

Experiment 57: Optische Eigenschaften dünner Halbleiterschichten

Table of Contents

Question 1	1
Question 2	1
Question 3	2
Question 4	3
Question 5	4
Question 6	5
Question 8	7
Question 9	8
Question 10	13
Question 11	14
Question 12	16

Table of Figures

Figure 1: Transmission Spectra of GaN, A-Si, and C-Si	3
Figure 2: Reflection Spectra of GaN, A-Si, and C-Si	4
Figure 3: Refractive Index of the Thin Film for Amorphous Silicon	5
Figure 4: Sum of Reflection and Transmission for GaN	7
Figure 5: Average Transmission for A-Si in Area of High Absorption	10
Figure 6: Average Reflection for A-Si in Area of High Absorption	10
Figure 7: Average Transmission for GaN in Area of High Absorption	11
Figure 8: Average Reflection for GaN in Area of High Absorption	11
Figure 9: Absorption Coefficient Calculated from R and T	12
Figure 10: Calculated Bandgap Energies from $\alpha = 0$	12
Figure 11: PDS Measurement	13
Figure 12: Absorption Coefficient from PDS	14
Figure 13: Absorption Coefficient of Amorphous Silicon	15
Figure 14: Absorption Coefficient of C-Si	15
Figure 15: Absorption Coefficient of GaN	16
Table 1: Calculated Bandgap Energies from the Absorption Coefficient (R and T)	9

Question 1

PDS stands for Photothermal Deflection Spectroscopy. PDS is a technique, which is very sensitive over several orders of magnitude down to regions of very weak absorption. PDS is used to calculate the absorption coefficient in areas of low absorption where information cannot be obtained from transmission and reflection measurements. In the areas of weak absorption, information about defects, and disorder can be obtained.

In PDS, two laser beams are used. One is the probe laser beam, which passes through the sample and the other is the modulated pump laser beam, which is absorbed by the sample at a given wavelength. The sample is in a weak-absorbing liquid with a strong temperature dependent refractive index. Any heating of the liquid due to light absorption of the sample results in a change of its refractive index, which leads to a deflection of the probe beam. This deviation of the probe beam can be easily detected with a position sensitive detector. The absorption coefficient is calculated from PDS by

$$\alpha = -\frac{1}{d} \ln(1 - K\Delta\phi) \quad \text{Equation 1}$$

where d is the sample thickness, $\Delta\phi$ is the deflection angle, and K is a constant depending on the experimental setup.

PDS is a very sensitive method because small deviations of the probe beam caused by absorption from the sample can be detected very accurately with a position sensitive detector.

Question 2

The advantages of PDS are we can measure regions of very weak absorption where we cannot obtain information from traditional transmission and reflection measurements. Also, information on dangling bonds and disorders can be obtained with PDS.

Question 3

The purpose of a Lock-In-Amplifier is to filter out the noise and amplify a signal with a given frequency ω and phase ϕ .

The Lock-In-Amplifier consists of an AC amplifier, a voltage controlled oscillator, a multiplier, a low-pass filter, and a DC amplifier. The AC amplifier amplifies a signal with frequency ω . Since this signal is at a frequency ω , it is not necessary to amplify other frequencies. The unwanted frequencies are eliminated by placing filters in the AC amplifier to pass only a narrow band of frequencies around the desired frequency ω .

The oscillator produces a signal proportional to $\cos(\omega t + \phi)$, and the multiplier produces an output voltage that is a product of the two voltages at its inputs, which is given by $f(t)\cos(\omega t)$. One of the input voltages is from the AC amplifier and the other input voltage is from the oscillator. The low-pass filter integrates this multiplied signal and is given by

$$c(\omega, \phi) = \frac{2}{T} \int_{-T/2}^{T/2} f(t) \cos(\omega t + \phi) dt \quad \text{Equation 2}$$

Mathematically, this integral is equivalent to the Fourier Transform. Therefore, one can imagine that the Lock-In-Amplifier is a convolution of the measured signal and a signal generated by the oscillator at a given frequency. All signals that do not have a given frequency will be averaged out to zero over time and only the desired signal will remain.

The Lock-In-Amplifier amplifies the selected frequency, which can be selected by the chopper. Now, let us assume that the voltage V is maximal and we change the phase by 90° . A signal that has a phase of 90° with respect to the reference signal will be sorted out and made zero. When we calculate this we get:

Let the phase ϕ be so that the voltage $V(t) = \int v(t) \sin(\omega t + \phi) dt$ is maximal, then

$$V'(t) = 0 = \omega \int u(t) \cos(\omega t + \phi) dt = \omega U(\phi + \pi/2) \quad \text{Equation 3}$$

If the phase is changed by 180° one obtains:

$$V(\phi + \pi) = \int u(t) \sin(\omega t + \phi) dt = -V(\phi) \quad \text{Equation 4}$$

Question 4

Figure 1: Transmission Spectra of GaN, A-Si, and C-Si

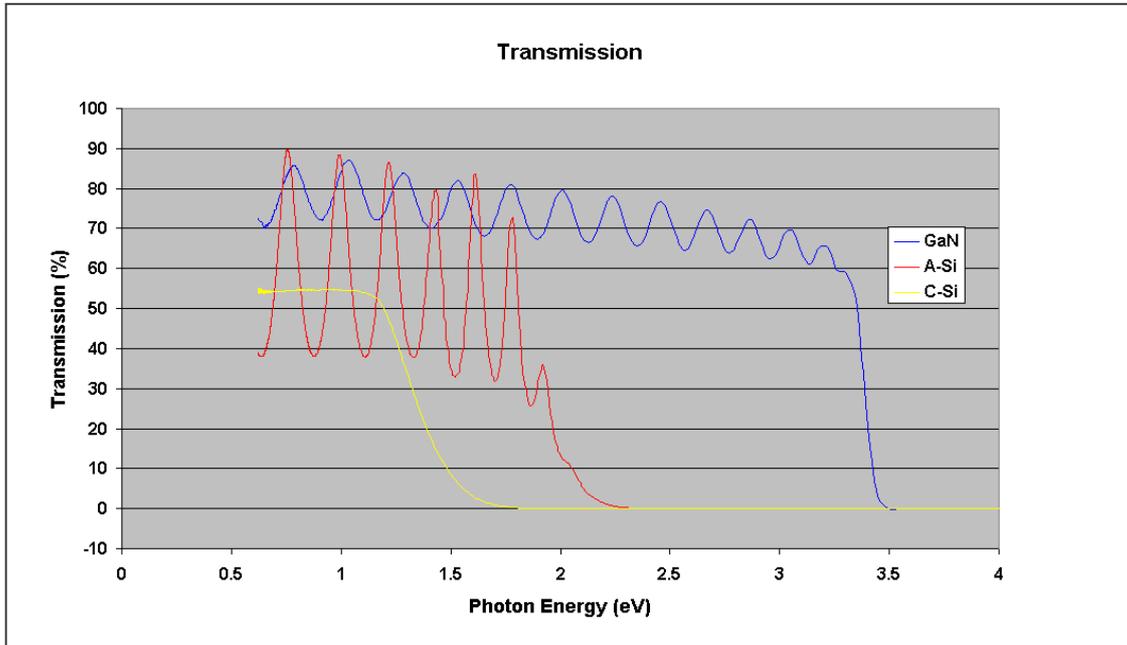


Figure 1 is a plot of the transmission spectra as a function of photon energy of all three samples. The three samples measured for transmission are GaN, A-Si, and C-Si.

