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Behavior of Optical Parameters of $CuZnSnO_4$Thin Films
سلوك العوامل البصرية لاغشية $CuZnSnO_4$ الرقيقة

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Abstract

A compound ($CuZnSnO_4$) as thin films is deposited by thermal evaporation method at room temperature onto glass substrates at film thicknesses (100 & 300) nm. The structure of $CuZnSnO_4$films is amorphous as indicated by X-ray diffraction pattern. Optical parameters like, transmittance, energy gap, constants of direct transition, Urbach energy, refractive index, extinction coefficient, and complex dielectric constant are studied. A good property for this compound, it can be used as window layer or absorbance layer with the variation of film thickness.

Keywords: Thermal Evaporation, Thin Films, Film Thickness

الخلاصة

رسب مركب ($CuZnSnO_4$) كاغشية رقيقة بطريقة التبخير الحراري في درجة حرارة الغرفة على قو زجاجية ولاسماك غشاء nm (100 &300) . التركيب عشوائي لاغشية ($CuZnSnO_4$) كما بين نموذج ح الاشعة السينية . درست العوامل البصرية مثل النفاذية، فجوة الطاقة، ثابت الانتقال المباشر، طاقة اورباخ، مع الانكسار، معامل الخمود وثابت العزل المركب. خاصية جيدة لهذا المركب حيث يمكن استخدامه كطبقة نافذة ماصة بتغير السمك.

1. Introduction

A compound ($CuZnSnO_4$)**,** which composes from the mixture of the compounds CuO, ZnO, and SnO_2 at relative atomic weights, is studied. These compounds are almost all of II –VI compounds which crystallize in such a manner that each atom of one element is located at the center of a regular tetrahedron, the apices of which are occupied by atom of the other element, can be formed in wurtzite structure and zincblende structure[1]. The structure of $CuZnSnO_4$ compound was studied in a previous research, for more details, see ref. [2]. The optical properties of a semiconductor are related to intrinsic effect, Based on the intrinsic location of the top of the valence band (V.B) and the bottom of the conduction band (C.B) in the band structure, the electron–hole pair generation occurs directly or indirectly. In this study, optical properties of $CuZnSnO_4$ films are studied. Cu_2ZnSnO_4 films are semiconductor with direct band gap. This property made it useful material for the manufacture of light emitting diodes and semiconductor lasers.

2. Experimental Work

($CuZnSnO_4$) compound were prepared from the mixture of the compounds CuO, ZnO, and SnO_2 at relative atomic weights. The mixture puts in evacuated tube and heated in a furnace at 900 C^o in steps of 200 C^o for 48 hours. Thermal evaporation is used to prepare $CuZnSnO_4$films for two film thickness (100 & 300) nm at room temperature. The deposition by thermal evaporation method is very convenient and most widely used for producing thin films. This method consists of heating the material with resistivity heated boat (Molybdenum) by passing electric current through it in vacuum chamber at pressure between 10^{-5}-10^{-6} Torr.. The rate of deposition is 10 nm/min. In this research, X-Ray diffraction was used to determine the structure of the prepared films by using Philips X-Ray diffract meter system record the intensity as function of Bragg's angle. The source CuKa with radiation of wavelength **λ**=15405A˚ is used. The optical measurements were studied in the wavelength range (250–1100) nm by using UV/V Centre 5 Spectrometer to GBC scientific equipment PTY ltd.

3. Results and Discussions

3.1Structural properties of $CuZnSnO_4$thin films

Fig 1 shows the X-ray diffraction pattern for $CuZnSnO_4$ thin film. The structure is amorphous due to oxygen vacancy in the structure of atomic bound between Zn-Cu-O and Due to the properties of oxygen defect.

