Structure and optical properties of polycrystalline ZnSe thin films: validity of Swanepoel’s approach for calculating the optical parameters

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Abstract

Ultrasonically cleaned glass slides are used as substrates for receiving the different thickness of Zinc selenide (ZnSe) films. The deposition processes of our investigated films were done at room temperature using physical thermal evaporation mechanism under vacuum ≈ 2 × 10^5 mbar. We investigated the optical and structural parameters of ZnSe thin films in correlation with film thickness (200–650 nm). Various techniques such as UV–vis–NIR spectrophotometer, x-ray diffraction lines and field emission scanning electron microscope were used to investigate aforementioned parameters. Structural analysis indicate that the films exhibited cubic preferred orientation along the plane (111) and the crystallinity and crystallite size of films increases linearly with film thickness. The optical band gap ranges from 2.69 to 2.81 eV and it is founded that it increases with film thickness. According to the applied Swanepoel’s approach, it is possible to estimate the optical parameters and average thickness of the ZnSe thin films of different thicknesses with higher accuracy.

1. Introduction

Recently, Zinc selenide (ZnSe), has received considerable attention because of possible application which results from its unique physiochemical properties [1–3]; such as, large band gap with direct transition and low optical absorption in the visible region, suitable refractive, high-rise electrical conductivity, high photo-catalytic activity and environment friendliness [4–7]. Its large exciton binding energy (22 meV) makes ZnSe a good choice to fabricate excitation-related devices. For instance, ZnSe based devices may be used as; green, blue and red light-emitting diodes, photo-detectors, photo-catalysis, solar cells, laser screens and optically sensitive devices. Among the II–VI semiconductor materials, CdS is considered the most extensively used as buffer layer in Cu(In, Ga)Se2 (CIGS) and window layer for the CdS/CdTe solar cells respectively [8]. Much attention has been centered on developing Cd-free layer because of the toxic nature of CdS layers, by using ZnSe instead of CdS as a buffer or window layer material in CdS/CdTe and CIGS based solar cells respectively. Using ZnSe over CdS in solar cell fabrication has many advantages which are related to its non-toxicity, its large band gap which is compared to CdS (≈ 2.4 eV), its high optical transparency (~90%) and its ability to provide a better lattice parameter matching with both CdTe and CIGS absorber layers. Moreover, ZnSe has a great potential for photocatalytic application as a promising photo-catalysis material. So that, the knowledge of structural, morphological, optical and electrical properties of ZnSe thin films is considered so important for improving its applications.

Different deposition methods may lead to different thickness dependencies of the optical parameters of ZnSe thin films [9]. Various physiochemical routes such as, thermal evaporation, pulsed laser deposition, electron beam evaporation, RF-sputtering, molecular beam epitaxy, atomic layer epitaxy, sol-gel deposition, metal organic chemical vapor deposition, hydrothermal, spray pyrolysis and chemical bath deposition can fabricate ZnSe thin films [10–19]. Among these methods, thermal evaporation techniques are useful for large area
applications and supports many advantages, because they are relatively simple, inexpensive and the film development under a thermal equilibrium condition without wasting used material. Moreover, the main parameters of fabrication process such as deposition rate, film thickness and surface morphology can be well controlled [20–23]. Recently, many authors have been considered Swanepoel’s approach for an accurate computation of the optical parameters of ZnSe thin films with different thicknesses [9, 24–26].

In this work, we noted that the film thickness is one of the most significant parameters which affect the physical properties of ZnSe thin films. High quality ZnSe polycrystalline films with various thicknesses are physically prepared by thermal evaporation technique, in which their structural, morphological and optical properties are systematically investigated. The applied Swanepoel’s approach was used for computing the index of refraction and film thickness. That approach depends basically on the extremes of the interference fringes of transmission spectra. The transmission and reflection spectra in the visible region were used to compute the energy band gap values of ZnSe thin films. In addition, the refractive index also calculated by Cauchy dispersion relationship.