The photon energy in eV is calculated by

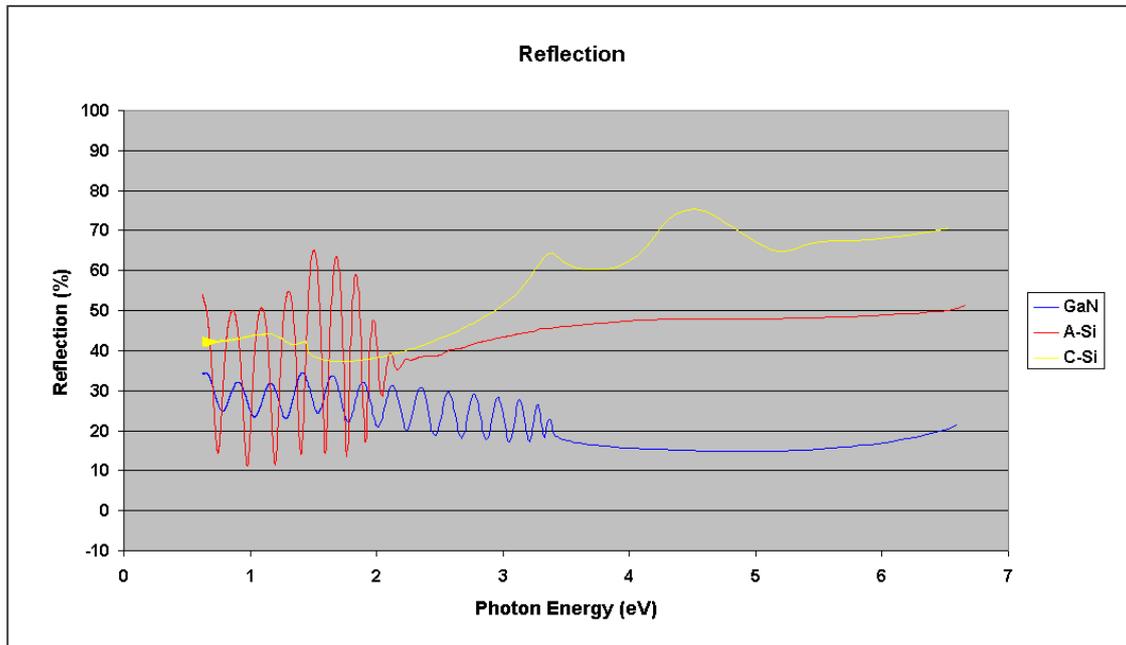
$$E[eV] = \frac{1240}{\lambda[nm]} \quad \text{Equation 5}$$

where λ is the wavelength in nm, and 1240 is a constant calculated from hc , where h is Planck's constant and c is the speed of light.

For all three samples, we see a strong drop off in the measured transmission signal at the absorption edge. The absorption edge observed is different for all three samples and is dependent on the band gap of the material. For GaN, the energy band gap is 3.4 eV and we observe no transmission signal at approximately 3.5 eV. Above the energy gap, the material exhibits high absorption. For GaN, and A-Si, we see interference effects at energies below the band gap energy. For C-Si, no interference is observed.

Question 5

Figure 2: Reflection Spectra of GaN, A-Si, and C-Si



The maxima that appears in the spectrum of C-Si is caused by direct optical transitions from the valence band to the conduction band.

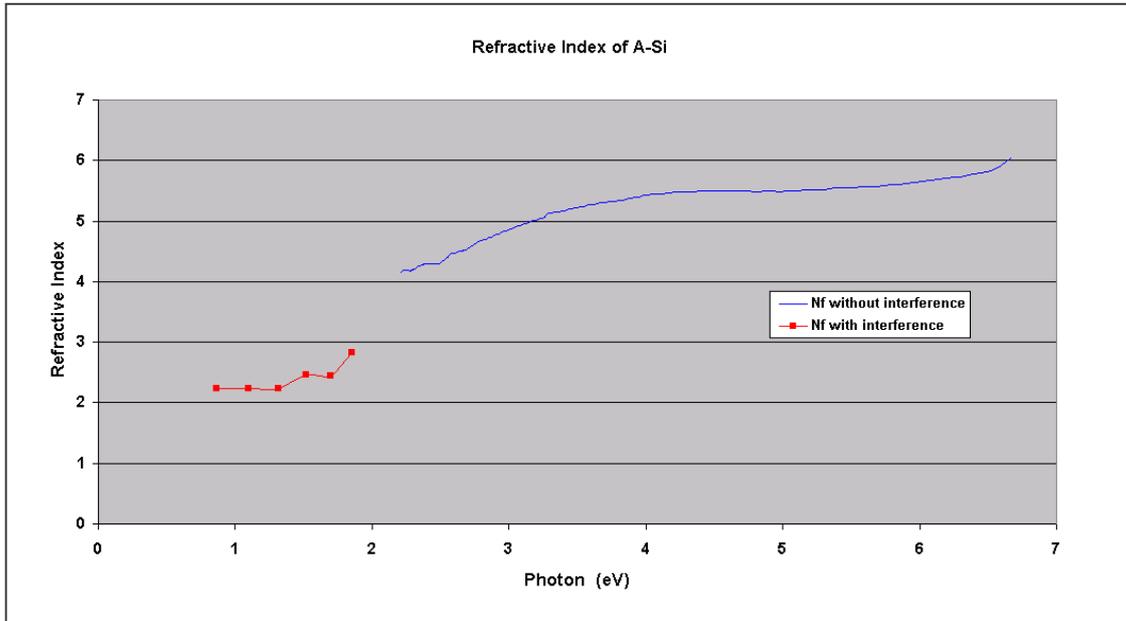
Propagation of light through a medium with a complex index of refraction can be described by an electromagnetic wave which consists of electric field and magnetic field oscillations. The real part of the oscillating waves is the propagation in space and the imaginary part is the absorption.

