} \tag{34}$$

with the factor of 1.960 being needed to bring the confidence bounds down to $68.269\%$.

As the error on the x intercept could not be calculated using (33), the error of the points around the intercept were used. These were interpolated to estimate the error on the intercept. It was assumed that the error of the points around the x intercept will be similar to that of the error itself.

# 5    Discussion of Results

The calculation of the reflection coefficient for both the GaAs and GaP sample was a relatively straightforward procedure. The values were found to be GaAs $0.21 \pm 0.03$ & GaP $0.30 \pm 0.04$ respectively compared to expected values of 0.31 for GaAs and 0.32 for GaP. The value for GaP was consistent as the error on our results means it included the experimental value. However the value for GaAs was around 33% different and therefore not consistent with the expected result. The value of R is derived from the calculation of the average value of T, the only error in which is the mean, (31), the uncertainty of the equipment having been accounted for in the line of best fit by weighting the points in MATLAB. This error on T was then propagated to obtain a value of R using (33). This does not however explain the significant difference in the value R. The value for R could potentially be wrong due to calibration error or an offset in the lock-in amplifier signal or it could be related to the sample, e.g. impurities or surface contamination. Because the source of the error was uncertain, to determine the band gap, the theoretical value of R was used instead of the experimental value.

The Urbach slope of the GaAs exponential band tail was calculated to be $(6.8 \pm 0.3) \times 10^{-3} meV$ which falls within the region stated in literature of $(5 - 7)meV$, and is therefore consistent with other experimental results.

Using the theoretical value for R, the band gap for GaAs was found to be $1.38 \pm 0.05$eV with the value in literature being 1.42eV at 300K. The results were therefore consistent with the known value for the value of the band gap. The band bap of GaP was found to be $2.1 \pm 0.2$eV experimentally, which is consistent with the value given in literature of 2.25eV. As the experiment was done with almost identical equipment the discrepancy between the errors for GaAs and GaP are due to the analysis. With the GaP sample, as the region of interest was smaller, there were less data points which therefore contributed to this higher error. Initially, to calculate the error on the x intercept, the confidence bounds of the gradient produced by MATLAB were used. However, knowing the number of points on the plot and looking at the graph it became clear that this was an overestimation. To estimate the error more accurately in this experiment the error was therefore estimated using the error of points around the x intercept. A more robust method of calculating the error on the x intercept would be to take the standard error on each point and estimate the x intercept using that data.

There are numerous factors which contribute to errors in this experiment. One potential source of error is the misalignment of the apparatus meaning the maximum intensity is not achieved. In addition there were will be an error associated with the values of the refractive index used to calculate R, the errors for which were not quoted in the literature. It is also possible that the samples that we used in this experiment had impurities which would lead to the Fermi level being closer to the valence or conduction band, affecting the band gap calculated. To improve the experiment a sample which is quoted to be very pure could be used, which should yield more accurate results.

One assumption made was that the reflection coefficient and the refractive index varied only to a small degree. However, the refractive index varied from 3.5 - 3.7 in the region recorded for GaAs. In addition, the assumption was made that the Extinction coefficient, k was 0 to make the mathematics simpler. However, as shown from the same source as the refractive index, k does have a value. Retrospectively accounting for this the new value is around 0.8% different. Both of these could have added to the error. Despite not being a big

error, it is still significant especially when error propagation is used. However, for the GaP sample the extinction coefficient does actually have a value for 0 in the region of interest so this error does not come into play. Similarly, the refractive index for GaP varies over a similar range between $3.4 - 3.6$. For both the samples the varying refractive index in the region of interest would affect the results. A potential solution to improve the experiment would be to calculate the reflection coefficient at each wavelength by using the refractive index at every point, the value of which can be found online.[25]

An error which could be introduced but not accounted for is the analysis of the graph to produce the line of best fit to find the band gap. As shown in the Figures 12, 13, 14, there are potentially multiple lines of best fit (due to the error bars) which could result in additional errors when extrapolating the results, affecting the value of the band gap obtained.

In this experiment the systematic error is considered to have a greater effect than random errors. In some experiments the systematic error has little affect as only the gradient is needed. In this experiment it plays a crucial role as the line of best was extrapolated to the intercept with the x axis; if there was any shift this would effect the results of this experiment directly. Random errors are accounted for in the error calculations so their effect is minimised. However accounting for systematic errors requires knowing what could go wrong making the analysis more complex. A possible systematic error in this experiment is that of the monochromator which was used; it only operates on a discrete scale and is therefore only accurate to one digit. It does not therefore have a high precision. As a result, the monochromator occasionally ended up being in between two values. This could be easily resolved by using a better monochromator with a higher level of precision. Another possible systematic error could be human error. As shown in the MATLAB script, the user needs to an input a wavelength. As only one reading was taken for each data set, there could possibly be human error in inputing the wrong starting or final wavelength with will result in results being shifted, affecting the x intercept of the line of best fit. A solution would be to repeat the experiment multiple times not only so that the data sets could be averaged out but also to diminish this systematic error. If a wrong wavelength wavelength was inputted it would be visible once the results are plotted as the region of interest would be in a different place.

