

Ultraviolet-Visible Spectroscopy to Determine the Nature of Band Gap and its Estimation

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In this experiment, we use UV-Vis spectroscopy to determine the bandgap energies of different materials. Specifically, we use the Tauc method to plot the absorption coefficient as a function of energy for three direct band gap materials – CdS, ZnTe and ZnO – to estimate their band gap values.

I. THEORY

A. Direct and Indirect Band Gap Semiconductors

The band gap of a material is the minimum difference in energy between the highest energy state of the valence band and the lowest energy state of the conduction band. However, these values may not occur at the same value of electron momentum. When the top of the valence band and the bottom of the conduction band align at the same value of momentum, the material is called a direct band gap material. Otherwise, it is called an indirect band gap material.

In optical devices, the difference between the two are quite significant. A typical photon energy is of the order of 10^{-19} J and since $p = E/c$, it equates to very small momentum.

In semiconductor devices, a photon of energy E_g can produce an electron-hole pair. In direct band gap materials, the process is much easier since the electron does not need to be given much momentum. But in an indirect band gap semiconductor, the electron must also undergo a significant change in its momentum for a photon of energy E_g to produce the same (Fig. 1). This means that in addition to interacting with a photon to gain energy, it also needs to interact with a lattice vibration called a phonon to lose/gain momentum.

This indirect process happens at a slower rate as it requires the interaction of an electron, a photon and a phonon. Since the same principle also applies to recombination of electrons and holes, that process is also faster for direct band gap semiconductors. Even though a broad spectrum of phonons are available in a crystal lattice, those phonons which conserve the momentum participate for indirect transitions.

B. UV-Vis spectroscopy for optical band gap measurement

UV-Vis spectroscopy measures light absorption as function of wavelength. It gives information on electronic transitions occurring in semiconductor material and can be used to estimate the optical band gap.

For a sample of thickness d , the absorption coefficient

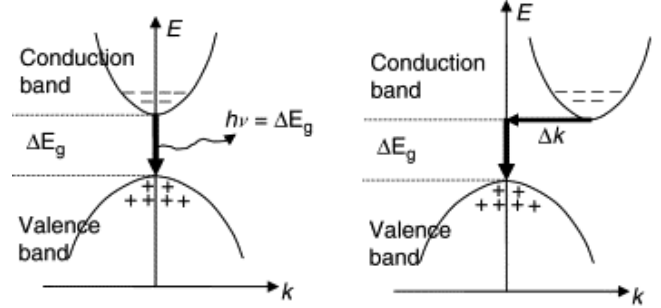


FIG. 1: Illustration of direct bandgap (left) and indirect bandgap (right) of semiconductor materials [1].

of light α is given by,

$$\alpha \text{ (cm)}^{-1} = \frac{2.303A}{d} \quad (1)$$

where A is the absorbance of the sample, given by

$$A = \log_{10} \left(\frac{I_0}{I_T} \right) \quad (2)$$

Here, I_T is the transmitted light and I_0 is the incident light, which are related by the Beer-Lambert's law.

$$I_T = I_0 e^{-\alpha d} \quad (3)$$

Energy band gap of a given material can be precisely calculated using *Tauc method* as,

$$\alpha(h\nu) = A(h\nu - E_g)^n \quad (4)$$

where $n = 1/2$ for direct allowed transitions and $n = 2$ for indirect allowed transitions [2]. Therefore, for direct band gap materials,

$$\alpha(h\nu) = A(h\nu - E_g)^{0.5} \quad (5)$$

Hence they exhibit a sharp rise in absorption above the E_g in the plot of energy of light source of Uv-vis setup

versus absorption coefficient α . For indirect band gap materials,

$$\alpha(h\nu) = A(h\nu - E_g \pm E_p)^2 \quad (6)$$

where E_p refers to the addition energy for the phonon interaction. The sign '+' corresponds to phonon emission, and the sign '-' corresponds to phonon absorption. The band gap is estimated by plotting $\sqrt{\alpha}$ versus energy and finding the intercept of the linear region.