2. Experimental details

2.1. ZnSe thin films preparation

ZnSe thin films with many thicknesses (200–650 nm) were prepared by using stoichiometric ZnSe powder of high purity ≥99.999% obtained from Sigma Aldrich Corporation. This powder was used as a source material for thermal vacuum evaporation process. ZnSe thin films have been deposited from a single source using a coating unit (Manufactured using Technology Licensed from Edwards Ltd, Auto 306, 2014) on ultrasonically cleaned microscopic glass substrates. The ultrasonic tool model (T-9) used to wash the substrate using filtered deionized water and acetone. Then, it has been left to dry in a muffle furnace at 120 °C. The glass substrate temperature during deposition process was kept at 300 K. The precipitation rate (2–2.4 Å s−1) and the approximate film thickness were monitored using a digital film thickness monitor model TM200 Maxtek. Figure 1 indicates the schematic diagram of thin film deposition procedure by thermal evaporation technique.

2.2. Investigation technique

The microstructure analysis of ZnSe thin films was performed using Philips x-ray diffractometer (model PW1710, Netherlands) using the copper-κα radiation (λ = 0.15418 nm) with diffraction angle 2θ range from 10 to 80. The surface morphology of ZnSe films were studied by scanning electron microscope model JSM-6100 microscope (JEOL, Japan) with an acceleration voltage of 40 KV. The chemical composition of ZnSe films was also analyzed using energy dispersive x-ray technique (EDX). UV–visible–NIR spectrophotometer model Jasco V-700 was used to determine the optical transmittance T(λ) and reflections R(λ) spectra in wavelength range between 400 and 2500 nm.

The film thickness and the deposition rate were monitoring by means of a digital film thickness monitor model INFINICON (SQM-160). Furthermore, the thickness of the films under study was verified again by using a profilometer model Talsysurf 50. It was found that the film thickness value estimated by optical analysis is around the value obtained from profilometer measurements and thickness monitor with a maximum experimental error about ±4%.

3. Result and dissuasion

3.1. Microstructure analysis by XRD

The typical XRD patterns of ZnSe thin films which are deposited on glass substrates at various thicknesses are presented in figure 2. It is revealed in XDR analysis that the films are described to be polycrystalline in nature and the crystallinity of the films increases by increasing the thickness of the film. Increased crystallinity by increasing film thickness is verified by several authors [27–29]. This is may be attributed to enhancement of forming the cluster, the reordering of atoms and reduced the stress of the film during the film growthindicating that there is an enhancement in the films’ crystallinity. The sharp diffraction peaks observed at 2θ = 27.22° and 72.7° corresponding to (111) and (331) orientations of the cubic ZnSe structure, respectively (ICPDS Data file code: 05-0566). XRD analysis investigated the structural parameters of ZnSe thin films. The films average grain size (Dav) (i.e. coherently diffracting domains) is calculated by using Debye-Scherer formula [30–36].

$$D_{av} = \frac{0.9 \lambda}{\beta \cos \theta}$$  \tag{1}

Where λ is the wavelength of x-radiation source (λ = 1.5418 Å), β is the full width at half-maximum (FWHM) in radians and θ is the Bragg diffraction angle in degrees. We have estimated the average grain size of ZnSe thin
films via XRD line expanding analysis by using Gaussian function in the procedure of fitting as illustrated in figure 3. It is indicated that, the grain size increases linearly with the film thickness and it is observed to be in the range of 14.5–18 nm. Ganbvle et al observed a similar behavior for spray deposited WO3 thin films [37] and Prasada Rao et al for ZnO thin films [28].

Moreover, one can investigate various structural parameters of polycrystalline ZnSe thin films with different thicknesses including the dislocation density ($d_D$), the average lattice strain ($\varepsilon_{av}$), the value of unit cell ($V$) and the number of crystallites ($N_c$) via XRD line expanding analysis by using equations (2)–(5) Respectively [38, 39].

\[
\varepsilon_{av} = \frac{\beta \cos \theta}{4}
\]  
\[
d_D = \frac{15\beta \cos \theta}{4aD_{av}}
\]  
\[
V = a^3
\]  
\[
N_c = \frac{d}{D_{av}}
\]

