

Determination of Optical Transition Nature using R^2 Value

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ABSTRACT

The present paper reports about determination of direct/indirect optical transition nature of material from UV-Vis transmission spectrum. Determination of transition nature is a pre-requisit to attain optical bandgap value from Tauc's plot, which is a conventional method of optical bandgap approximation. The present work shows how the transition nature can be concluded with R^2 value using R-Software, which is an open-source statistical tool. For the case study, amorphous $As_{40}Se_{60}$ is taken, which is a well-known optical material. This study can be generalized for the investigation of any optical material.

Key words: Optical bandgap, Direct/Indirect transitions, Transmission Spectrum, R-Software.

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INTRODUCTION

Optical bandgap E_g is energy bandgap, which can be defined as the gap or region between valence and conduction band in which there is no level of energy. The absorption spectra, with a rapid increase in absorption at shorter wave-length, can be used to determine the energy bandgap (E_g) of the material. Every solid has its own characteristic energy band structure. The conduction and valence band are the regular features of all the solids. Only difference is up to which they are occupied and vertical separation between them i.e. energy bandgap (E_g). Material becomes transparent for the EM radiations of energy greater than optical bandgap of the material. The bandgap (E_g) may be classified as direct and indirect bandgap depending up on electron transition [1]. As the photon of incident light is absorbed by the material, an electron is excited from lower to upper energy level. This transition of electron can be direct (without phonon participator) or indirect (in which the interaction with a phonon takes place). In a direct transition an electron in the conduction band can fall to an empty state in the valence band giving of the energy difference E_g as photon of light. CdTe, GaAs are examples of direct bandgap material. On the other hand, in an indirect transition, an electron in the conduction band can not fall directly to the valence band but must undergo a momentum change as well as changing its energy. Silicon is a well known example of indirect bandgap material. The difference between direct and indirect band structure is very important for deciding that what material can be used in device requiring light output.

Determination of optical bandgap for a material can be done using Tauc's method [2]. However, before determining optical bandgap, it must be known if a material is direct bandgap material or indirect bandgap material. To resolve this problem R^2 value can be calculated using R Software to determine category of the optical bandgap (direct or indirect) of the material [3].

THEORY

Determination of optical bandgap is done by extrapolation of Tauc's plot, which is:

$$(\alpha h\nu)^{1/n} = B^{1/n} (h\nu - E_g) \quad (1)$$

In the above equation, $n = 1/2$ for direct allowed transition, $n = 2$ for indirect allowed transitions. Hence, equation for direct bandgap material is:

$$(\alpha h\nu)^2 = B^2 (h\nu - E_g) \quad (n = 1/2 \text{ for direct bandgap material}) \quad (2)$$

And the equation for indirect bandgap material is:

$$(\alpha h\nu)^{1/2} = B^{1/2} (h\nu - E_g) \quad (n = 2 \text{ for indirect bandgap material}) \quad (3)$$

Here, B is band tailing parameter, E_g is energy bandgap and α is absorption coefficient, which is defined as the fraction of power absorbed in a unit length of the medium. To determine E_g by extrapolating Tauc's plot, value of α and n should be known. From absorption spectra, absorption coefficient (α) is calculated as a function of photon energy. Value of n can be determined by calculating R-squared value from R Software, which provides a wide variety of statistical and graphical techniques (linear and nonlinear modeling, statistical tests, time series analysis, classification, clustering etc.). If the R-squared value is greater for $n = 2$, then material is indirect bandgap material or vice-versa as higher R-squared value indicates higher quality of linear regression.

In this study, this analysis is applied for a well known indirect bandgap material – $\text{As}_{40}\text{Se}_{60}$. The steps and results are shown only for a subset of data as the actual data is too big to fit in the document.

DETERMINATION OF R² VALUE

The determination method assumes that value of absorption coefficient (α) is already determined from absorption or transmission spectra [4,5]. A datasheet needs to be prepared with three columns containing $h\nu$, $(\alpha h\nu)^{1/2}$ and $(\alpha h\nu)^2$ respectively in a spreadsheet tool such as OpenOffice or Microsoft Excel. Now, following steps can be performed to determine R² value:

- Select these columns (leave column headers) and press Ctrl + C to copy the data into the clipboard.

