Band gap estimation using UV-VIS Spectroscopy

Biswaranjan Meher
Integrated M.Sc.
Roll No.-2011050
School of Physical Sciences
National Institute of Science Education and Research, Bhubaneswar
(Dated: April 9, 2023)

In this experiment, we compare the characteristics of semiconductors with direct and indirect band gaps. While phononic and photonic interaction are necessary for electronic transitions in indirect band gap semiconductors, only photonic interaction causes electronic transitions in direct band gap semiconductors. We employ UV-vis spectroscopy, which measures light absorption as a function of wavelength and can offer information on the electronic transitions as a function of incident light wavelength.

I. OBJECTIVES

- Estimation of the band gap for direct and indirect band gap materials using Uv-vis spectroscopy.

II. THEORY

A. Energy band gap

The **band gap** is defined as the difference between the lowest energy of the conduction band and the highest point energy of the valence band.
There are two basic types of band gaps:

- Direct band gap
- Indirect band gap

1. *Direct band gap*

For direct band gap, the lowest energy difference between the valence and conduction band occurs at the same k value.
In a direct band gap semiconductor, an electron-hole pair can be created fairly readily by a photon of energy E_g, where Eg is the band gap energy, as the electron only needs to be supplied a small amount of momentum.

2. *Indirect band gap*

For indirect band gap, the lowest energy difference between the valence and conduction band occurs at different k values.
For a photon of energy E_g to generate an electron-hole pair in an indirect band gap semiconductor, an electron must also experience a sizable change in its momentum. This is feasible, but it necessitates that the electron interact not only with the photon to obtain energy but also with a phonona (a type of lattice vibration) to change its momentum.

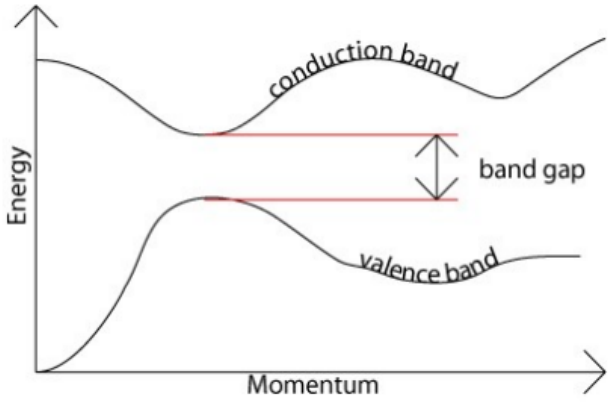

FIG. 1. Direct band gap for semiconductors

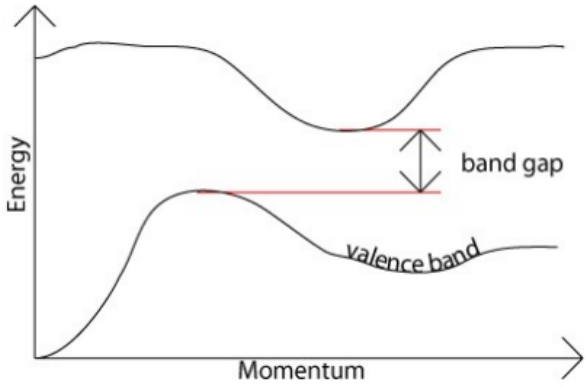

FIG. 2. Indirect band gap for semiconductors

Semiconductors are materials that have a considerably low band gap. These materials have a varied use due to their "on - off" feature.

B. Process of electron excitation

The indirect process moves significantly more slowly since it needs the intersection of three different entities: an electron, a photon, and a phonon. The production of photons from the recombination of electrons and holes follows the same general rule. For a direct band gap semiconductor, the recombination process is far more effective than for an indirect band gap semiconductor, where the process needs to be mediated by a phonon. Although a crystal lattice has a wide range of phonons, only those phonons that conserve momentum participate in indirect transitions.

C. Uv-vis spectroscopy for optical band gap measurement

In order to determine the optical band gap, UV-VIS spectroscopy, which measures light absorption as a function of wavelength, provides information on the electronic transitions that take place in semiconductor materials as a function of incident light wavelength. Electronic band gap, which is defined as the energy difference between the conduction band maximum and the valence band lowest, is roughly equivalent to the optical band gap.

1. *Beer-Lambert's law*

Beer-Lambert's law states that:

$$A = \epsilon cl = -log_{10}\left(\frac{I_T}{I_o}\right) \tag{1}$$

where A is the absorbance, ϵ is the molar absorption coefficient , c is the concentration of the absorbing species, and l is the length of the path taken by the light.