Where $a$ is the lattice constant for (111) plane and $d$ is the film thickness. The computed structural parameters of the ZnSe thin films are summarized in table 1. It was found that the average lattice strain decreases when the film thickness increases which may be related to a decrease in the concentration of lattice imperfections and then, the grain boundaries decreases as the film becomes thicker. The dislocation density of ZnSe thin film ($d_D$), which represents the defects mount in the film has not changed with the thickness of the film, clarifies the formation of crystallinity films which is described to be good and with high quality. Moreover, the unit cell almost constant; however, the number of crystallites increases with film thickness increase.
3.2. Surface morphology investigation by FESEM

The surface morphologies of ZnSe thin films were studied using the field emission scanning electron microscope (FE-SEM) which comes up with extremely-high resolution imaging at small working distances and low accelerating voltages. The FESEM images of the ZnSe thin films which deposited on glass substrate at different thicknesses are shown in Figure 2. The XRD diffraction patterns of as-deposited ZnSe films at various thickness deposited on glass substrate are shown in Figure 3. The variation of the average grain size ($D_{av}$) and average lattice strain ($\varepsilon_{av}$) of as-deposited ZnSe films at various thickness deposited on glass substrate is also shown in Figure 3.

Figure 2. The XRD diffraction patterns of as-deposited ZnSe films at various thickness deposited on glass substrate.

Figure 3. Variation of the average grain size ($D_{av}$) and average lattice strain ($\varepsilon_{av}$) of as-deposited ZnSe films at various thickness deposited on glass substrate.
thicknesses \( a = 224 \text{ nm} \) and \( b = 633 \text{ nm} \) are shown in figure 4. We observed that the size of the average crystallite increases while thickness increases at the same time. The ZnSe layer is recrystallized by increasing the film thickness in a way that some of the small crystallites group together to larger ones. This is a good matching with what have been previously interpreted in XRD analysis.

### 3.3. Optical analysis of ZnSe films by UV–vis-NIR spectrophotometer

#### 3.3.1. Optical spectra and band gap estimation

The variation of absolute values of transmittance \((T)\) and reflectance \((R)\) spectra in the wavelengths which range from 400 to 2500 nm are presented in figure 5. It is observed that all transmittance spectrums showed the interference fringes in all wavelength range with a sharp fall at the band edge in the range of 400–500 nm; whereas the interference effects disappear below this rang. The intensity value of interference fringe around 90% in the transparent region this value gradually decreasing when the wavelength approaching the absorption edge region. In addition, a blue shift observed in transmittance spectra increases from longer to shorter wavelength with film thickness. Optical flatness and thickness homogeneity of the deposited ZnSe films are indicated by the uniform sequential maxima and minima of the fringes at the transparent wavelength region. This indicates the close relationship between optical band gap and film thickness [40].

The absorption coefficient \(\alpha(h\nu)\) was calculation from the experimental values of transmittance \((T)\) and reflectance \((R)\) by using the following relation [41]:

\[
\alpha = \frac{1}{d} \ln \left[ \frac{(1 - R)^2}{2} + \sqrt{(1 - R)^4 + 4R^2T^2} \right]
\]

(6)

Where \(d\) is considered the film thickness

We evaluated the optical band gaps \((E_g)\) of ZnSe films from the optical transmittance and reflectance data using the Tauc’s relation [42–44]:

![Figure 4. FE-SEM images of as-deposited ZnSe films with two different thickness (a) 224 nm and (b) 633 nm deposited on glass substrate.](image-url)
Here hv is the incident photon energy, K is a constant and r is a number which depends on the nature of electronic transition, according to the electronic transition, the values of r may be taken 1/2, 3/2, 2 and 3 for forbidden direct transition, allowed direct transition, allowed direct transition, and also for forbidden indirect transition respectively. Consider figure 6, which plot the variation of \((\alpha hv)^2\) various hv for ZnSe films with different thickness is linear at the absorption edge, which confirmed direct band gap transition. The film thickness dependence of optical band gap can be related to various factors such as (i) crystal defects which produce localized states that may be change the effective Fermi level, (ii) crystallites size which may be produce quantum confinement effect, (iii) improvement of the phase crystallinity in thin films can be reduce the number of localized states and defects, and thus increasing the band gap [45]. The computed optical band gap values are shown in figure 6. It is noticeable that the band gap is increased from 2.69 eV for the 224 nm thickness to 2.81 eV for the 633 nm thickness. Further, we found that there is a comparison between the calculated band gap and the value of the optical band gap reported for the bulk ZnSe (2.7 eV). It is indicated by these results that ZnSe thin films as a solar cell window layer provides a large band gap which allows transmission of higher energy photons than the band gap of CdS layer.

