

Determination of Optical Energy Gap for Copper oxide at Different Temperatures

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Abstract— In this work, thin films of copper oxide (CuO) have been prepared using spraypyrolysis technique. The energy gap was determined for samples of the copper oxide (CuO) at different temperatures ranging from (150 to 330) °C. The absorption and transmission spectra, shows the energy gap for (CuO) in the range from (2.44- 2.19) eV. These values are comparable to the actual values.

Keywords— Optical Energy Gap, Copper oxide, semiconductors.

I. INTRODUCTION

Determination of the band gap energy of semiconductors and specially semiconductor nanostructures is of great interest since it is directly related to the nanometer sized particles. Therefore, many efforts have been focused on the evaluation of the band gap energy to investigate the optical properties. Semiconductor nano particles produced by various methods constituting different sizes, thereby particles size distribution introduces many consequences on the optical properties due to the corresponding band gap. Therefore studying the particle size and their size distribution could be considered an crucial point.

Copper oxides CuO are the main semiconductor phases of copper oxides. CuO has monoclinic crystal structure and indirect band gap of 1.4eV, CuO also been reported [2,3].

Due to copper oxides potential applications, such as, in solar cells [4], catalysis [5], and magnetic devices [6], much attention has been attracted. Recently, extraordinary efforts have been made to investigate the optical properties of Cu₂O. Mishinia et al have studied the structure of Cu/Cu₂O multilayer preparation using non-linear electrochemical deposition with high precision in control thicknesses and number of layers. Their results lead to significant changes in the linear and nonlinear optical properties of Cu₂O and CuO multilayer structure [7]. Liu et al reported the structural and optical properties of film select rods deposited on different substrates. Their results illustrate that, the kind

of substrate strongly affect film morphology, crystal structure and optical properties [8]. Prevot et al studied the near infrared optical and photoelectric properties of Cu₂O under oxygen atmosphere. The absorption near the fundamental edge was characterized by several absorption bands with peak position at 0.65μm, 0.75μm, 0.88μm, 1.1μm with strongest one at 1.28μm, The aim of this work is to find an appropriate theoretical consideration to obtain the value of the optical energy gap at the different temperatures [9].

II. THEORETICAL BACKGROUND OF OPTICAL BAND

A common and simple method for determining whether a band gap is direct or indirect uses absorption spectroscopy. By plotting certain powers of the absorption coefficient against photon energy, one can normally tell both what value the band gap has, and whether or not it is direct. For a direct band gap, the absorption coefficient is related to light frequency according to the following formula [10].

$$\alpha \approx A^* \sqrt{hf - E_g} \quad (1)$$

$$A^* = \frac{q^2 x_{vc}^2 (2m_r)^{\frac{3}{2}}}{\lambda_0 \epsilon_0 \hbar^3 n} \quad (2)$$

Where: α is the absorption coefficient, f is light frequency, h is Planck's constant, \hbar is reduced Planck's constant

n is the (real) index of refraction, E_g is the band gap energy, q is the elementary charge, ϵ_0 is the vacuum permittivity

A^* is a certain frequency-independent constant, with formula above, Type equation here is a "matrix element", with units of length and typical value the same order of magnitude as the lattice constant [11].

$$m_r = \frac{m_h^* m_e^*}{m_h^* + m_e^*} \quad (3)$$

Where: m_e^* and m_h^* are the effective masses of the electron and hole, respectively, (m_r is called a "reduced mass")

This formula is valid only for light with photon energy larger, but not too much larger, than the band gap (more specifically, this formula assumes the bands are approximately parabolic), and ignores all other sources of absorption other than the band-to-band absorption in question, as well as the electrical attraction between the newly created electron and hole. It is also invalid in the case that the direct transition is forbidden, or in the case that many of the valence band states are empty or conduction band states are full [12].

On the other hand, for an indirect band gap, the formula is:

$$\alpha \propto \frac{(hf - E_g + E_p)^2}{\exp\left(\frac{E_p}{KT}\right) - 1} + \frac{(hf - E_g - E_p)^2}{1 - \exp\left(\frac{-E_p}{KT}\right)} \quad (4)$$

Where: E_p is the energy of the phonon that assists in the transition, K is Boltzmann's constant,

T is the thermodynamic temperature, (This formula involves the same approximations mentioned above.)