Reflection and transmission of electromagnetic radiation occur when a beam of light strikes an interface between two media with different indices of refraction. If the surface is smooth, then the transmitted wave and reflected wave follow the law of refraction and reflection respectively. If the surface is not smooth, then the electromagnetic (EM) wave is diffusely scattered into all directions.

In the area of low absorption below the bandgap of the material, A-Si and GaN demonstrate interference, while C-Si does not. This is due to the fact that below the bandgap of the material, there is minimal absorption. Here, the transmission and reflection spectra dominate. In the case of A-Si and GaN, the surface is not smooth. The EM wave is reflected at the first interface between air and thin film, and the transmitted wave is reflected at the second interface between the thin film and substrate. These two reflected waves clearly interfere and are observed in Figure 2 above. Above the bandgap of the thin film, interference is no longer observed. The reason C-Si does not demonstrate interference is because of the smooth surface. Therefore, there is no interference of the reflected beams from the substrate and thin film.

Question 6

Figure 3: Refractive Index of the Thin Film for Amorphous Silicon



Amorphous Silicon has a band gap energy somewhere between 1.7eV and 1.9eV. Figure 3 demonstrates the refractive index of the thin film for A-Si as a function of photon energy. As the photon energy increases, the refractive index increases. Therefore, as the absorption of the material increases for A-Si, so does the refractive index.

The blue curve is the refractive index of A-Si calculated above the band gap energy. Above the band gap, there is no interference. Here, equation 5 is valid and is used to calculate the refractive index as a function of photon energy. The Fresnel reflection coefficient is given by

$$R_f = \frac{(n_f - 1)^2}{(n_f + 1)^2} \quad \text{Equation 6}$$

where n_f is the refractive index of the thin film material.

When there is no interference, we can set the reflection spectra equal to the Fresnel reflection coefficient

$$R = R_f = \frac{(n_f - 1)^2}{(n_f + 1)^2} \quad \text{Equation 7}$$

Rearranging for the refractive index of the thin film material, we get

$$n_f = \frac{1 + \sqrt{R}}{1 - \sqrt{R}} \quad \text{Equation 8}$$

where R is taken from the reflection spectrum as a function of photon energy.

The red curve in figure 3 is the refractive index of A-Si calculated below the band gap energy. Below the band gap energy, interference of the reflected beams from the substrate and thin film are observed. In this region, we use equation 6 to equation 9 to first calculate the index of refraction of the substrate, and then the index of refraction of the thin film. The index of refraction of the substrate is given by:

$$n_s = \frac{1 - \sqrt{R}}{1 + \sqrt{R}} \quad \text{Equation 9}$$

where R is given by

$$R = \frac{1 - T_{\max}}{1 + T_{\max}} \quad \text{Equation 10}$$

where Tmax is the maximum of all maximums in the transmission spectra shown in Figure 1: Transmission Spectra of GaN, A-Si, and C-Si on page 3.

With Tmax calculated to be 89.7%, the index of refraction of the substrate was found to be $n_s = 0.622$. Substituting this value of n_s back into the following equation verifies this calculation.

$$T_{\max} = \frac{2n_s}{n_s^2 + 1} \quad \text{Equation 11}$$

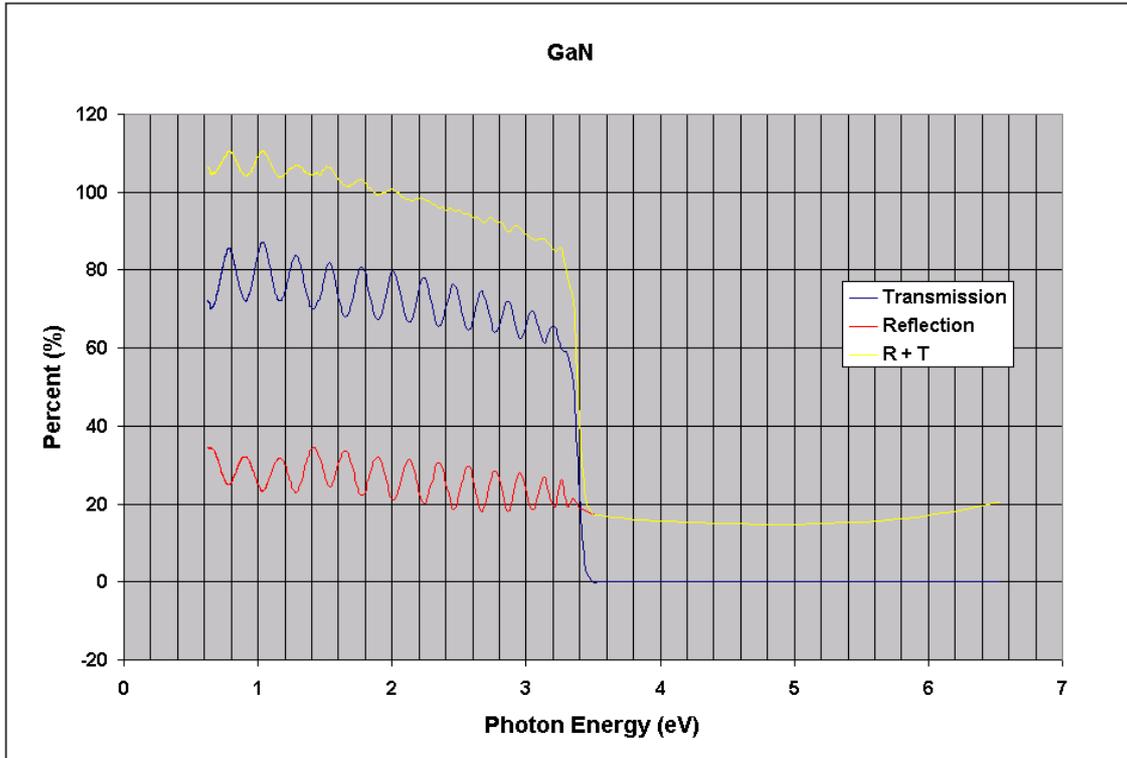
With interference, the refractive index of the thin film is given by

$$n_f = \sqrt{M + \sqrt{M^2 - n_s^2}}; \quad \text{where } M = \frac{2n_s}{T_{\min}} - \frac{n_s^2 + 1}{2} \quad \text{Equation 12}$$

T_{\min} is taken from the transmission spectra of A-Si in Figure 1 for the energy region below the energy gap. T_{\min} is then taken at each point where destructive interference occurs.

Question 8

Figure 4: Sum of Reflection and Transmission for GaN



In Figure 4 above, the yellow curve shows the summation of the transmission and reflection curves. In the area of interference, each maximum in the reflection curve corresponds to a minimum in the transmission curve and vice versa. Therefore, in the sum of both transmission and reflection, we do not see these interference phenomena.