### 3.3.2. Evaluation of Urbach energy

The optical absorption spectra of semiconducting compounds study is considered an important thing as it gives the main details about the optical band gap and composition. Three main regions contained the optical absorption spectra of the semiconductor; (i) the region generating from defects and impurities which is known as weak absorption region, (ii) the region generating from system disorder and structural perturbation which is known as absorption edge region, and (iii) the strong absorption region which determine the optical energy gap. The exponential part is known as Urbach tail which indicates the characteristic phenomena of absorption curve with respect to photon energy [46, 47]. By using the band tail energy or Urbach energy \((E_{\text{urb}})\) value one can estimate the disorder level of the film structure. \(E_{\text{urb}}\) value can be evaluated using the Urbach empirical relation [48], which is given by use the inverses slope of the liner plot of absorption coefficient \(\ln(\alpha)\) versus photon energy \((hv)\) as presented in figure 7.

\[
(\alpha hv) = K (hv - E_g)^r
\]

\[
\alpha = \alpha_0 \exp \left( \frac{hv}{E_{\text{urb}}} \right)
\]

\[
\ln(\alpha) = \ln(\alpha_0) + \exp \left( \frac{hv}{E_{\text{urb}}} \right)
\]

Where \(\alpha_0\) is the material—depending constant

It is shown in figure 8 that the \(E_{\text{urb}}\) decrease by increase the film thickness and the optical band gap that may be in a relation with the improvement in the structure and suggests that the optical band gap is controlled by the disorder in the film network [49].

![Figure 5](image-url) The spectral distribution of transmittance and reflectance of as-deposited ZnSe films at various thickness deposited on glass substrate.
Figure 6. Direct optical band gap determination by Tauc relation of as-deposited ZnSe films at various thickness deposited on glass substrate.

Figure 7. Plot of the absorption coefficient $\ln(\alpha)$ versus photon energy ($h\nu$) of as-deposited ZnSe films at various thickness deposited on glass substrate.
3.3.3 Evaluation of the film thickness and refractive index

Considering Swanepoel’s enveloped approach that developed the Manifacier et al. idea (Manifacier’s idea) of creating envelops of interference maximum and minimum to estimate ZnSe thin films thickness and the refractive index as can be seen from figure 9. The basic approximate refractive index value of the film \( n_R \) in the spectral bands of medium and weak absorption can be estimated as in the following equation [8]

\[
 n_R = [N_t + (N_t^2 - s^2)^{1/2}]
\]

Where,

\[
 N_t = 2s \left( \frac{T_M - T_m}{T_M T_m} \right) + \frac{S^2 + 1}{2}
\]

In this part, \( T_M \) and \( T_m \) are the utmost values of transmittance and the least values at a certain wavelength, respectively. There are two values, one of them comes from an experimental interference extreme and the other value is evaluated from the corresponding envelope by using the Origin Lab 8 program. In addition, the refractive index of the substrate (here glass) which calculated by the following expression:

\[
 s = \frac{1}{T_s} + \left( \frac{1}{T_s} - 1 \right)^{1/2}
\]

Where \( T_s \) is the utmost value of the transmittance spectrum of glass substrate (figure 9).

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Figure 8. Optical band gap (\( E_g \)) and Urbach energy of as-deposited ZnSe films at various thickness deposited on glass substrate.