3.2 The Transmittance Spectra

The transmittance Spectra for $CuZnSnO_4$ thin films can be shown in Fig. 2, we note that the transmittance of film has minimum value at wavelength 330 nm for the two film thickness (100 &300) nm. For film thickness (100 nm), the transmittance is more than film thickness (300 nm) between wavelength range (250 – 690) nm. For film thickness 300 nm, the transmittance increases in the wavelength range (690-1100) nm. The maximum of transmittance shits towards longer wavelengths with the increase of thickness and this can be attributed to the amorphous structure with increases the defects and dangling bonds [3, 4].

3.3 The Optical Energy Gap

The optical energy gap was measured in the fundamental absorption edge by using the expression for the absorption coefficient, for allowed direct energy gap [5], as

$$(\alpha h\gamma) = B\left(h\gamma - E_g\right)^r \qquad (1)$$

Where hע is photon energy, E_g represents optical energy gap, r indicates the type of transition ($r = \frac{1}{2}$ for allowed direct, $r = \frac{3}{2}$ for forbidden direct , r =2 for allowed indirect and $r = 3$ for forbidden indirect transition) and B is a constant transition.

Fig. 3 shows the relation between $(\alpha h\nu)^2$ against $h\nu$. From the figure, the energy gap was determined by the intercept of the linear part of the curve with X-axis and was found to be (3.3 and 2.7) eV at room temperature for film thicknesses (100 and 300) nm respectively with allowed direct transition . The decrease in energy gap for higher film thickness is due to the increase the atoms with different bonds due to amorphous structure [5]. The constant of allowed direct transition can be found from the slope of the straight line of Fig. 3 according to the relation, $B = (slope)^r$, as indicated in Table 1.

3.4 Urbach Energy

The tail width of localized states of the amorphous structure can be found according to the relation of absorption coefficient (α) as [6]:

$$\alpha(\omega) = \alpha_\circ exp^{(\hbar\omega/E_e)} \qquad (2)$$

The Urbach energy (E_e) in the optical energy gap can be determined from the plot of (lnα(ω)) as a function of (ħω) according to relation (2). E_e represents the reciprocal of the slope of the straight line in Fig. 4 and its values are indicated in Table with the variation of film thickness.

3.5 The Refractive index

The refractive index (n) was determined from the reflectance data using equation [7]:

$$n = \left(\frac{4R}{(R-1)^2} - k^2\right)^{1/2} - \left(\frac{R-1}{R+1}\right) \qquad (3)$$

The variation of refractive index versus wavelength in the range (250–1100) nm for films with thicknesses (100 &300) nm is shown in Fig. 5. The refractive index has high refractive index more than the glass substrate. It has minimum value at 400 nm due to high absorption with the increase of film thickness [8,9]

3.6 Extinction Coefficient

The extinction coefficient was determined by using the equation:

$$k = \frac{\alpha\lambda}{4\pi} \qquad (4)$$

Fig. 6 shows the variation of extinction coefficient with the wavelength. The Extinction Coefficient (k) for the thin film decreases with the increase of wavelength at thickness (300) nm due to increasing transmittance in the infrared region. But for less thickness (100) nm, the opposite behavior can be noticed due to increasing transmittance in the infrared region [10, 11].

3.7 Complex Dielectric Constant

The complex dielectric constant (ε^*) can be represented by the equation:

$$\varepsilon^* = \varepsilon_r - i\varepsilon_i \qquad (5)$$

The real $\varepsilon_r$and imaginary part ε_i of dielectric constant can be calculated by using the following equations

$$(n - ik)^2 = \varepsilon_r - i\varepsilon_i \qquad (6)$$

Where

$$\varepsilon_r = n^2 - k^2 \qquad (7)$$

And

$$\varepsilon_i = 2nk \qquad (8)$$

Figs. (7&8) show the variation of real and imaginary parts of the dilectric constant with wavelenght . the imaginary part repersent the absorption of radiation by free carrier. From the figure we can see the real part for the thin film decreses with wavelenght . Also the imaganry part of dielectric constant of films decreases with wavelenght range. The behavior of real part is the same for refractive index and the behavior of imaginary part is the same for extinction coefficient.