Despite the seeming simplicity of absorption there are several possible transitions which might take place and the band structure assumed in this experiment is simplified. There are in fact multiple valleys and band gaps from which electrons from the valence can be promoted to the conduction band and, in combination with splits of bands, heavy holes and light holes, a more complex picture starts to emerge. In future experiments, accounting for these more complex ideas so the results do not conflict should enable more accurate results to be obtained.

## 6   Conclusions

Being able to determine accurately the band gap of semiconductors is important if their performance is to be optimised, eg for converting light to electrical power in solar cells. This experiment gave accurate results for the GaP sample and could therefore be used for this purpose. The values obtained for the band gap were $1.38 \pm 0.05$eV and $2.10 \pm 0.19$eV for GaAs and GaP respectively. In addition, the phonon energy for GaP was calculated to be $0.05 \pm 0.01$eV and the Urbach energy for GaAs to be $(6.8 \pm 0.03) \times 10^{-3}$eV. These results were consistent with those expected.

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## A    MATLAB Code

---

## Table of Contents

```
% Harry Spratt
% Optical absorption of semiconductors
% 24th Feburary 2020
```

## Setting Up Motor

Setting up output & input, involving automation of data

```
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 wavelenght change with time for GaP
% comment off the r value not used

Optical_Function
% calls on the function optical thing

% the following configures the analog input channel AI0 on the NI DAQ
 card
s1 = daq.createSession('ni');
% creates session object
s1.addAnalogInputChannel('Dev1',0,'Voltage');
% Adds 1 anolog input channel (numbered 0) on the DAQ card
s1.Rate = 2; s1.DurationInSeconds = (deend-startw)/r;
% Set the sampling rate and the number of samples to be collected per
 trigger

% get the data collected by channel AI0
pause(3);
disp('Ready!')
[Voltage,time] = startForeground(s1);
wavelength = (time.*r) + startw;

%plot(wavelength ,Voltage)
title('Data sampled from signal generator')
xlabel('Wavelength(nm)')
ylabel('Voltage(volts)')

% Graph above plot graph of volatge vs weavelength so the data can be
 check
```

---

1

```
% to see if its roughly correct

Error using input
Cannot call INPUT from EVALC.

Error in nonlivetest (line 6)
startw = input('Enter starting wavelength: ')
```

# Anaylsis of Direct Band Gap (GaAs)

Data and graphs relating to GaAs

```
close all; clc;

load('V0_As.mat');
load('V1_As.mat');
load('wavelength_As.mat');

% Loads data for GaAs

% This includes data for volatage without sample (V0), volatge with
 sample
% (V1). These sets are mapped against the wavelength data (wavelength)

V0_1 = smooth(V0);
% smooths V0 data
V1_1 = smooth(V1);
% smooths V0 data
V0abs = abs(V0_1);
% Takes the absolute value as the voltage input was negative
V1_1offset = max(V1_1);
% find the maximum value of V1
negV1_1 = V1_1 - V1_1offset;
% Uses the max value to corerct the offset so no negative values
V1abs = abs(negV1_1);
% Takes the absolute value as the voltage input was negative

T = V1abs./V0abs;
% Finds the Transmission values for each wavelength

meanInsideInterval = mean(T(2070:2255))
% find average transmsission value on flat region at the end of the
 graph


R = (1-meanInsideInterval)/(1+meanInsideInterval)
% Value of R found via transmission graph
R = (3.5160 - 1)^2 / (3.5160 + 1)^2
% Approximate value of R to check

x = 0.417.*10.^(-3); % error = 0.001 %actually
% thickness of sample, error = 0.001
h = 6.62607004*10^(-34) ;
% plancks constant
```