Therefore, if a plot of hf versus α forms a straight line, it can normally be inferred that there is a direct band gap, measurable by extrapolating the straight line to the $\alpha = 0$ axis. On the other hand, if a plot of hf versus $\alpha^{\frac{1}{2}}$ forms a straight line, it can normally be inferred that there is an indirect band gap, measurable by extrapolating the straight line to the $\alpha = 0$ axis (assuming $E_p \approx 0$) we get [13].

$$(\alpha hf) = A(hf - E_g)^{\frac{1}{2}} \quad (5)$$

The photon energy (hf) for y-axis can be calculated using Eq. (6).

$$hf = E = \frac{hc}{\lambda} \quad (6)$$

Where h is Planck's constant (6.626×10^{-34} J/s), c is speed of light (3×10^8 m/s) and λ is the wavelength.

Band gap obtained from Eq(5) where

$$(\alpha hf)^2 = A(hf - E_g) \quad (7)$$

Setting $y = \alpha hf, x = hf$ (8)

One gets $y = A(x - E_g)$ (9)

The tangent is given by $\frac{dy}{dx} = A$ (10)

It is important to note according to eq (9) at $y = 0$

$$x = E_g \quad (11)$$

Thus the tangent eq is given by

$$y = ax + b \quad (12)$$

The slope is given according to Eq (2.10)

$$a = \frac{dy}{dx} = A \quad (13)$$

Thus substituting eq (13) in eq (11) yields

$$y = Ax + b \quad (14)$$

The straight line of eq (9) and tangential (13) are the same.

Thus

$$y = Ax + E_g \quad (15)$$

In general if even eq (9) to be generalized to be in the form

$$y = A(x - E_g)^n \quad (16)$$

The equation of tangent is $y = ax + b$ (17)

The slope of the tangent at $x=x_0$ is given by

$$a = \left. \frac{dy}{dx} \right|_{x_0} = nA(x_0 - E_g)^{n-1} \quad (18)$$

The tangent intersect with x-axis, when

$$y = 0, ax = -b, x = \frac{-b}{a} \quad (19)$$

It is clear that for $x < E_g$:

$$y_{real} + y_{imag} = (x - E_g)^n = (-1)^n (E_g - x)^n$$

$$= \left[(-1)^{\frac{1}{2}} \right]^{\frac{n}{2}} (E_g - x)^n = i^{\frac{n}{2}} (E_g - x)^n \quad (20)$$

$$\text{Thus: } y_{real} = 0, \dots, y_{imag} = i^{\frac{n}{2}} (E_g - x)^n \quad (21)$$

But since $y = y_{real}$ hence $y=0$ $x \leq E_g$ (22)

Thus one can for a good approximation requires that

$$y=0 \quad x = E_g \quad (23)$$

Sub this relation in eq(17) to get $0 = aE_g + b$, $b = -aE_g$ (25)

Substance eq (25) in eq (16) to get

$$y = a(x - E_g) \quad (24)$$

Which is the equation of the tangent of the curve described by Eq (15).

To see the intercept of this tangent with the x-axis, substance $y = 0$ in Eq (25) to get

$$0 = a(x - E_g) \quad , \text{ Thus intercept exists at } x = E_g \quad (25)$$

Thus the energy gap is the value of x at the point where the tangent of the curve (16) intersect meet the x-axis.

III. EXPERIMENTAL METHOD

Work method summarized in the following steps:

1. 0.2M solution of Copper acetate dehydrate ($\text{Cu}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$) diluted in methanol and deionized water (3:1) was used for all the films. A few drops of acetic acid were added to improve the clarity of solution.
2. Nitrogen was used as the carrier gas, The nozzle to substrate distance was 30 cm and during deposition, solution flow rate was held constant at $4\text{ml}\cdot\text{min}^{-1}$.
3. The CuO films were deposited onto glass slices, chemically cleaned, using the spray pyrolysis method at different substrate temperature.
4. The optical measurements of CuO films were carried out at room temperature using Shimadzu UV-VIS-1240 scanning spectrophotometer in the wavelength range from 190 to 1100 nm. The substrate absorption is corrected by introducing an uncoated cleaned glass substrate in the reference beam. Energy Band Gap: According to the curve obtained from UV-absorption, the energy band gaps can be measured experimentally. These curve explain the connection between the determined energy E_g from Eqs. (5) and (28) and the square of absorption $(\alpha E)^2$.