Question 9

Figure 5 on page 10 and Figure 6 on page 10 exhibits the transmission and reflection spectra respectively for A-Si. The envelope function of the max and the min are calculated using a polynomial fit of 3rd and 4th order respectively. The average of the maximum envelope and minimum envelope for transmission and reflection are calculated by the following two equations.

$$T_{avg} = \sqrt{T_{max} T_{min}} \quad \text{Equation 13}$$

$$R_{avg} = \sqrt{R_{max} R_{min}} \quad \text{Equation 14}$$

where T_{max} and T_{min} correspond to the maximum and minimum transmission of the envelope function at the same photon energy, R_{max} and R_{min} correspond to the maximum and minimum reflection of the envelope function at the same photon energy.

Now, using the calculated averages for transmission and reflection, we can use equation 12 to calculate the absorption coefficient

$$T = (1 - R)^2 e^{-\alpha d} \quad \text{Equation 15}$$

where T is the transmission, R is the reflection at a given photon energy, α is the absorption coefficient, and d is the sample thickness

Solving for the absorption coefficient α , we get

$$\alpha = -\frac{1}{d} \ln \frac{T}{(1 - R)^2} \quad \text{Equation 16}$$

The following value of the sample thickness is used in the calculation of the absorption coefficient ($d=10^{-4}$ cm).

The absorption coefficient of GaN is calculated analogously to A-Si. The average transmission and reflection of GaN in area of high absorption is calculated in Figure 7 on page 11 and Figure 8 on page 121 respectively. The absorption coefficient of C-Si is calculated with the above equation for the absorption coefficient α , without averaging. This is due to the fact C-Si does not have the same observed interference.

The area of the transmission curve that do not give us useful values is at low photon energies below the band gap energy, which corresponds to the area of weak absorption. Here, the transmission is zero and the equation above is invalid.

Plotted in Figure 9 on page 12 are the absorption coefficients as a function of photon energy for GaN, A-Si, and C-Si. The energy gap of each sample is then calculated

according to equation one and two for direct and indirect bandgap when the absorption coefficient crosses the x-axis (i.e. $\alpha = 0$). When $\alpha = 0$, the equations of the energy bandgap for direct and indirect bandgap simplify to

$$E_g = \hbar\omega = \textit{photon energy}$$

That is, where the absorption curve crosses the x-axis for the semi logarithmic plot, this corresponds to the energy bandgap of the sample. Table 1 displays the bandgap energies for the three samples.

Table 1: Calculated Bandgap Energies from the Absorption Coefficient (R and T)

Sample	Bandgap Energy (Theory)	Bandgap Energy (Experimental)	% difference
GaN	3.4 eV	3.15 eV	7.3%
A-Si	1.7-1.9 eV	1.76 eV	2.2%
C-Si	1.11 eV	1.3 eV	4.6%

The calculation above for A-Si is for E_{04} . E_{04} for A-Si is 1.8eV. Figure 10 on page 12 shows how the intercept of the absorption coefficient with the x-axis was calculated.