2

```matlab
c = 299792458;
% speed of light

Joules_energy = (h*c)./(wavelength.*10.^(-9));
% calculates energy in joules

eV_energy = Joules_energy./(1.602176634*10^(-19));
% converts joules to eV

alpha_GaAs = -(x.^(-1)).*log(((( 1 - R).^4 + 4.*(T.^2).*(R.^2)).^0.5 -
 (1 - R).^2)./(2.*T.*(R.^2)));
% calculate each alpha for each wavelength

offset_As = min(alpha_GaAs)
% finds alpha offset

offsetalpha = alpha_GaAs + abs(offset_As);
% correct alpha offset so no negative values

square_alpha = offsetalpha.^2;
% finds alpha squared

squarealpha = smooth(square_alpha);
% smooths values

Log_alpha_GaAs = log10(offsetalpha);
%logs alpha

plot(wavelength,V0abs)
hold on
plot(wavelength,V1abs,'r')
hold off
xlabel('Wavelength (nm)','Interpreter','latex')
ylabel('Volatage','Interpreter','latex')
% plots V1 and V0 against wavelength

plot(wavelength,T,'b')
xlabel('Wavelength (nm)','Interpreter','latex')
ylabel('Transmission Coefficient','Interpreter','latex')
% plots T against wavelength

plot(eV_energy,Log_alpha_GaAs)
xlabel('Optical Energy (eV)','Interpreter','latex')
ylabel('Logaritm of Absorption Coefficient','Interpreter','latex')
% plots log alpha vs energy

plot(eV_energy,squarealpha)
xlabel('Optical Energy (eV)','Interpreter','latex')
ylabel('Absorption Coefficient Squared','Interpreter','latex')
% plots alpha squared vs energy, the graph of interest

plot(eV_energy(1:40:end),offsetalpha(1:40:end),'*')
set(gca, 'YScale', 'log')
hold on
```

3

```matlab
plot(x,y,'r--')
hold on
plot(eV_energy(1:30:1070),offsetalpha(1:30:1070),'r--')
legend('experimental values', 'theoretical values')
% plots theroetical vs experimental values
```

## Anaylsis of Indirect Band Gap (GaP)

Data and graphs relating to GaP

```matlab
close all; clc;

load('V0_P.mat');
load('V1_P.mat');
load('wavelength_P.mat');

% Loads data for GaP

% This includes data for volatage without sample (V0), volatge with
 sample
% (V1). These sets are mapped against the wavelength data (wavelength)

V0_1 = smooth(V0);
% smooths V0 data
V1_1 = smooth(V1);
% smooths V0 data
V0abs = abs(V0_1);
% Takes the absolute value as the voltage input was negative
V1_1offset = max(V1_1);
% find the maximum value of V1
negV1_1 = V1_1 - V1_1offset;
% Uses the max value to corerct the offset so no negative values
V1abs = abs(negV1_1);
% Takes the absolute value as the voltage input was negative


T = V1abs./V0abs;
% Finds the Transmission values for each wavelength

plot(wavelength(1:11:834),T(1:11:834),'*')
hold on
plot(wavelength(834:11:895),T(834:11:895),'r*')
xlabel('Wavelength (nm)','Interpreter','latex')
ylabel('Transmission Coefficient','Interpreter','latex')
% Plots wavelength vs T to in order to find plateau region of graph

meanInsideInterval = mean(T(797:895))
% Calculates average of plateau region

R = (1-meanInsideInterval)./(1+meanInsideInterval) % calculates
 experimental R
R = (3.5860 - 1)^2 / (3.5860 + 1)^2 % Approximate value of R to check
```

4

```matlab
x = 0.408.*10.^(-3);
% thickness of sample, error = 0.001e-3
h = 6.62607004*10^(-34) ;
% plancks constant
c = 299792458;
% speed of light

Joules_energy = (h*c)./(wavelength.*10.^(-9));
% calculates energy in joules

eV_energy = Joules_energy./(1.602176634*10^(-19));
% converts joules to eV

alpha_GaP = -(x.^(-1)).*log(((((1 - R).^4 + 4.*(T.^2).*(R.^2)).^0.5
 - ...
    (1 - R).^2)./(2.*T.*(R.^2)));
% calculate each alpha for each wavelength

offset_P = min(alpha_GaP(828:895))
%finds offset of alpha

offsetalpha_P = alpha_GaP + abs(offset_P);
% correct alpha offset so no negative values

smooth_offset_alpha = smooth(offsetalpha_P);
% smooths data

sqrtalpha_P = sqrt(smooth_offset_alpha);
% takes the square root

sqrt_alpha_P = smooth(sqrtalpha_P);
% smooths data

plot(wavelength,V0abs)
hold on
plot(wavelength,V1abs,'r')
xlabel('Wavelength (nm)','Interpreter','latex')
ylabel('Voltage','Interpreter','latex')
hold off
% plots V0 and V1 against wavelength to check

plot(wavelength,T,'b')
xlabel('Wavelength (nm)','Interpreter','latex')
ylabel('Transmission Coefficient','Interpreter','latex')
% plots wavelength against transmission coefficient

plot(eV_energy,offsetalpha_P)
xlabel('Optical Energy (eV)','Interpreter','latex')
ylabel('Absorption Coefficient','Interpreter','latex')
% plots energy in ev vs alpha

plot(eV_energy,sqrt_alpha_P)
xlabel('Optical Energy (eV)','Interpreter','latex')
ylabel('Square Root of Absorption Coefficient','Interpreter','latex')
```