Figure 9. A typical transmittance \( T(\lambda) \) and reflectance \( R(\lambda) \) spectra of the as-deposited ZnSe films at \( d = 633 \text{ nm} \) evaluated by Swanepole’s envelops method.
The precision of this first calculation of the refractive index is enhanced after evaluating \(d\). The fundamental relation who gives the description of the interference fringes as shown in the following equation:

\[
2nd = m\lambda
\]

where \(m\), \(n\), \(d\), and \(\lambda\) are half integer for minima and integer for maxima, radiation wavelength, film thickness and refractive index respectively. Furthermore, if \(n_{R1}\) and \(n_{R2}\) are the refractive indices evaluated at two neighboring maximum or minimum at \(\lambda_1\) and \(\lambda_2\), respectively, then the film thickness \(d\) is given by the following expression:

\[
d = \frac{\lambda_1 \lambda_2}{2(\lambda_1 n_{R1} - \lambda_2 n_{R2})}
\]

Table 2 shows the thickness of the film (\(d\)) and the index of refractive (\(n\)) values which evaluated by using equations (10) and (14). The estimated refractive index values which are corresponding to the film thickness (224–633 nm) range from 2.14 to 2.48. ZnSe thin films at lower thickness which have high refractive index values make these films suitable for solar cells and antireflective applications [50]. The values of refractive index (\(n\)) in whole wavelengths which calculated using Cauchy’s dispersion relationship as:

\[
n(\lambda) = A + \frac{B}{\lambda^2}
\]

Where \(A\) and \(B\) are Cauchy’s constant and they depend on the type of thin film material. These constants were determined from \(n\) versus \(\lambda^{-2}\) linear plot. The spectral reliance of refractive index (\(n\)) on the wavelength (\(\lambda\)) for ZnSe thin films at various film thickness are present in figure 10. It is indicated that when refractive index (\(n\)) decreases, wavelength (\(\lambda\)) increases at the same time which shows the normal dispersion behavior of ZnSe thin films. It is noticeable that that the refractive index increases linearly with the film thickness which may lead to the increase of crystallite size and decrease in micro-strain as shown in figure 2 [51]. It is expected that the refractive index value depend in its increase on crystallite size value because of the effect of quantum confinement [52].

### 3.3.4. Electronic polarizability

One of the most significant characteristics in examining the optical properties of any material is the average electronic polarizability of ions. The electronic polarizability (\(\alpha_p\)) can be derived according to Clausius–Mossotti’s relationship of dielectric constant as given in the following formula [53, 54]:

\[
\alpha_p = \left( \frac{n^2 - 1}{n^2 + 2} \right) \left( \frac{3M}{4\pi Nd} \right)
\]

This formula provides a connection between a macroscopic quantity (the dielectric constant) and a microscopic quality (polarizability). In addition, it is utilized to calculate the electronic polarizability (\(\alpha_p\)) of the compound through the index of refractive (\(n\)), whereas \(d\) and \(M\) are the density of material and the molecular weight respectively, and \(N\) is the number of Avogadro. The proportion \((n^2 - 1)/(n^2 + 2)\) in equation (16) is named the reflection loss (RL). Figure 11 presents the RL of the ZnSe films at various thicknesses as a function of \(h\). Table 2 summarizes the electronic polarizability (\(\alpha_p\)) values of ZnSe thin films estimated by extrapolation of linear part towards \(\gamma\)-axis in equation (16). It is shown by the results that the electronic polarizability (\(\alpha_p\)) increases while the film thickness increases as well and this may be attributed to increase the average particle size.

### 3.3.5. Dispersion studies

The study of refractive index (\(n\)) dispersion or single oscillator energies which proposed by Wemple and DiDomeneicco (WD), plays a significant role for optical materials investigation. The refractive index dispersion is considered an important factor in telecom mutation and also in devices modeling for spectral dispersion. Below the absorption region, the dispersion energy (\(E_d\)) and oscillator energy (\(E_o\)) of ZnSe thin films can be obtained using curve fitting the of Wimple-DiDomeneicco dispersion relationship [55].

\[
(n^2 - 1) = \frac{E_d E_o}{[E_o^2 - (\hbar \nu)^2]}
\]