Figure 5: Average Transmission for A-Si in Area of High Absorption

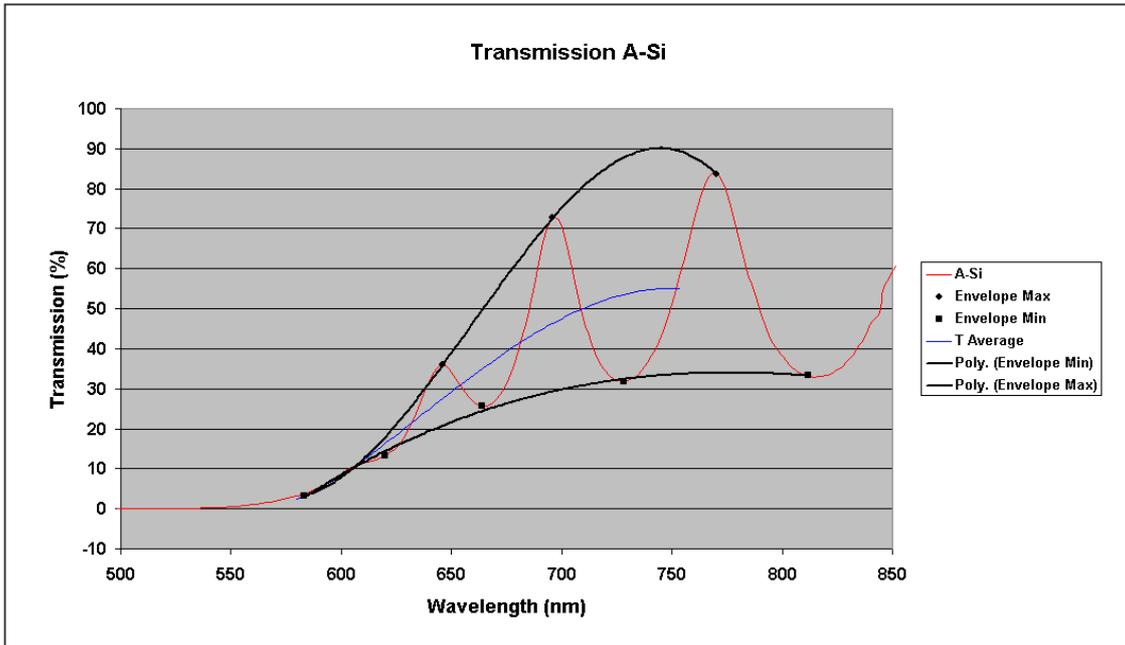


Figure 6: Average Reflection for A-Si in Area of High Absorption

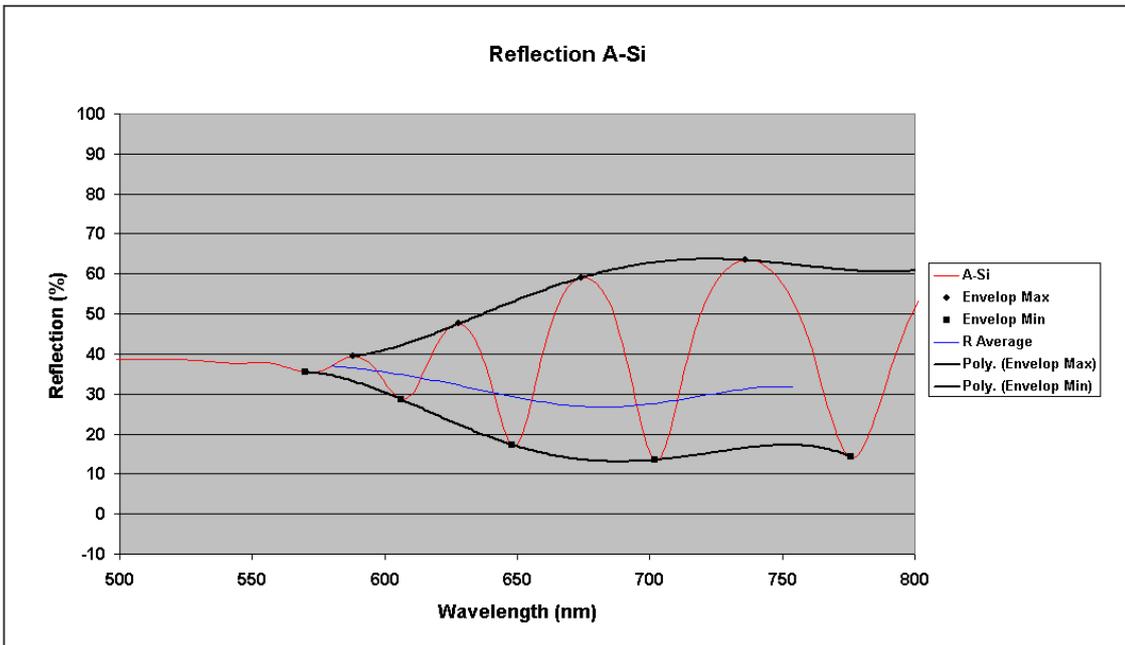


Figure 7: Average Transmission for GaN in Area of High Absorption

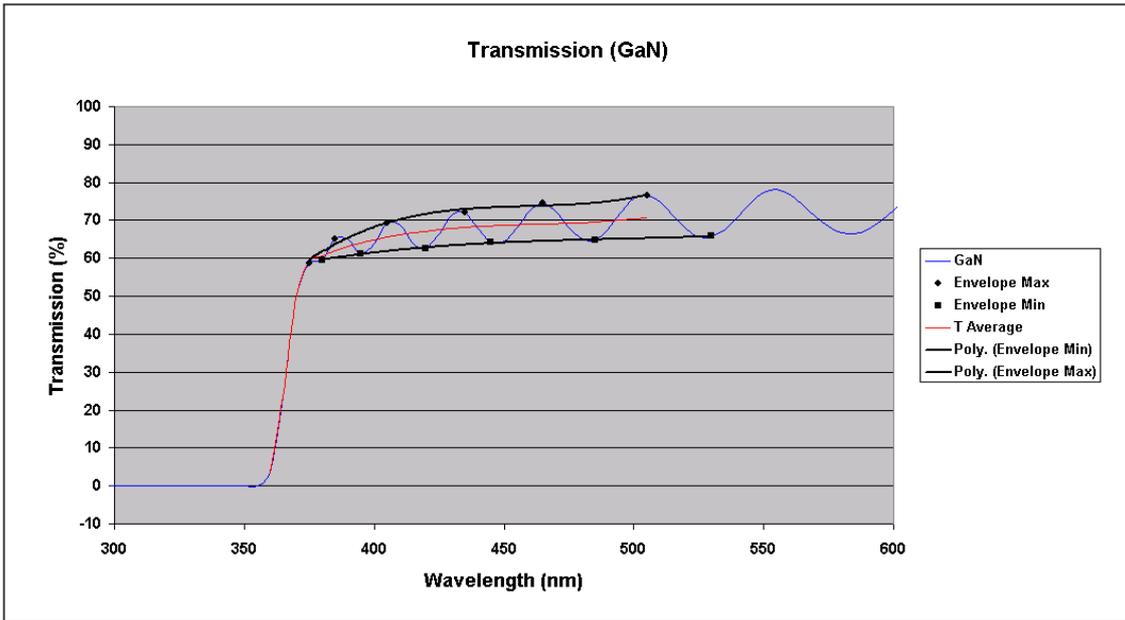