2. *Absorption coefficient*

The absorption coefficient is given by:

$$\alpha = \left(\frac{ln(10)A}{l}\right) \tag{2}$$

3. *Tauc method*

Energy band gap of a given material can be precisely calculated using Tauc method as given below:

$$\alpha = C(h\nu - E_g)^n \tag{3}$$

where n = 2 for indirect transitions and n = 0.5 for direct transitions.
For indirect band gap semiconductor:

$$\alpha = C(h\nu - E_g \mp Ep)^2 \tag{4}$$

In the above equation for indirect band gap, - sign corresponds to phonon absorption and + sign corresponds to phonon emission. But in some of the cases, phonon absorption and emission are not clearly seen in the indirect band gap data.

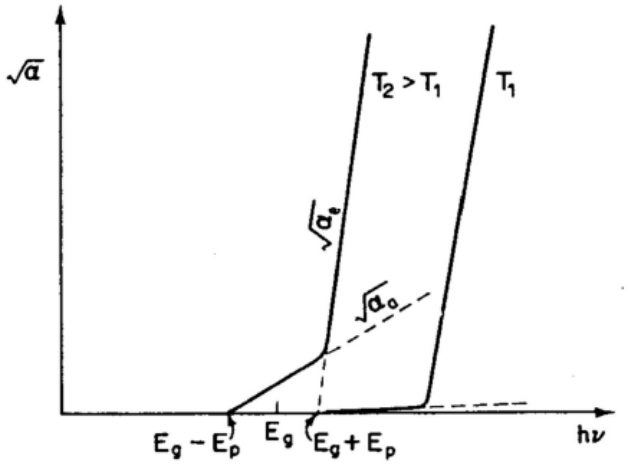

FIG. 3. Plot of $\sqrt{\alpha}$ vs Energy for indirect transitions

III. EXPERIMENTAL SETUP

Components required:

- **Samples:** CdS and ZnTe
- **PC with the software**
- **Chamber:** To hold the sample material and pass light through it.
- **Connecting cables and optical fibres**