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```
hold on
plot(fittedmodel)
% plots energy in ev vs alpha^(0.5) with fitted line to find Eg - Ep

c = 202.2/97.96
%value of Eg - Ep

alpha_a = (eV_energy - c).^2; % alpha a over c
% calculates value of alpha a needed for alpha e


alpha_e = (smooth_offset_alpha - alpha_a).^(0.5);
% calculates value of alpha e^(0.5)


plot(eV_energy,alpha_e)
xlabel('Optical Energy (eV)','Interpreter','latex')
ylabel('Absorption Coefficient of e to the
 half','Interpreter','latex')
% plots alpha_e vs enegy to find Eg + Ep
```

## Matlab Error anaylsis

Error propagation relating to GaAs and GaP

```
%Error Anaylsis of follwing equation
```

$$\alpha = \frac{1}{x} \ln \left( \frac{((1-R)^4 + 4T^2R^2)^{0.5} - (1-R)^2}{2T^2R^2} \right)$$

```
%where b is the section within the ln
where
x = R;
y = T;
z = 0.000407;
```

$$\frac{d}{dx} = \frac{x^2 y^2 \left( \frac{\frac{8xy^2 - 4(1-x)^3}{2\sqrt{4x^2y^2+(1-x)^4}} + 2(1-x)}{2x^2y^2} - \frac{\sqrt{4x^2y^2+(1-x)^4}-(1-x)^2}{x^3y^2} \right)}{z(\sqrt{4x^2y^2+(1+x)^4}-(1-x)^2)}$$

which in plain text is

```
dx = (2.*x.^2.*y.^2.*(((8.*x.*y.^2-4.*(1-x).^3)./
(2.*sqrt(4.*x.^2.*y.^2+(1-x).^4)) +2.*(1-x))./(2.*x.^2.*y.^2)
 - (sqrt(4.*x.^2.*y.^2+(1-x).^4)-(1-x).^2)./(x.^3.*y.^2)))./
(z.*sqrt(4.*x.^2.*y.^2+(1-x).^4)-(1-x).^2);
```

$$\frac{d}{dy} = \frac{2x^2 y^2 \left( \frac{2}{y\sqrt{4x^2y^2+(1-x)^4}} - \frac{\sqrt{4x^2y^2+(1-x)^4}-(1-x)^2}{x^2y^3} \right)}{z(\sqrt{4x^2y^2+(1+x)^4}-(1-x)^2)}$$

which in plain text is

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```
dy = (2.*x.^2.*y.^2.*(((2)./(y.*sqrt(4.*x.^2.*y.^2+(1-x).^4))
 - (sqrt(4.*x.^2.*y.^2+(1-x).^4)-(1-x).^2)./(x.^2.*y.^3)))./
(z.*sqrt(4.*x.^2.*y.^2+(1-x).^4)-(1-x).^2));
```

$$\frac{d}{dx} = \frac{1}{z^2} \ln\left(\frac{((1-R)^4+4T^2R^2)^{0.5}-(1-R)^2}{2T^2R^2}\right)$$

which in plain text is

```
dz = ((1)./(z.^2)).*log((sqrt((1-R).^4+4.*T.^2.*R.^2)-(1-R).^2)./
(2.*T.^2.*R.^2));

    % Errors of respective variables

% error on voltage
errVoltage = 0.001*ones(size(V0_1));
% error on Transmission Coefficient
errT = T.*(((errVoltage./V0_1).^2+(errVoltage./V1_1).^2).^0.5);
SE = (std(T(795:895)/sqrt(5))) % check error T
% error on R
errR = 0.01;
% error on Z which is thickness
errz = 0.0001;
%error on X which is reflection coefficient
errx = errR*ones(size(V0_1));
%error on y which is transmission
erry = errT;

err_alpha = sqrt((dx.*errx).^(2)+(dy.*erry).^(2)+(dz.*errz).^(2));
% error on alpha
%err_alphasquared = 2.*err_alpha.*alpha_GaAs;
% error on alpha squared
err_alphasqrt = real((1/2).*err_alpha.*(alpha_GaP).^(-1/2));
% error on square root of alpha
```