Figure 8: Average Reflection for GaN in Area of High Absorption

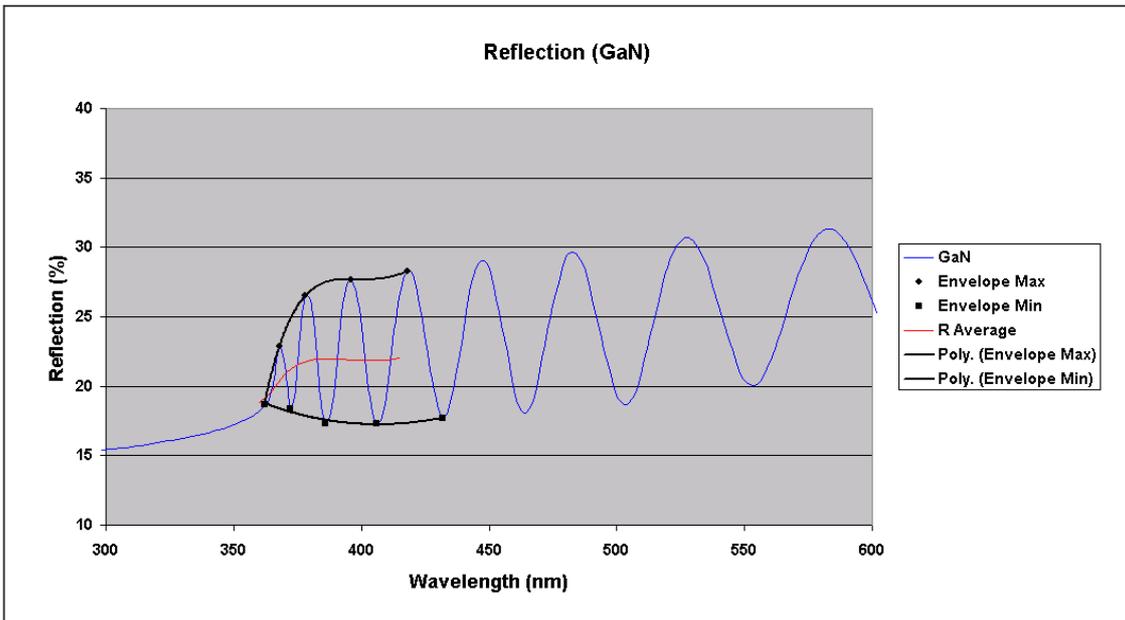


Figure 9: Absorption Coefficient Calculated from R and T

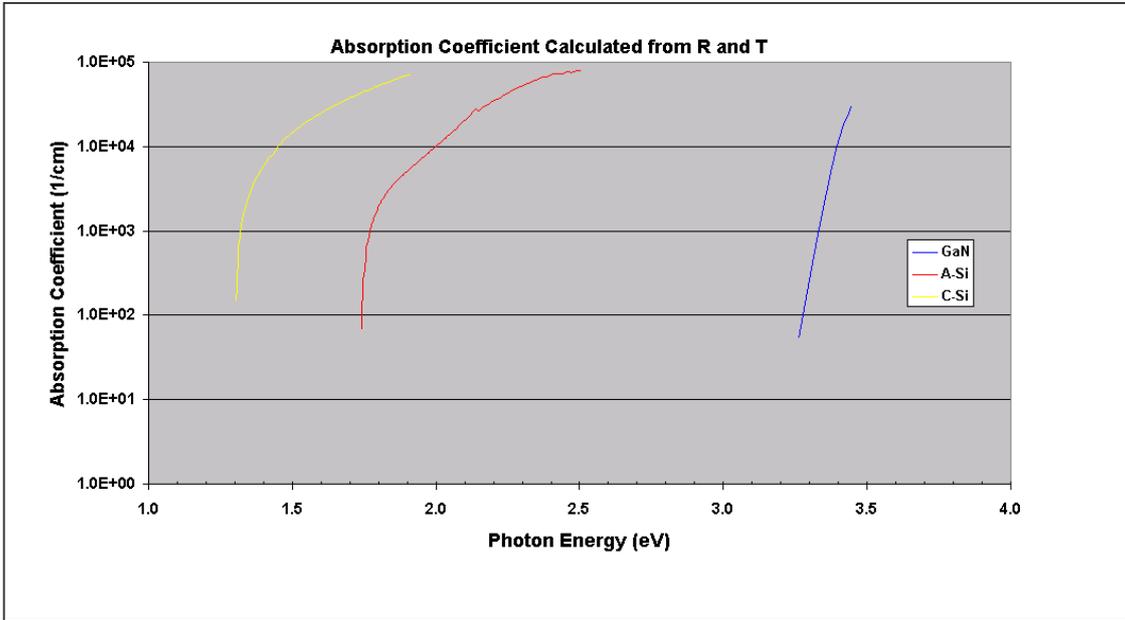
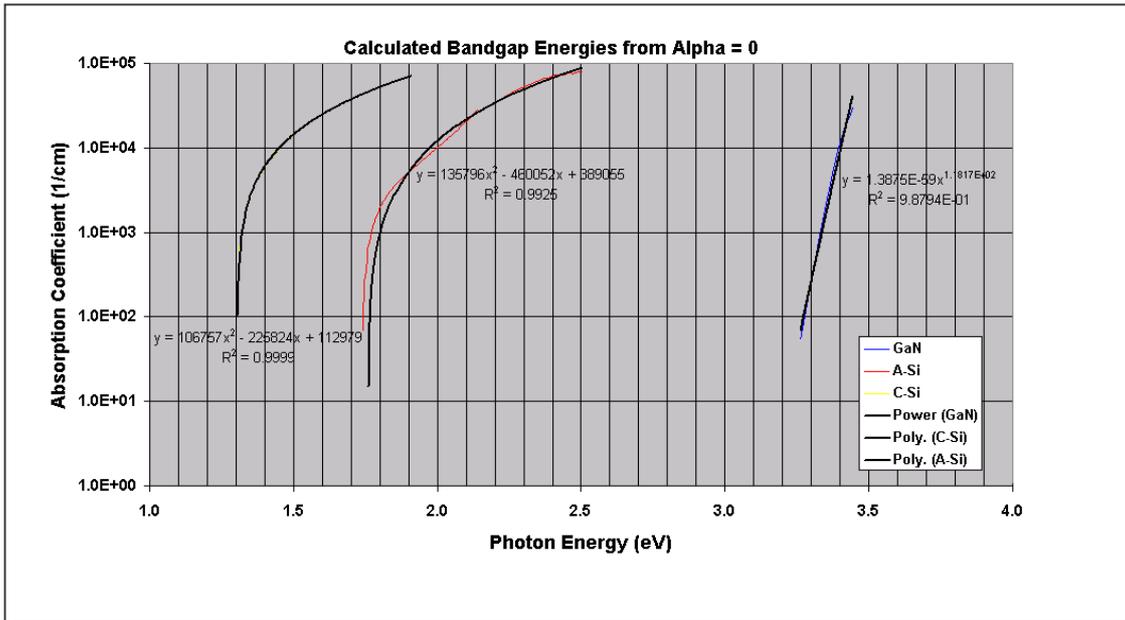
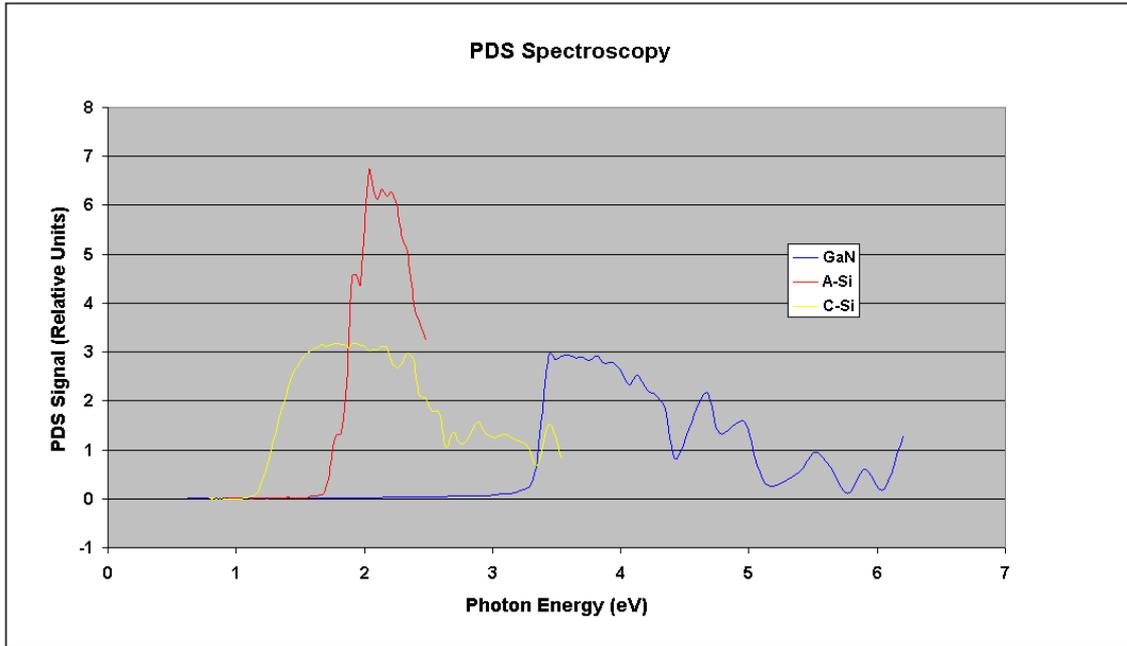