IV. OBSERVATIONS AND CALCULATIONS

A. Material: CdS

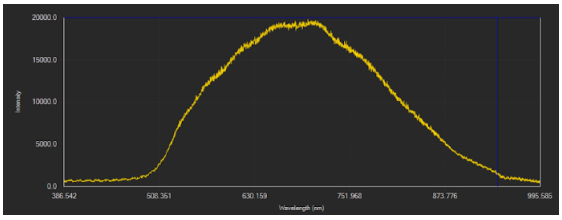

FIG. 4. Intensity vs wavelength for CdS

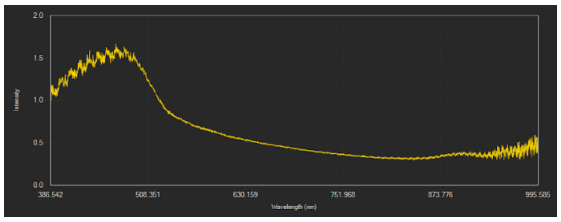

FIG. 5. Absorption spectrum of CdS

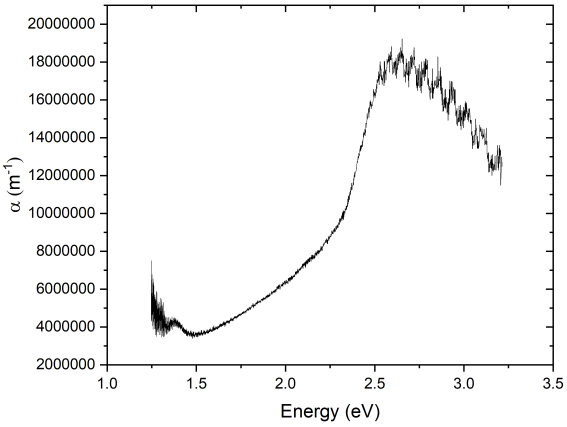

FIG. 6. Plot of Energy vs absorption coefficient for CdS

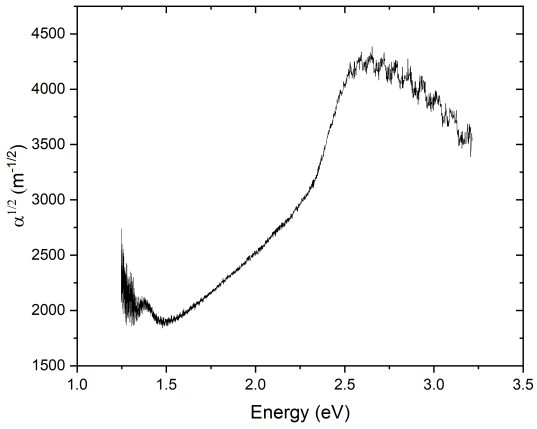

FIG. 7. Plot of Energy vs $\sqrt{\alpha}$ for CdS

-

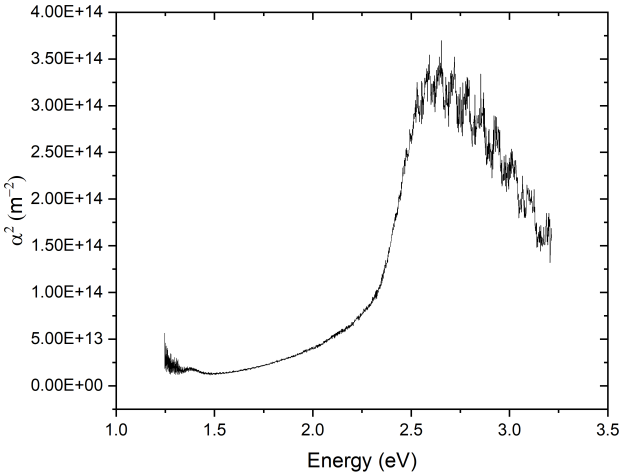

FIG. 8. Plot of Energy vs α^2 for CdS

-

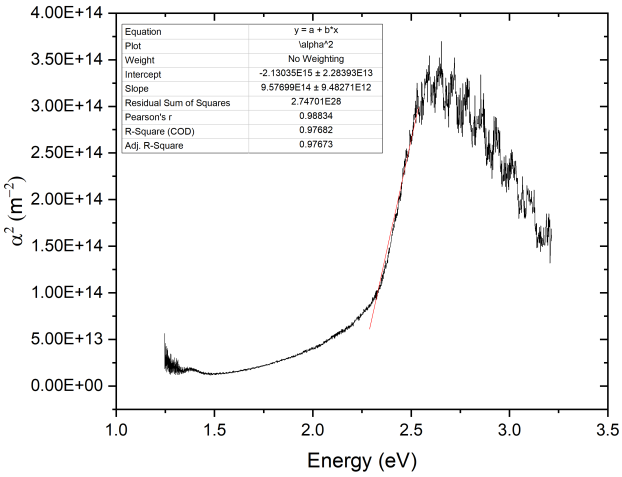

FIG. 9. Plot of Energy vs α^2 with fit for CdS

From the fit:

$$Slope = (9.577 \pm 0.095) \times 10^{14} m^{-2} eV^{-1}$$

$$Intercept = (-2.13 \pm 0.028) \times 10^{15} m^{-2}$$

The band gap energy for CdS:

$$E_g = \frac{intercept}{slope} = 2.224eV$$

Error: $\frac{\delta E_g}{E_g} = \sqrt{\left(\frac{\delta intercept}{intercept}\right)^2 + \left(\frac{\delta slope}{slope}\right)^2} = 0.0166$