By fitting the lines and plotting \((n^2 - 1)^{-1}\) versus photon energy \((\hbar \nu)^2\) for ZnSe film as presented in figure 12. The values of both dispersion energy (\(E_d\)) and oscillator constants (\(E_o\)) directly calculated from the slope \((1/E_o E_d)\) and the intercept \((E_o/E_d)\), respectively (i.e., table 2). The increase of film thickness and the reduction of oscillator energy \(E_o\) can be interpreted to the optical transmission spectra shift toward the higher wavelengths [56]. In addition, the basic information about the film structure and density such as static refractive index \(n_0\) can be estimated from the oscillator parameters \(E_o\) and \(E_d\) values by using the following relation:

\[
n_0 = \sqrt{1 + \frac{E_d}{E_o}}
\]
Table 2. The refractive index (n), static refractive index (n₀), high frequency dielectric constant (ε∞), dispersion energy (E_d), single oscillator energy (E₀), static dielectric constant (εs), free carrier concentration (N), plasma frequency (ω_p), relaxation time (τ), oscillator wavelength (λ₀), oscillator strength (S₀) and electronic polarizability (α_p) respectively, of as-deposited ZnSe thin film at various thickness deposited on glass substrate.

| Thickness (nm) | n     | n₀    | ε∞   | E_d  | E₀   | ε_s  | N x 10¹⁹ (cm⁻³) | ω_p x 10¹⁴ (s⁻¹) | τ x 10⁻¹⁰ (s) | λ₀ (nm) | S₀ x 10⁹ (m⁻²) | α_p x 10⁻²⁴ |
|---------------|-------|-------|------|------|------|------|-----------------|-----------------|-------------|--------|----------------|------------|
| 224           | 2.14  | 2.100 | 4.76 | 13.2 | 3.88 | 4.413| 5.14            | 2.89            | 1.50        | 320    | 3.33           | 5.90       |
| 261           | 2.30  | 2.109 | 4.85 | 13.3 | 3.86 | 4.448| 5.52            | 3.00            | 1.20        | 319    | 3.38           | 6.39       |
| 313           | 2.30  | 2.121 | 4.90 | 14.4 | 3.84 | 4.498| 5.21            | 2.90            | 0.64        | 369    | 3.38           | 6.40       |
| 352           | 2.31  | 2.122 | 5.00 | 11.7 | 3.35 | 4.501| 5.40            | 2.96            | 0.590       | 303    | 2.57           | 6.42       |
| 557           | 2.31  | 2.142 | 5.15 | 10.9 | 3.05 | 4.590| 5.41            | 2.97            | 0.9        | 405    | 2.18           | 6.44       |
| 633           | 2.48  | 2.168 | 5.47 | 9.89 | 2.67 | 4.703| 6.90            | 3.35            | 1.00        | 462    | 1.73           | 7.88       |
One the other hand, the complex dielectric constant consists of two main parts (real \( \varepsilon' \) and imaginary \( \varepsilon'' \) parts) according to the following relation:

\[
\varepsilon(h\nu) = \varepsilon'(h\nu) - i\varepsilon''(h\nu)
\]

(19)

The \( \varepsilon' \) and \( \varepsilon'' \) values can be calculated by using the following formulas [57]:

\[
\varepsilon'(h\nu) = n^2(h\nu) - k^2(h\nu)
\]

(20)

\[
\varepsilon''(h\nu) = 2n(h\nu) - k(h\nu)
\]

(21)

In the real part, the high frequency dielectric constant \( \varepsilon_{\infty} \), which describes the contribution of free carrier electric susceptibility and lattice vibration modes of dispersion, can be written as in the following relation [58, 59]:

\[
\varepsilon' = n^2 - k^2 = \varepsilon_{\infty} - \frac{\varepsilon^2}{4\pi^2\varepsilon_0} \left( \frac{N}{m^*} \right) \lambda^2
\]

(22)

where \( \varepsilon' \) is the real part of residual dielectric constant or the high frequency dielectric because of the ion core, \( k \) is the extinction coefficient \( (k = \alpha \lambda / 4\pi) \), \( c \) is the speed of light, \( e \) is the charge of electron, \( m^* \) is the charge carrier effective mass, \( \varepsilon_0 \) is the free space permittivity and \( N \) is the conduction band free carrier concentration. Obeying
the free electron Drude model ε′ has a linear function of \( \lambda^2 \) with negative slope as shown in figure 13. Values of \( N \) and \( \varepsilon_\infty \) which were calculated from the slope and intercept of Drude model relationship (equation (22)). The electron plasma frequency at which the electrons pair with oscillating electric field is in the form:

\[
\omega_p^2 = \frac{N}{m^*} \left( \frac{\varepsilon^2}{\varepsilon_0 \varepsilon_\infty} \right)
\]

The calculated values of \( n_0, \varepsilon_\infty, N \) and \( \omega_p \) at various thicknesses were reported in table 2.