II. EXPERIMENTAL SETUP

Apparatus

1. A laser lamp
2. Glass plates
3. ZnTe, CdS and ZnO coated glass slides
4. UV-Vis spectroscope and Analysing software
5. Optical Cables for connection

In the experiment, we use a spectrum analyzer software which samples wavelengths from 340 to 1000 nm, which lie in the UV-Vis range. The thin films are held in a sample holder box through which the light source is passed. To get the corrected spectrum of the sample, we first take a dark measurement with the lights turned off I_{dark} . Now, we take the spectrum of the empty glass slide as reference (I_{ref}). Finally, the sample data is taken by placing the sample in front of the light source (I_{sample}). The final absorbance is calculated using Eq. 2 after subtracting the dark values.

$$A = \log_{10} \left(\frac{I_{\text{ref}} - I_{\text{dark}}}{I_{\text{sample}} - I_{\text{dark}}} \right) \quad (7)$$

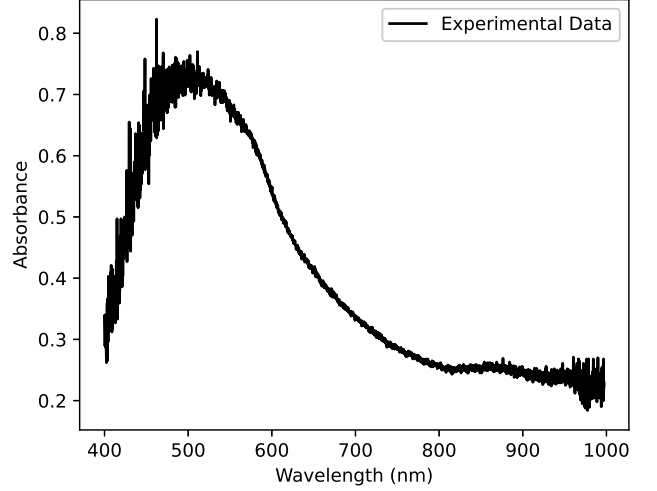
III. OBSERVATION AND CALCULATIONS

Figs. 2a, 3a and 4a show the absorbance vs. wavelength plots obtained from the spectrometer for three materials – ZnTe, CdS and ZnO. All the materials used in this experiment are direct band gap materials.

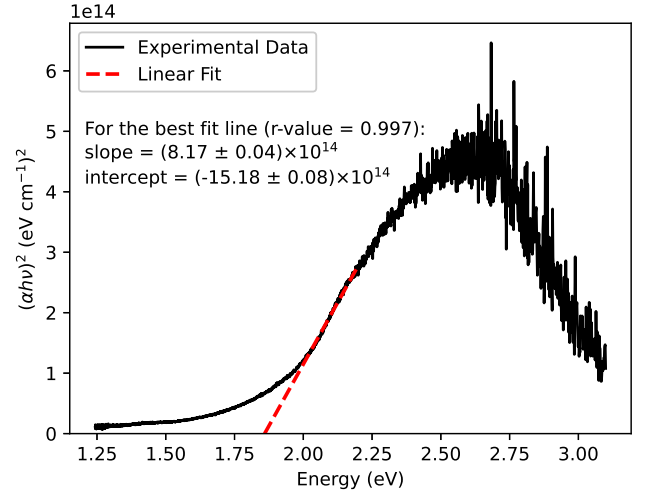
Using the obtained values of A , we have calculated α using Eq. 1. Figs. 2b, 3b and 4b show the $(\alpha h\nu)^2$ vs. $h\nu$ plots for ZnTe, CdS and ZnO respectively. By fitting a straight line over the linear region we have obtained the slope and intercept parameters. We have used the Savitzky–Golay filter for ZnO to smoothen the plot as the experimental data had a very high signal to noise ratio.