- Start R Software. On the R Console, enter the following command:

```
Data = read.table("clipboard")
```

The above command copies excel sheet's data into an internal structure of R Software and we may process this data using R Console commands.

- To ensure that the data is ready to process, enter following on the R Console:

```
Data
```

The above command displays the data copied from clipboard. The output shows that Columns V1, V2 and V3 hold the values for photon energy ($h\nu$), $(\alpha h\nu)^{1/2}$ and $(\alpha h\nu)^2$ respectively.

- To calculate the R-squared value for $(\alpha h\nu)^{1/2}$, enter the following command on the R Console:

```
M1 = lm(V1~V2, data=RSqr1)
```

- To check the R-squared value for $(\alpha h\nu)^{1/2}$ (i.e. for $n=2$), enter the following:

```
Summary(M1)
```

It displays processed data along with R-squared value for $n = 2$ (Indirect bandgap material).

- To calculate the R-squared value for $(\alpha h\nu)^2$, enter the following command on the R Console:

```
M1 = lm(V1~V3, data=RSqr2)
```

- To check the R-squared value for $(\alpha h\nu)^2$ (i.e. for $n=1/2$), enter the following:

```
Summary(M1)
```

It displays processed data along with R-squared value for $n = 1/2$ (Direct bandgap material).

RESULTS AND DISCUSSIONS

Using the method, R-squared value for indirect transition is 0.9929, whereas for direct transition, it is 0.9794. As R-squared value for indirect transition is greater than that of direct transition, hence, it can be concluded that the material is a indirect bandgap material. Hence its optical bandgap (E_g) is calculated using Tauc's plot for indirect bandgap material, which is shown in the following figure:

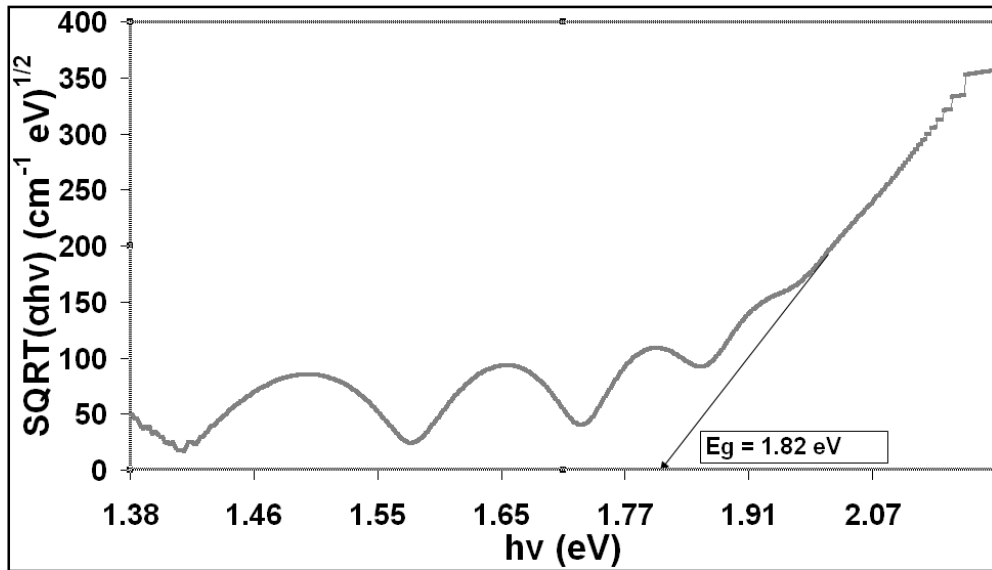


Fig. 1: Tauc's Plot for As₄₀Se₆₀ [6]

Using this analysis, optical bandgap (E_g) of As₄₀Se₆₀ thin film is 1.82 eV, which is as per reported in the literature [5].

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