In the imaginary part, according to the free electron Drude model the dielectric loss \( \varepsilon'' \) should be a linear function of \( \lambda^2 \) in the following relation (figure 14):

\[
\varepsilon'' = 2nk = \frac{1}{4\pi^2\varepsilon_0} \left( \frac{\varepsilon^2}{\varepsilon_0} \right) \left( \frac{N}{m^*} \right) \left( \frac{1}{\tau} \right) \lambda^2
\]

The optical relaxation time \( \tau \) value can be estimated from the slope quantity \left[ \frac{1}{4\pi^2\varepsilon_0} \left( \frac{\varepsilon^2}{\varepsilon_0} \right) \left( \frac{N}{m^*} \right) \left( \frac{1}{\tau} \right) \right] \) (i.e., table 2) which is resulted from linear regression of equation (24).

Furthermore, oscillator wavelength (\( \lambda_0 \)) and the oscillator strength (\( S_0 \)) for the ZnSe thin film can be also determined by using the single term Sellmaier oscillator [59]:

Figure 12 Variation of \( 1/(n^2 - 1) \) versus of \((hv)^2\) of the as-deposited ZnSe films at various thickness deposited on glass substrate.

Figure 13. Variation of the dielectric constant \( \varepsilon' \) versus \( \lambda^2 \) of the as-deposited ZnSe films at various thickness deposited on glass substrate.
This relation can be modifying as the following:

\[
\frac{(n_0^2 - 1)}{(n^2 - 1)} = 1 - \left(\frac{\lambda_0}{\lambda}\right)^2
\]

(25)

This relation can be modifying as the following:

\[
(n^2 - 1)^{-1} = \frac{1}{S_0\lambda_0^2} - \frac{1}{S_0\lambda^2}
\]

(26)

Figure 15 illustrate the variation of \((n^2 - 1)^{-1}\) versus \(\lambda^{-2}\) of as-deposited ZnSe films at various thickness deposited on glass substrate. \(S_0\) and \(\lambda_0\) values which estimated from the slope \((1/S_0)\), and the intercept \(\left(\frac{1}{S_0\lambda_0^2}\right)\) on the vertical axis are given in table 2.

4. Conclusion

In summary, we investigated the dependence of the structural and optical properties of ZnSe thin films on film thickness. Thermal evaporation technique is employed to deposit different films thickness from 200 to 650 nm on glass substrates. It is revealed by XRD examination that the films have a nanocrystalline nature and zinc-blende structure with preferred reflection (111). By using XRD line broadening analysis, various structural parameters were extracted such as the average grain size \((D_{avg})\), the average lattice strain \((\varepsilon_{avg})\), the dislocation density \((\delta_d)\), the value of unit cell \((V)\) and the number of crystallites \((N_c)\). The calculated average grain sizes, for
investigated thin films, ranges from 14.5 nm to 18 nm and its values increase with increasing film thickness from 224 nm to 633 nm. The dislocation density and lattice strain calculated values indicate forming high quality and good crystallinity films. The straight forward analysis suggested by Swanepoel’s approach, which depends basically on the extremes of the interference fringes use has been used to calculate the refractive index and the film thickness. It was found that, the Swanepoel’s approach is an effective way to estimate the refractive index and film thickness of ZnSe thin films. In addition, the refractive indices for all investigated films were extrapolated by the relationship of Cauchy dispersion over the whole spectral zone from 400 to 2500 nm. ZnSe thin films at lower thickness which have high refractive index values make these films suitable for solar cells and antireflective applications. The average values of transmittance for all films were more than 90% in the visible zone. It was found that the optical band gap for investigated films increases when film thickness increases and ranges from 2.69 eV to 2.81 eV. Moreover, the refractive index, dielectric constant, urbah energy, electronic polarizability and dispersion energy parameters of ZnSe thin films have been discussed in detail.

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