$$\delta E_g = 0.037eV$$

B. Material:ZnTe

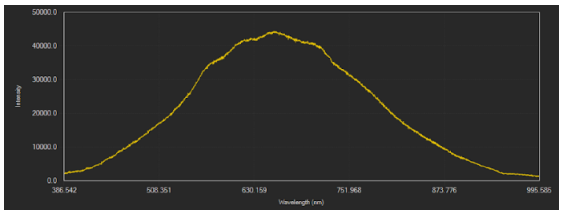

FIG. 10. Intensity vs wavelength for ZnTe

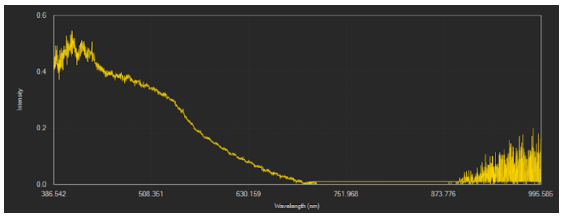

FIG. 11. Absorption spectrum of ZnTe

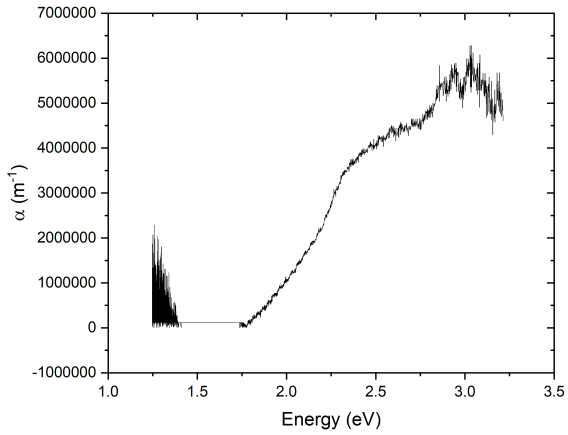

FIG. 12. Plot of Energy vs absorption coefficient for ZnTe

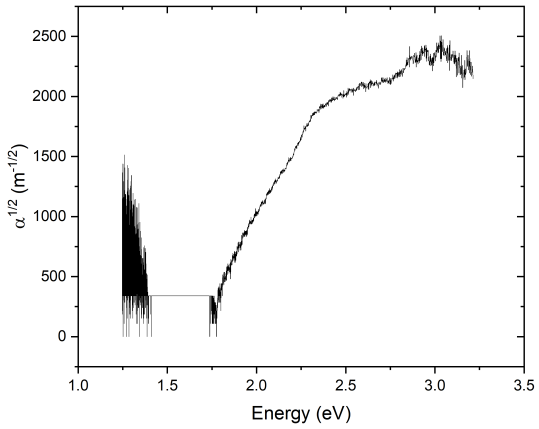

FIG. 13. Plot of Energy vs $\sqrt{\alpha}$ for ZnTe

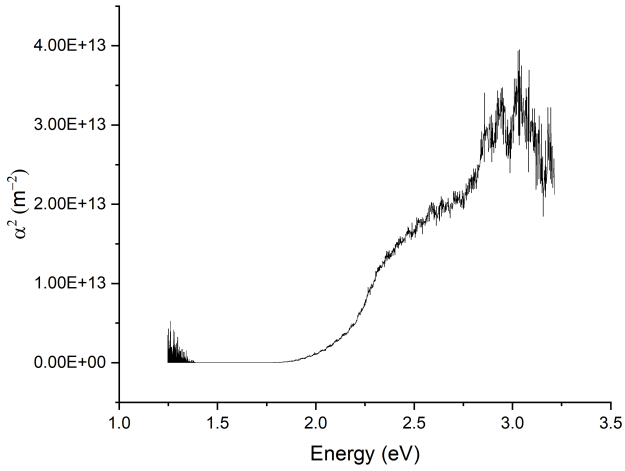

FIG. 14. Plot of Energy vs α^2 for ZnTe

-The fit plot is attached on the next page.

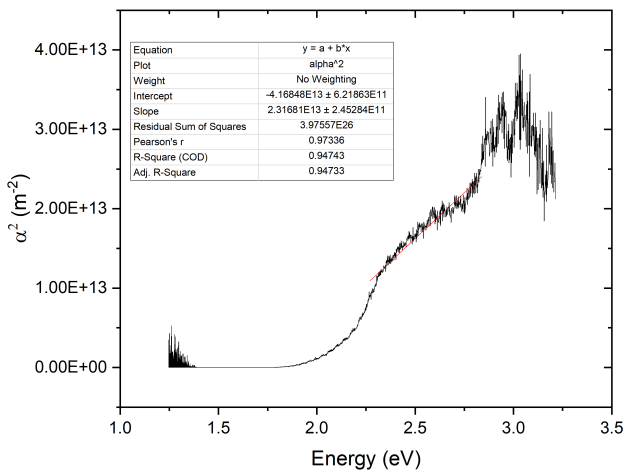

FIG. 15. Plot of Energy vs α^2 with fit for ZnTe

From the fit:

$$Slope = (2.317 \pm 0.0245) \times 10^{13} m^{-2} eV^{-1}$$

$$Intercept = (-4.168 \pm 0.0622) \times 10^{13} m^{-2}$$

The band gap energy for ZnTe:

$$E_g = \frac{intercept}{slope} = 1.799eV$$

Error: $\frac{\delta E_g}{E_g} = \sqrt{\left(\frac{\delta intercept}{intercept}\right)^2 + \left(\frac{\delta slope}{slope}\right)^2} = 0.0183$