4. Conclusions

This research study behavior the optical parameters for a compound $CuZnSnO_4$ as thin films which have amorphous structure for thicknesses (100 &300) nm. The transmittance spectra for films shift towards longer wavelengths with the increase of film thickness. The optical energy gap decreases with the increase of film thickness. The refractive index of films in the infrared region increases with the increase of film thickness but decreases in the visible region.

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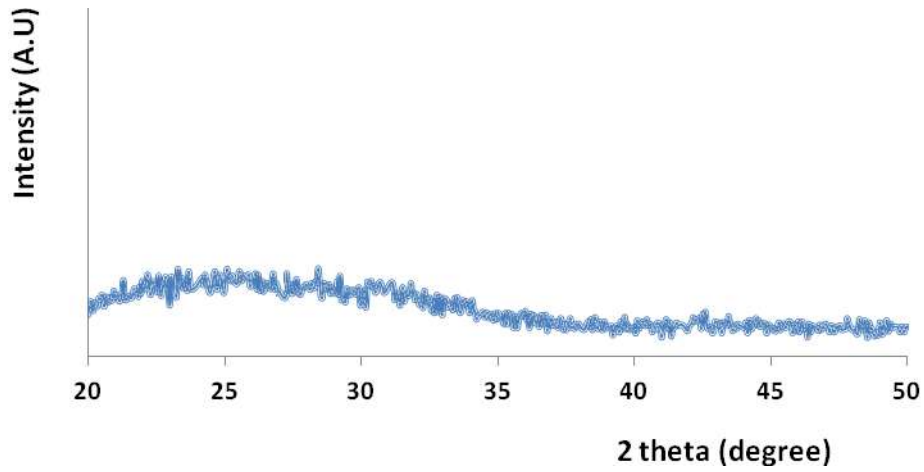