## Plotting Error Graphs GaAs

```
load('fittedmodel_GaAs_squared.mat')

% Graph of ev_energy vs alpha squared
% Coefficients (with 95% confidence bounds):
p1 = 1.263e+10; % gradient
error_p1 = p1 - 1.228e+10;
p2 = -1.745e+10; % y intercept
error_p2 = p2 - -1.794e+10;
xintercept = -p2/p1
error_xintercept = xintercept.*sqrt((error_p1./p1).^2+(error_p2./
p2).^2)

% plotting graph of energy vs alpha squared to obtain value of bandgap
errorbar(eV_energy(1:11:end),squarealpha(1:11:end),err_alphasquared(1:11:end),err_
pbs = predint(fittedmodel_GaAs_squared,eV_energy,0.68);
hold on
plot(eV_energy,pbs,'m--')
```

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```
hold on
plot(fittedmodel_GaAs_squared)
legend('off')
xlim([1.3435 1.4320])
ylim([-8014600 192218977])
hold off

% plotting graph for urbach curve
errorbar(eV_energy(1:50:end),Log_alpha_GaAs(1:50:end),log_e_alphaerror(1:50:end),l
pbs = predint(Urbach_fit,eV_energy,0.99999999999999);
hold on
plot(eV_energy,pbs,'m--')
hold on
plot(Urbach_fit)
legend('off')
xlabel('Optical Energy (eV)','Interpreter','latex')
ylabel('Natural log of Absorption Coefficient','Interpreter','latex')
xlim([1.277 1.472])
ylim([-0.0 12.5])
hold off

p1 = 145.8 % gradient
error_p1 = 146.9 - 145.8 % error
```

# Plotting Error Graphs for GaP

```
load('fittedmodel_alpha_P.mat')
load('fittedmodel_GaP_alpha_e')
hold off

% Graph of ev_energy vs alpha sqrt
p1 = 81;
error_p1 = p1 - 75.89;
p2 = -166.1;
error_p2 = p2 -- 176.8;
xintercept = -p2/p1;
error_xintercept = xintercept.*sqrt((error_p1./p1).^2+(error_p2./
p2).^2)
errorbar(eV_energy(1:11:end),sqrt_alpha_P(1:11:end),err_alphasqrt(1:11:end),err_al
pbs_a = predint(fittedmodel_alpha_P,eV_energy,0.95);
hold on
plot(eV_energy,pbs_a,'m--')
hold on
plot(fittedmodel_alpha_P)
legend('off')
xlabel('Optical Energy (eV)','Interpreter','latex')
ylabel('Square Root of Absorption Coefficient, $\alpha
$','Interpreter','latex')
hold off

xlim([2.027 2.257])
ylim([-6.8 93.2])
```

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```matlab
% Graph of ev_energy vs alpha_e sqrt
% Coefficients (with 95% confidence bounds):
p1 = 868.3;
error_p1 = p1 - 854.3;
p2 = -1868;
error_p2 = p2 - - 1899;
xintercept = -p2/p1
error_xintercept = xintercept.*sqrt((error_p1./p1).^2+(error_p2./
p2).^2)
errorbar(eV_energy(1:11:end),alpha_e(1:11:end),err_alphasqrt(1:11:end),err_alphasq
pbs_e = predint(fittedmodel_GaP_alpha_e,eV_energy,0.95);
hold on
plot(eV_energy,pbs_e,'m--')
hold on
plot(fittedmodel_GaP_alpha_e)
legend('off')
xlabel('Optical Energy (eV)','Interpreter','latex')
ylabel('Square root of Absorption Coefficient of emission of photon, $
\alpha_e^{\frac{1}{2}}$','Interpreter','latex')
xlim([2.044 2.362])
ylim([-2 115])

bandgap = (xintercept+x_intercept)/2
% calculates band gap
phonon = (xintercept-x_intercept)/2
% calculates phonon energy
generalerr = ((error_xintercept./xintercept).^2+(error_x_intercept./
x_intercept).^2).^0.5
err_bandgap = generalerr*bandgap
% error on band gap
err_phonon = generalerr*phonon
% error on phonon energy
```

## Optical function

Code for moving motor

```matlab
Optical Function
function Optical_Function
daq.reset
clear, close all
clc;
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

% The following creates 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);
```

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```matlab
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

% options.codeToEvaluate = 'startw = 1; Publish_Trials(c)';
% options.codeToEvaluate = 'startw = 500; deend = 1000'
% options.format = 'pdf';
% publish('Publish_Trials.m', options);
```

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