Eq. 5 can be rewritten as

$$(\alpha h\nu)^2 = Ah\nu - AE_g \quad (8)$$



(a) Absorbance vs. Wavelength



(b) $(\alpha h\nu)^2$ vs. Energy

FIG. 2: Absorbance plots for ZnTe

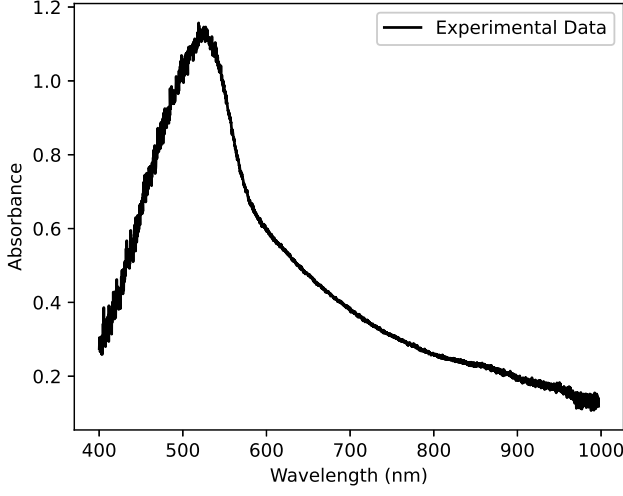
Here, AE_g is the y-intercept and hence $AE_g/A = E_g$ will be the x -intercept of the linear region.

The x -intercept can be calculated by taking the ratio of the intercept to the slope. The corresponding x -intercepts, which represent the band-gap energies are:

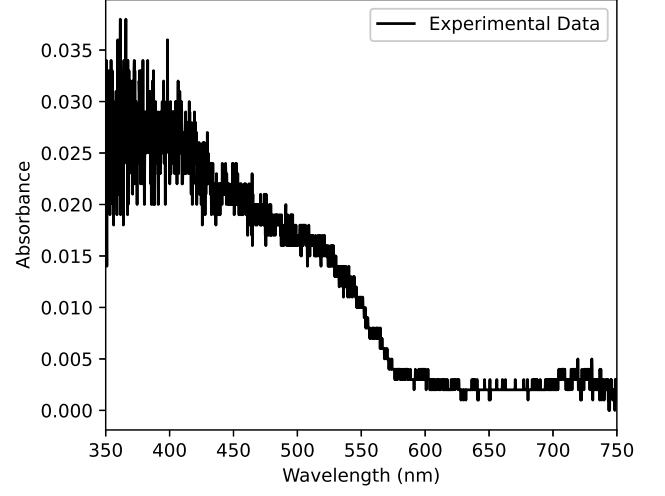
- For ZnTe: 1.859 eV
- For CdS: 2.074 eV
- For ZnO: 2.539 eV

IV. ERROR ANALYSIS

The error in the estimation of E_g can be calculated from the uncertainties in the slope and intercept of the linear region.