Fig. 1 X-ray diffraction of $CuZnSnO_4$ film

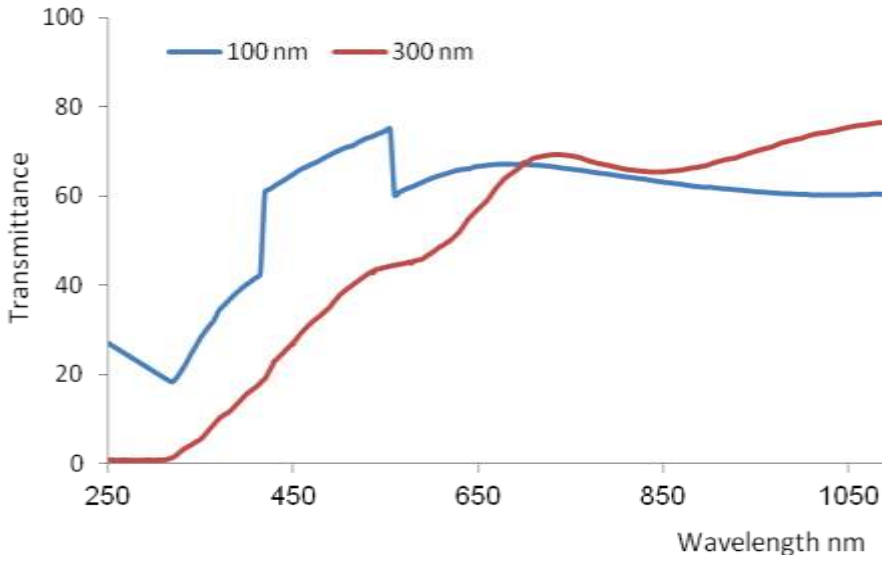

Fig. 2 The Optical transmittance of $CuZnSnO_4$ thin film

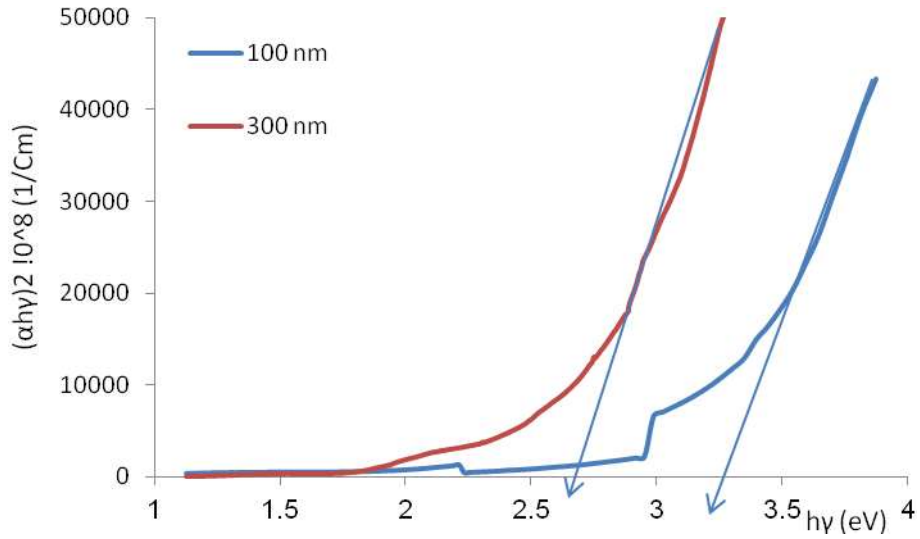

Fig. 3 The Optical Energy gap of $CuZnSnO_4$ thin film

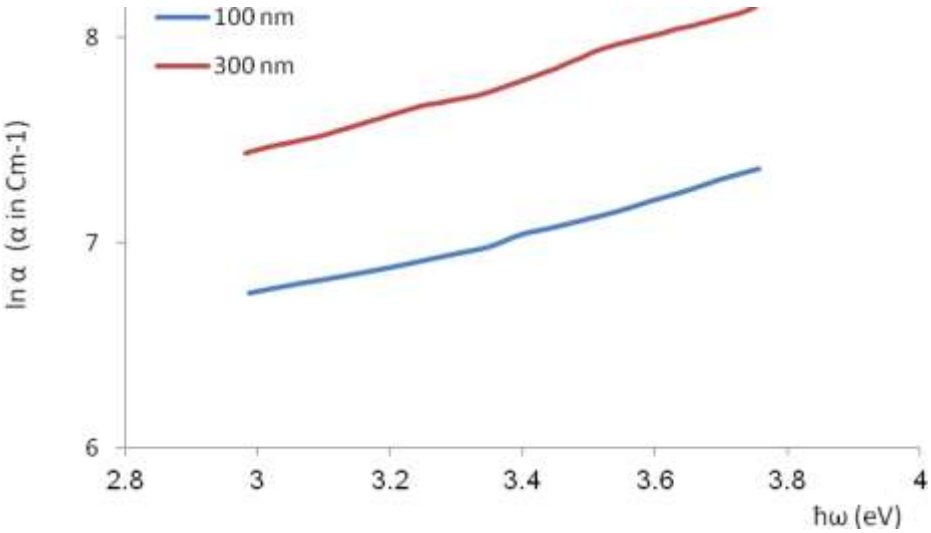

Fig. 4 The relation between lnα(ω) with ħω

Table 1 values of constant of allowed direct transition B and Urbach Energy

Thickness (nm)	E_g (ev)	B ($Cm^{-1}.eV^{1/2}$)	E_e (eV)
100	3.3	35541.5	1.27
300	2.7	40976	1.05