Figure 10: Calculated Bandgap Energies from Alpha = 0



Question 10

Figure 11: PDS Measurement



From the PDS curve above, the absorption coefficient is calculated by equation 22

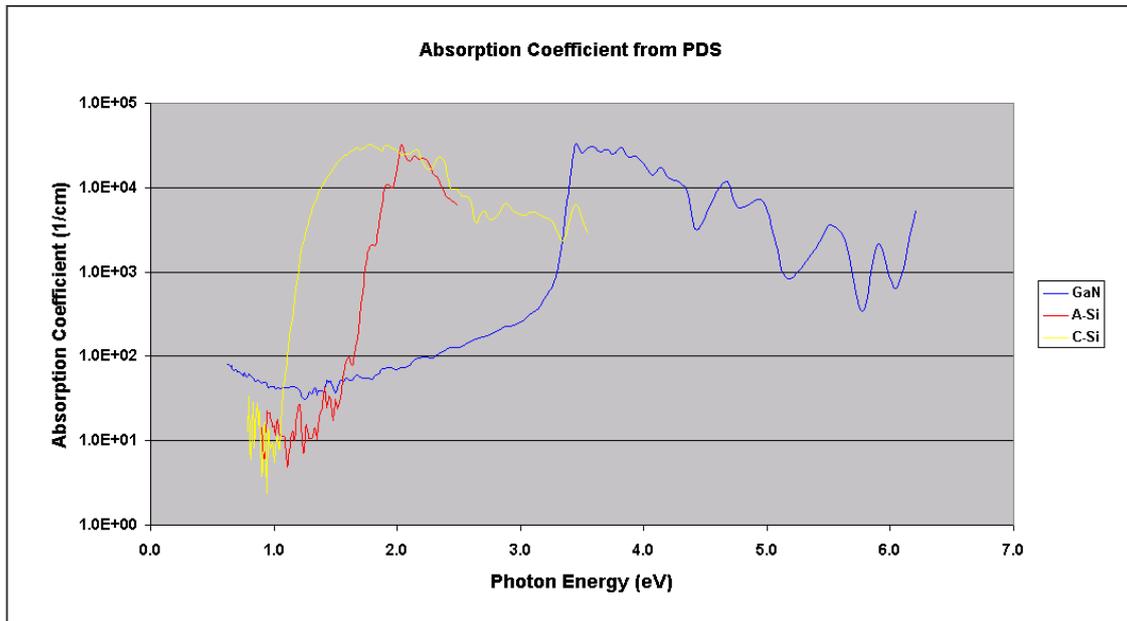
$$\alpha = -\frac{1}{d} \ln[1 - 0.96 \times PDS(\text{Normalized})]$$

where d is the sample thickness (10^{-4} cm), and the PDS curve is normalized to the maximum PDS signal.

Figure 12 on page 14 is the calculation of the absorption coefficient from the PDS measurement. The absolute value of this value is meaningless until we match up these results with the transmission and reflection measurements.

The saturation of the curve occurs at the maximum, and does not make sense to calculate the absorption coefficient above this photon energy, but is shown for completeness as asked in question 10.

Figure 12: Absorption Coefficient from PDS



Question 11

Figure 13, Figure 14, Figure 15, demonstrate the absorption coefficient as a function of photon energy for A-Si, C-Si, and GaN respectively. The blue curve is the absorption coefficient calculated from Reflection and Transmission measurements and the red curve is the absorption coefficient calculated from PDS. The PDS measurements are in normalized units; therefore the PDS spectra are fitted to the Reflection and Transmission spectra by a constant factor. The constant factor is calculated where the two curves overlap at the same photon energy to bring the PDS spectra in line with the Reflection, Transmission spectra. The following absorption spectra results from PDS and Reflection, Transmission overlap very well.