$$\delta E_g = 0.033eV$$

C. Material:Polymer

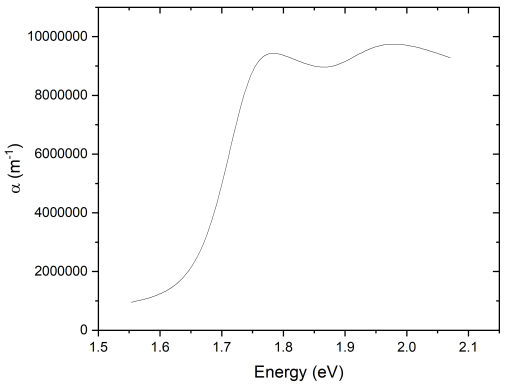

FIG. 16. Plot of Energy vs absorption coefficient for Polymer

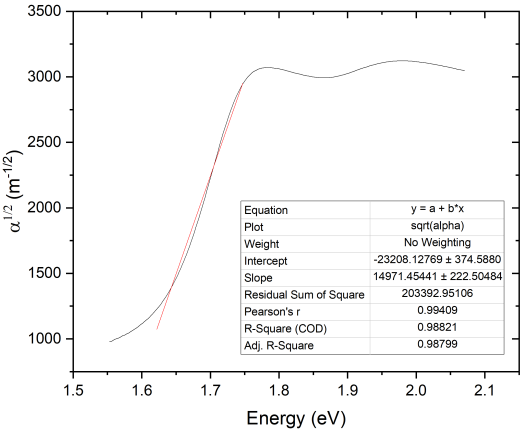

FIG. 17. Plot of Energy vs $\sqrt{\alpha}$ for Polymer with fit

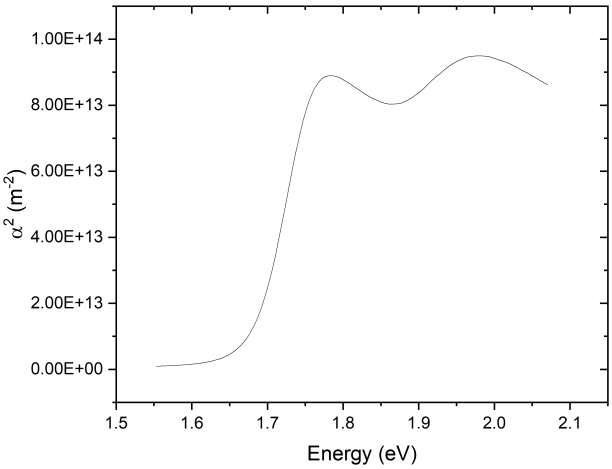

FIG. 18. Plot of Energy vs α^2 for Polymer

From the fit:

$$Slope = (14971.4544 \pm 222.5048) m^{-1/2} eV^{-1}$$

$$Intercept = (-23208.1277 \pm 374.588) m^{-1/2}$$

The band gap energy for Polymer:

$$E_g = \frac{intercept}{slope} = 1.55eV$$

Error: $\frac{\delta E_g}{E_g} = \sqrt{\left(\frac{\delta intercept}{intercept}\right)^2 + \left(\frac{\delta slope}{slope}\right)^2} = 0.022$

$$\delta E_g = 0.0341eV$$

V. RESULTS

- Direct band gap materials:
  - CdS: $E_g = (2.224 \pm 0.037)$ eV
  - ZnTe: $E_g = (1.799 \pm 0.033)$ eV
- Indirect band gap material:
  - Polymer: $E_g = (1.55 \pm 0.0341)$ eV

VI. CONCLUSIONS AND DISCUSSIONS

- We employed UV-VIS spectra to observe the band gap for both direct (CdS and ZnTe) and indirect band gap materials (polymer).
- The software's snapshot displays the absorption spectra. The graphs were also plotted to show how energy and absorption coefficient powers varied.
- The linear region of square absorption coefficient vs energy for direct band semiconductors and the linear region of square root absorption coefficient vs energy for indirect band gap semiconductors were both explored. This determines the nature of band structure for the different materials.

VII. SOURCES OF ERRORS

- Fluctuating light source intensity
- Impurities in the sample or inside the chamber
- The sample slide was broken which was a problem fitting in a proper way.

VIII. REFERENCES

- NISER Lab Manual
- `https://pubs.acs.org/doi/10.1021/acs.jpclett.8b02892`