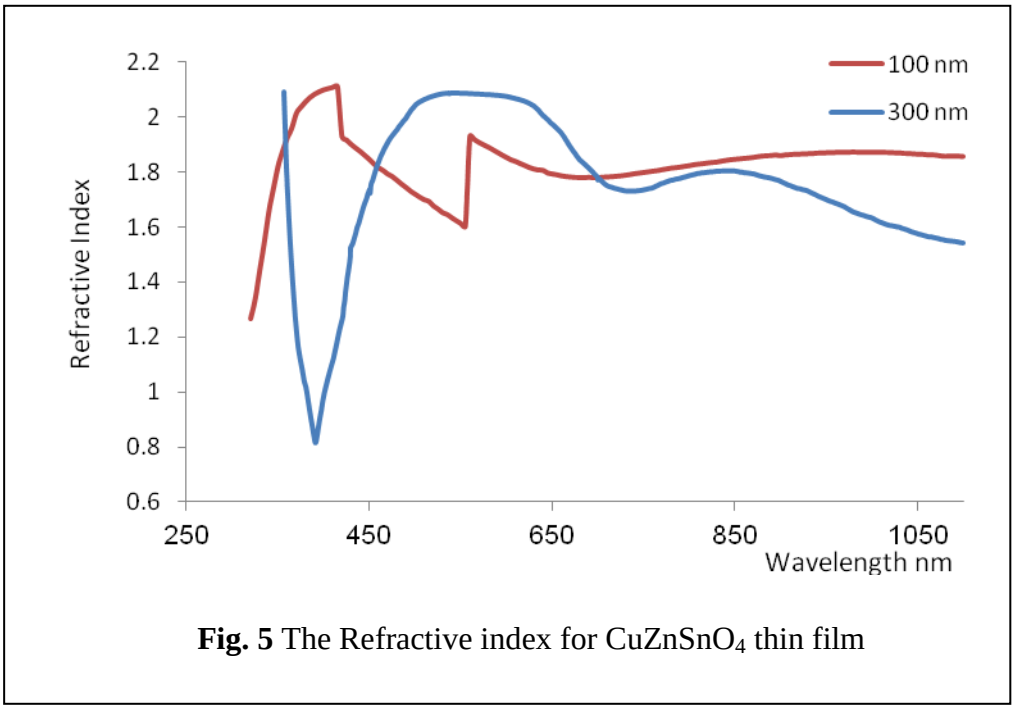

Fig. 5 The Refractive index for $CuZnSnO_4$ thin film

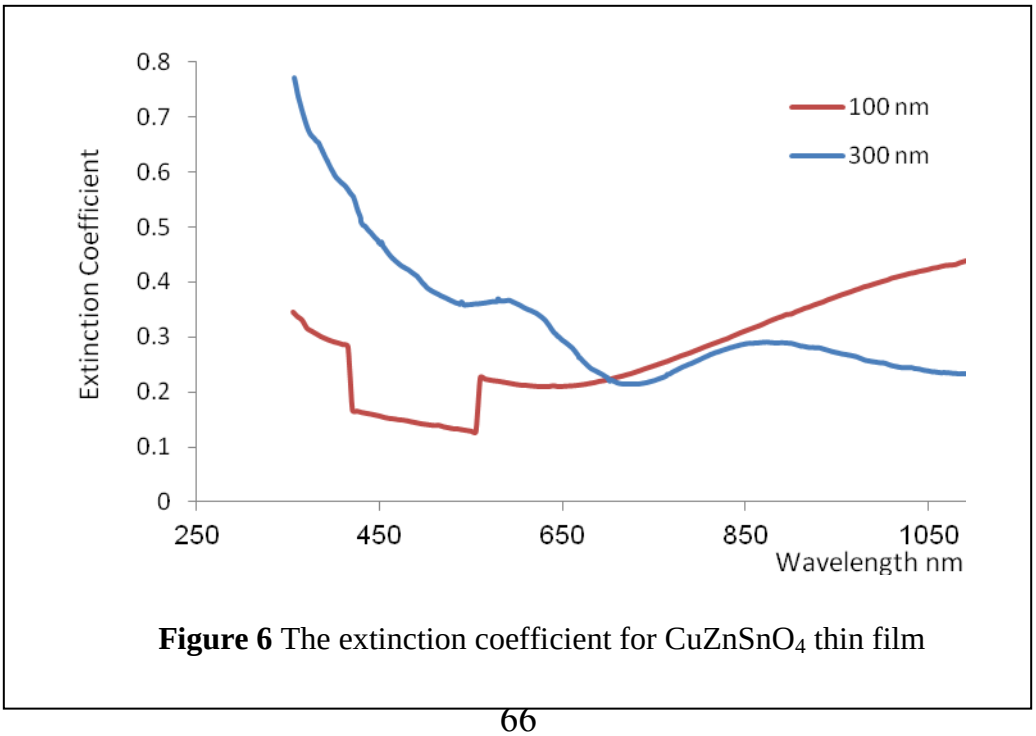

Figure 6 The extinction coefficient for $CuZnSnO_4$ thin film