IV. RESULTS BAND GAP OF COPPER OXIDE (CuO)

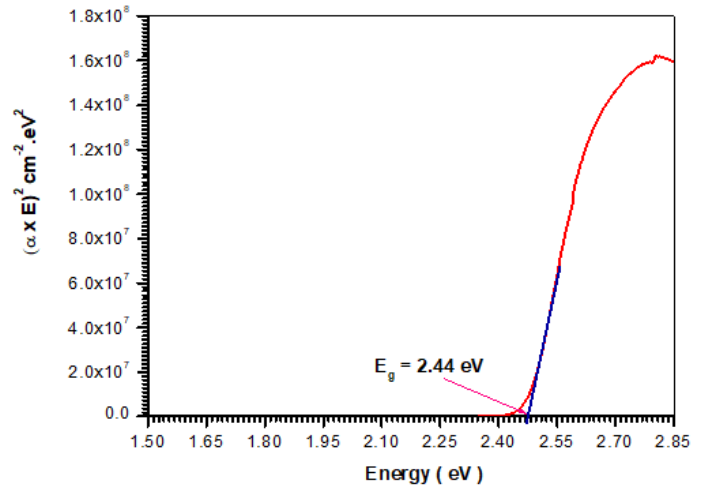


Fig.1: Band gap measurement of CuO at 150°C

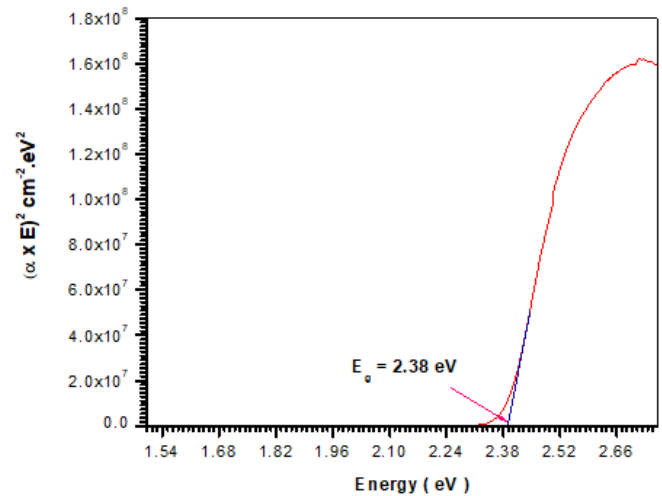


Fig.2: Band gap measurement of CuO at 190°C

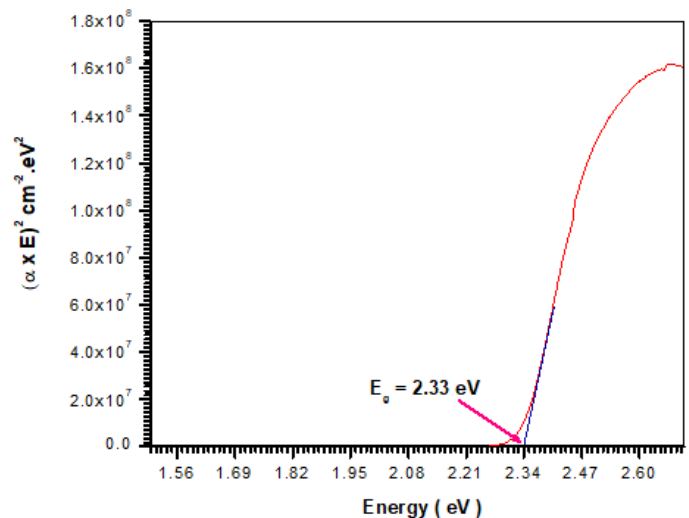


Fig.3: Band gap measurement of CuO at 230°C

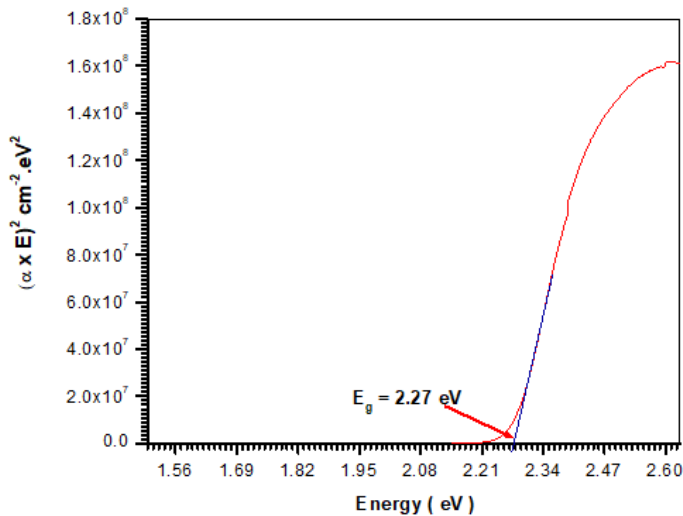


Fig.4: Band gap measurement of CuO at 270°C

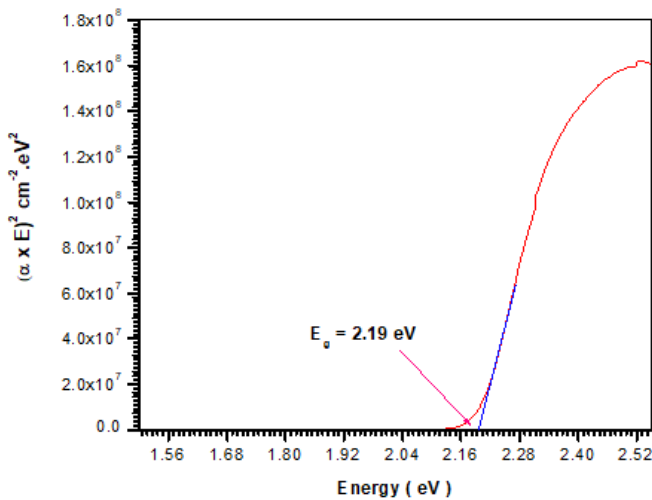


Fig.5: Band gap measurement of CuO at 330°C

Table.1: Variation energy gap with temperature (UV-VIS spectrophotometer)

No	Temperature (T °C)	Copper oxide E _g
1.	150	2.44
2.	190	2.38
3.	230	2.33
4.	270	2.27
5.	330	2.19

V. DISCUSSION

The determined optical band gap values for copper oxide are shown in Table (1). The band gaps of films were obtained at different temperatures ranging from 150°C to 330°C. The values of band gap decrease as temperature increase. It is very striking to note that this result agrees with equation (2.1) and Fig (5.1). The lower band gap of the copper oxide samples are at high temperature 330°C where

they reached 2.16 eV, 3.31eV respectively. The transmittance is min at $\lambda \approx 500 \text{ nm}$ or $500 \times 10^{-9} \text{ m}$ corresponding to photon energy for copper oxide

$$E = \frac{hc}{\lambda} = \frac{6.6 \times 10^{-34} \times 3 \times 10^8}{500 \times 10^{-9} \times 1.6 \times 10^{-19}} \text{ eV}, E = \frac{hc}{\lambda} = \frac{19.8 \times 10^{-26}}{8 \times 10^{-26}} = 2.475 \text{ eV} \quad (26)$$

It is very clear that photons of energy having this value are absorbed. This is not surprising as for as the energy of this photons is just greater than the band gap. Those having energy less than the band gap E_g, i.e E < 2.38 eV for copper oxide

VI. CONCLUSION

From previous results one can conclude that the chemical spray pyrolysis method that has been used to perform the experimental measurements required for this investigation was found to work fairly successfully.

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