(a) Absorbance vs. Wavelength



(a) Absorbance vs. Wavelength

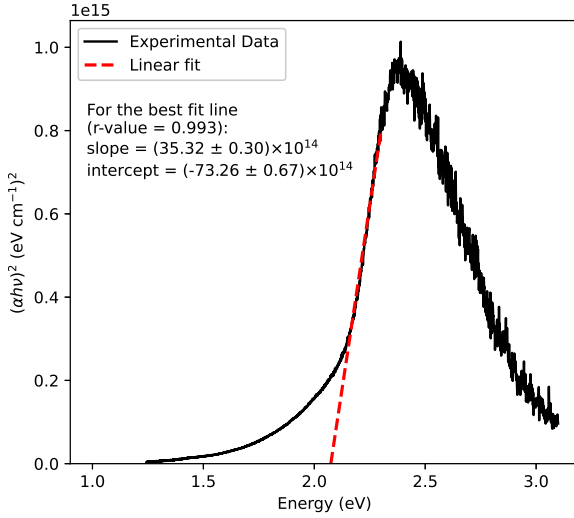
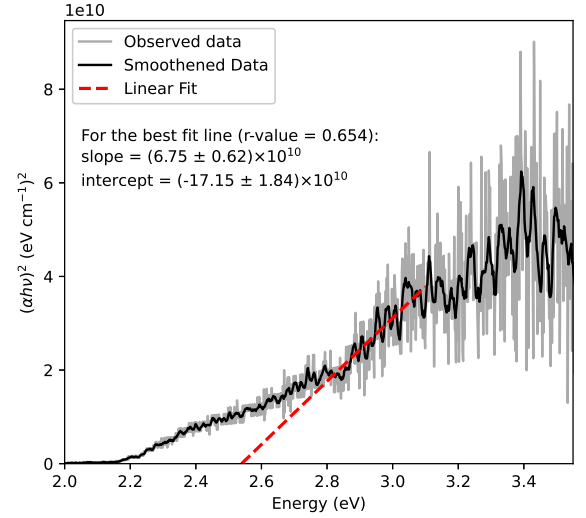
(b) $(\alpha h\nu)^2$ vs. Energy(b) $(\alpha h\nu)^2$ vs. Energy

FIG. 3: Absorbance plots for ZnTe

FIG. 4: Absorbance plots for ZnTe

$$\frac{\Delta E_g}{E_g} = \sqrt{\left(\frac{\Delta \text{slope}}{\text{slope}}\right)^2 + \left(\frac{\Delta \text{intercept}}{\text{intercept}}\right)^2} \quad (9)$$

Plugging in the values for all three plots, the corresponding ΔE_g 's are:

- For ZnTe: 0.026 eV
- For CdS: 0.013 eV
- For ZnO: 0.359 eV

V. DISCUSSION & CONCLUSION

In this experiment, we were able to determine the bandgaps for three different direct band-gap materials.

These are:

- ZnTe: (1.859 ± 0.026) eV
- CdS: (2.074 ± 0.013) eV
- ZnO: (2.539 ± 0.359) eV

We have found that the bandgap values obtained from this method are slightly lower than the literature values for all three materials (2.26 eV, 2.42 eV and 3.35 eV for ZnTe, CdS and ZnO respectively). Hence the percentage errors are 18%, 14% and 24% respectively. This could be attributed to impurities contaminating the sample. Since we did not use a vacuum chamber, there could also be dust and other particles interfering with the light matter interaction.

We can also see that the error in the band gap of ZnO is

significantly higher than the other two materials. This is expected as the absorbption vs. wavelength plot obtained for this material was very noisy (Fig. 4). This could be because that particular sample of ZnO deposition might have worn off or contaminated heavily. Uneven sample thickness could also contribute to the inaccuracy in the measurement.

VI. PRECAUTIONS

1. Make sure to not hold the sample by hand to avoid contamination.
2. Wait for a few minutes after switching on the light source for it to provide maximum intensity.

3. Take proper dark and reference readings to ensure proper calibration.

VII. APPLICATIONS

In conclusion, UV-Vis spectroscopy is an important analytical tool used in many fields, including chemistry, biology, environmental science, and pharmaceuticals. It can be used to identify and characterize molecules, measure their concentration, and determine the purity of a sample. Indirect bandgap materials also provide a more continuous and wider range of absorbance compared to direct bandgap materials which makes them better suited for use in solar cells.

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| <p>[1] R. Hui and M. O’Sullivan, Chapter 1 - fundamentals of optical devices, in <i>Fiber Optic Measurement Techniques</i>, edited by R. Hui and M. O’Sullivan (Academic Press, Boston, 2009) pp. 1–128.</p> | <p>[2] J. I. Pankove, <i>Optical processes in semiconductors</i> (1975).
 [3] SPS, <i>Ultraviolet-Visible Spectroscopy to determine the nature of band gap and estimation of the bandgap</i>, NISER (2023).</p> |
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