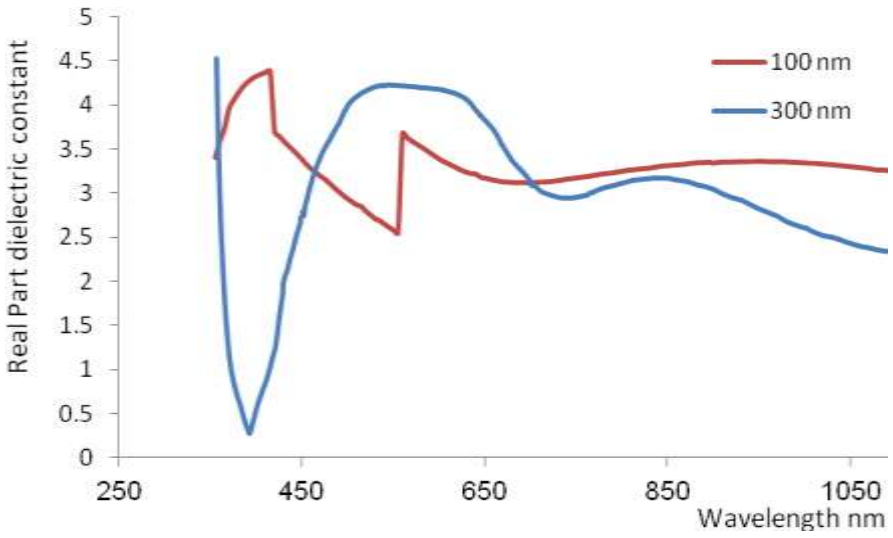

Fig. 7 Real dielectric constant (ε_1) of $CuZnSnO_4$ film

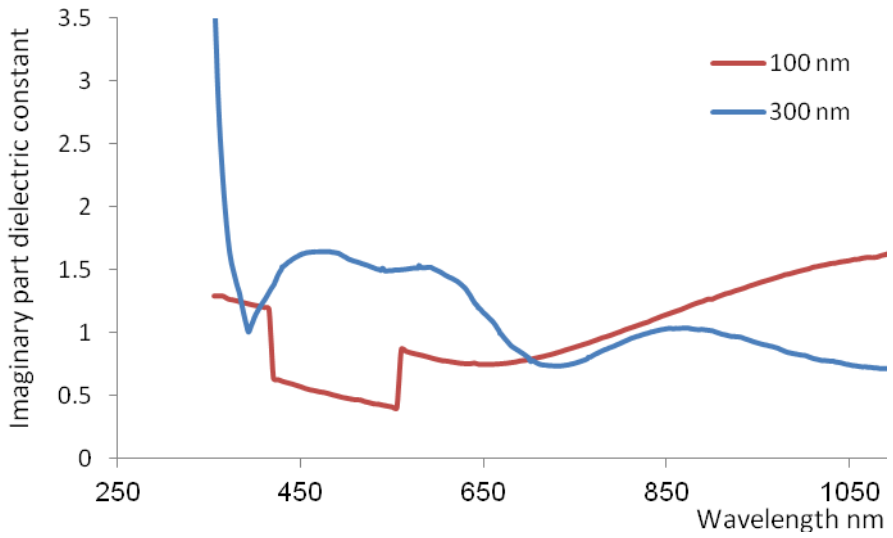

Fig. 8 Imaginary dielectric constant (ε_2) of $CuZnSnO_4$ film