Figure 13: Absorption Coefficient of Amorphous Silicon

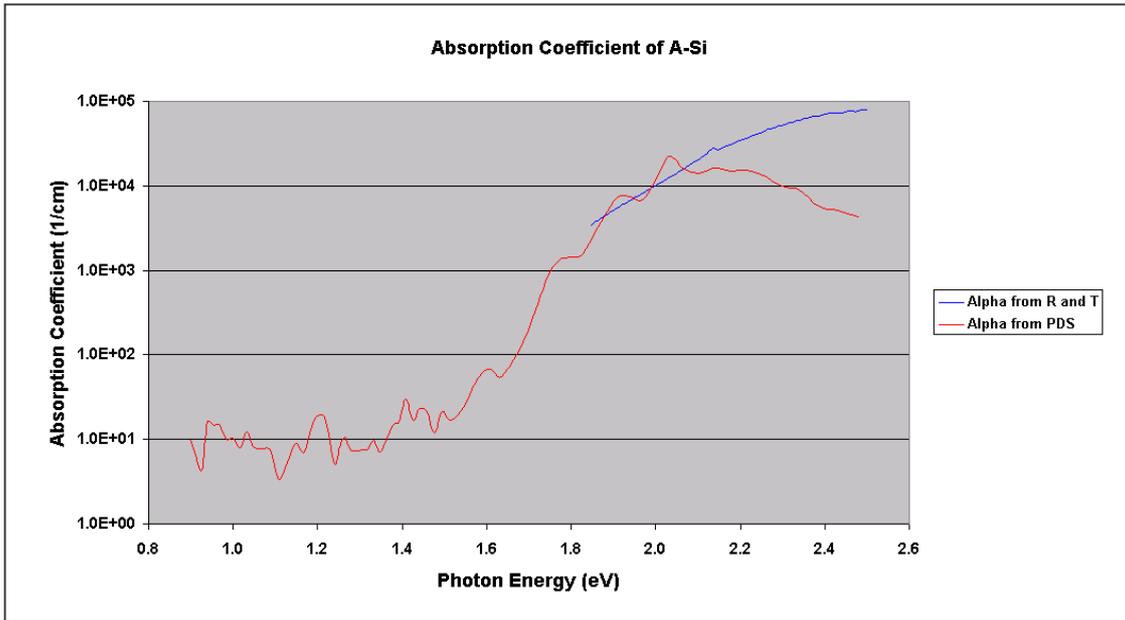


Figure 14: Absorption Coefficient of C-Si

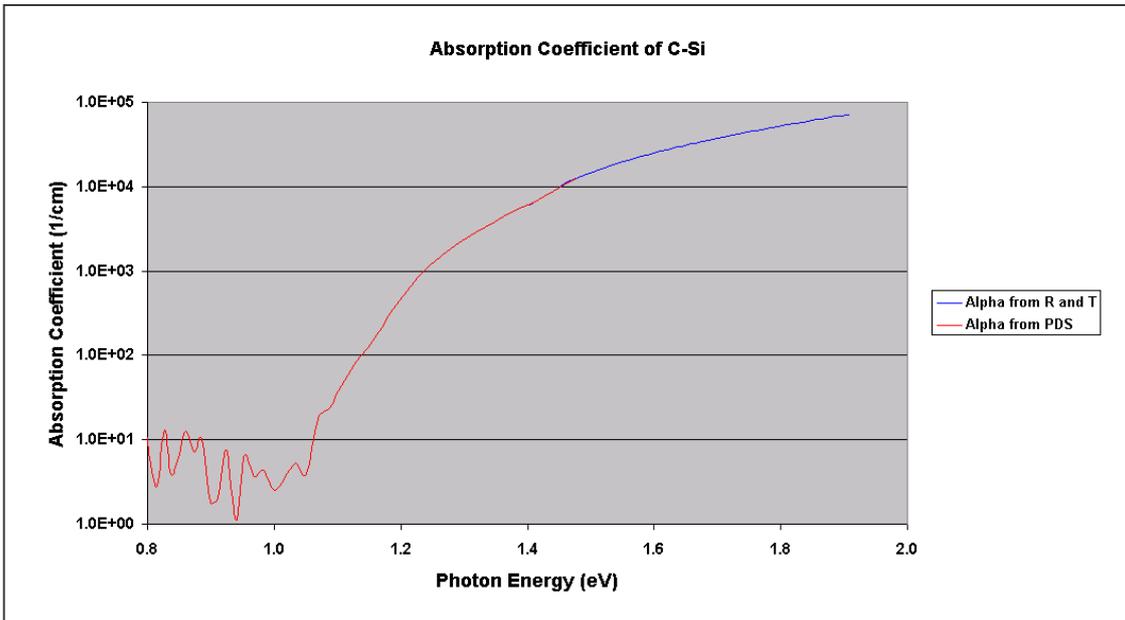
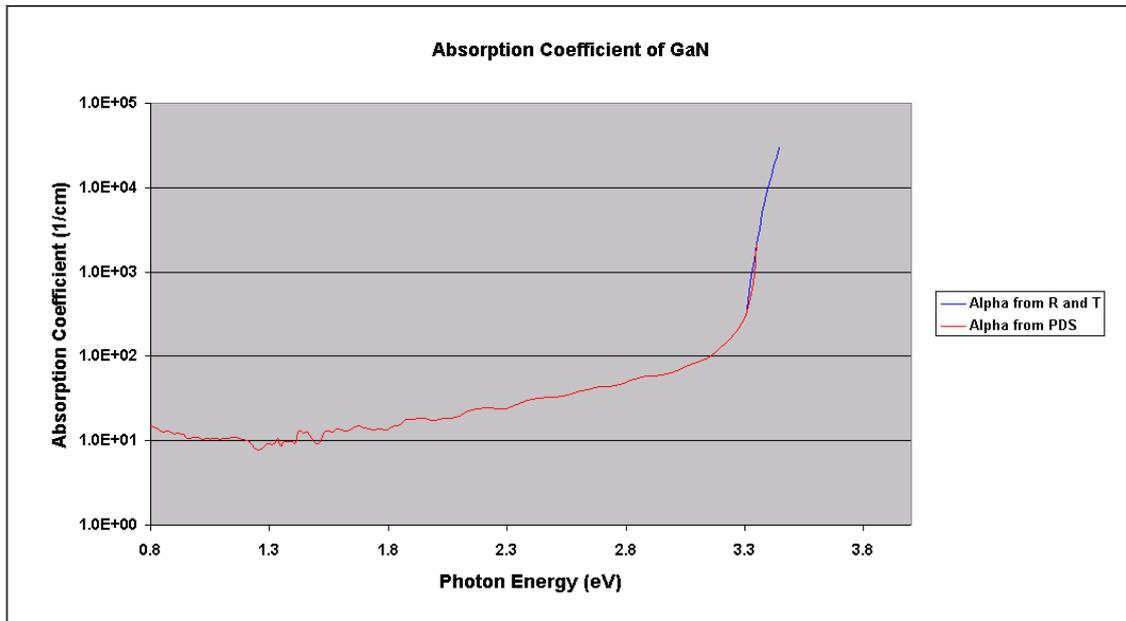


Figure 15: Absorption Coefficient of GaN



Question 12

The energy bandgap for each sample was calculated in Table 1: Calculated Bandgap Energies from the Absorption Coefficient (R and T) on page 9. The calculated values agree very well with the theoretical values. The energy bandgap of Si is indirect. An indirect bandgap means for a transition from the valence band maximum to conduction band minimum to occur, the addition of a phonon to conserve momentum and energy must be introduced. GaN is a direct bandgap semiconductor; therefore transitions from the valence band maximum to the conduction band minimum occur at the same point in the Brillouin zone by absorption of a photon.

The energy bandgap of GaN is the highest bandgap with energy of 3.4 eV, therefore strong absorption occurs in the UV and GaN appears transparent in the visible spectrum. A-Si has a higher band gap than C-Si due to the additional defects and dangling bonds in the structure. Si has a lower bandgap than GaN because Si is a group IV semiconductor and GaN is a group III-V semiconductor. Group IV semiconductors have covalent bonds and group III-V semiconductor have ionic bonds.

For each of the three absorption spectra: GaN, A-Si, and C-Si, they show a pronounced onset close to the bandgap and increase at higher photon energies. The absorption strength close to the bandgap is much weaker for Si than for GaN due to the indirect nature of the bandgap. In this case the absorption edge is more poorly defined, increasing gradually at energies above the bandgap. This is due to the indirect nature of the fundamental bandgap in Silicon and arises as the absorption process involves three particles; a photon, phonon and the electron. The probability of this three-particle process is much weaker than direct optical absorption as it requires a third particle to be present (the phonon) to conserve the total crystal momentum.

For a direct bandgap semiconductor, the absorption curve is steeper at the absorption edge than an indirect bandgap. This is due to reasons mentioned above. The absorption of the indirect bandgap semiconductor is a two-step process and therefore less probable for electrons and holes to recombine with absorption of a photon. From our results, we recognise the bandgap of C-Si as an indirect semiconductor.

The Dangling Bond Defect Density in the bandgap is given by

$$N_{DB} = 2 \cdot 10^{16} \text{ cm}^{-2} * \alpha(1.3\text{eV})$$

$$\text{At } 1.3 \text{ eV} \Rightarrow \alpha = 7.43 \text{ cm}^{-1}$$

$$\therefore N_{DB} = 1.93 \cdot 10^{17} \text{ cm}^{-3}$$