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Effect Of Thickness On Structural And Optical Properties Of ZnxCd1-xS Thin Films Prepared By Chemical Spray Pyrolysis

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Abstract: Zn0.5Cd0.5S polycrystalline thin films of different thickness were deposited on cleaned glass substrates by spray pyrolysis technique. X-ray diffraction was used to characterize the thin films. X-ray diffraction study showed that, all the films have the hexagonal, wurtzite structure. Grain sizes calculated from Scherer relation are in the range of 47.02-48.21 nm and the grain size of the thin films are observed to increase with the increase in the thickness of the sample. The optical properties of the polycrystalline thin films were investigated by the UV- spectroscopy. The band gap of the thin films is found to be direct allowed transition and decreases with the increase of thickness of films in the range of 2.85- 2.7 eV. Extinction coefficient k showed oscillatory behavior in lower band edge region. The Zn0.5Cd0.5S polycrystalline thin films are suitable for solar cell application.

Keywords: Control ZnS, CdS , ZnCdS thin films, structure properties, optical properties, ternary compounds.

1. Introduction

The synthesis and characterization of polycrystalline materials have attracted much attention not only because of their exceptional properties [1] , but also due to their structure and temperature dependent properties and great potential for many technological applications. Recently, the wide one of the most important properties leading to the great experimental interest in these materials. CdS and ZnS are a suitable window layer for solar cells [2] and also finds applications as interference filters, optical fibers, optical instruments, coated glazing for windows, solar energy collectors and low coast flat panel solar cells. Optical constant as input data in design process of the thin film devices gives the designer an additional tool for optimization of the product design, and thus an accurate knowledge of optical constant over wide range of wavelength is essentially important.

Many techniques have been reported for the deposition of ZnxCd1-xSthin films . These include are sputtering [3], pulse laser evaporation [4], physical vapour deposition [5], electrodeposition [6], screen printing [7], spray pyrolysis [8], and chemical bath deposition (CBD) [9–10] metal organic vapour phase epitaxial (MOVPE) /metal organic chemical vapour deposition (MOCVD) [11], The present study is centered over the effect of thickness on the structural and optical properties of spray pyrolysis ZnxCd1-xSpolycrystalline thin films. X-Ray diffraction (XRD), Ultraviolet-visible(UV–VIS-NIR) are used to characterize the samples. Optical constants, such as optical bandgap, absorption coefficient , ar evaluated from the optical spectra.

2. Experimental Details

ZnxCd1−xS thin films were produced on a glass substrate by the spray pyrolysis technique .The ZnCl2,CdCl2 salts and H2NCSNH2 were dissolved in deionized water in separate beakers .Aqueous solutions of ZnCl2,CdCl2 salts and H2NCSNH2 were used as the sources of Zn, Cd, S, respectively . The ZnCl2,CdCl2 and H2NCSNH2 solutions were mixed for 30 min. With a magnetic stirrer. The compositions of the solutions used to fabricate the ZnxCd1-xS thin films are shown in Table1 in terms of the nominal concentrations in the deposition solution. The substrate temperature was regulated at (400±20°C) during the deposition process using a resistive heater and a thermocouple. Glass substrates were prepared by cutting (2.5×2.5) cm2 pieces and cleaning them by water and they were placed in the microwave until we used them. In order to spray the solution onto the substrate using an ultrasonic atomizer, nitrogen (N2) Was used as the carrier gas at a pressure of 3bar with a deposition rate of 3cm3/min during the deposition process. At the end of the spraying process ,nitrogen (N2) was flowed onto the thin films formed on the glass substrate for 3min in order to dry them .

They were then cooled down naturally at room temperature .

Structural characterization of the ZnxCd1−xS thin films was carried out by XRD using Cu kα radiation in the Bragg configuration . The optical absorption spectra of the ZnxCd1−xSthin films were obtained in the wavelength range 300 to1200nm using a perkin-Elmer Lambda 2UV-Vis double –beam spectrometer.

Table 1: Solution used for the production of Zn_xCd_{1-x}Sthjn films.

NominalCompositionof $Zn_xCd_{1-x}S$	$CdCl_2$(0.1) M (ml)	ZnCl2(0.1) (ml)	$H_2NCSNH_2$0.1M (ml)
0.5	12.5	12.5	25

3. Results and Discussion

The thickness of the Zn0.5Cd0.5S thin films deposited on glass substrate as measured using SE was found to be 200 nm, 300 nm and 400 nm. Effect of the change in thickness of the film on the structural and optical properties using the XRD andUV-VIS absorption spectroscopy is presented in the following sections.

3.1 X-ray diffraction analysis

Fig. 1 shows the X-ray diffraction patterns of the three Zn0.5Cd0.5S thin films deposited on glass substrate. Deposited films were uniform, reflective, adherent and yellow in colour. A strong peak with 2θ value about 27.766° corresponds to the (002) crystalline plane of Zn0.5Cd0.5S is present in all the three XRD patterns. This peak in these XRD could be indexed to hexagonal structure of Zn0.5Cd0.5S and the 2θ value is consistent with the value in standard card (JCPDS).

The crystallites size of the grains in the films is estimated using the Scherer's formula [12] $D=0.9\lambda/\beta\cos\Theta$,
Where, β: is the full width at half maximum in radian, λ:is the X-ray wavelength (0.15406nm).

the dislocation density(δ)is found using[13] $\delta=1/D2$.
It is interesting to note that the grain size improves and the defects like dislocation density decrease with film thickness. This may be due to the improvement in crystallinity in the films with film thickness.
grain size (D)and Dislocation density (δ) for different thickness are shown in table2 Using the Miller indices of these planes, the lattice parameters a=b and c of the unit cell are evaluated according to the relation[12]: $1/d^2=4/3[(h^2+hk+k^2)/a^2]+(l^2/c^2)$, where: d is the interplaner spacing, and (h,k,l) are the Miller indices. The calculated value of the lattice parameter are a=b=4.16A°, and c=6.42A°. The interplaner distance (d), lattice parameters (a) are shown in table 3.

Table 2: grain size (D) and Dislocation density (ρ) for different thickness.

Dislocation density (δ)cm2	Grain size (D) nm	(h k l)	thickness nm
4.52	47.02	002	200 nm 300nm 400nm
4.3	48.21	002	
4.37	47.83	002	

Table 3: Structural parameters for Zn0.5Cd0.5S thin films.

film	2 θ	d(exp)nm	hkl	a(nm)
$Zn_{0.5}Cd_{0.5}S$	25.198	0.353	100	0.407
	27.766	0.321	002	-
	29.2465	0.305	101	0.4
	37.8334	0.2375	102	0.407
	43.5581	0.2069	110	0.4138
	49.0852	0.1854	103	0.48
	54.2176	0.1689	200	0.39

3.2 Optical Properties

Transmittance spectra of films were recorded as a function of wavelength in the range of 350-1200nm. The transmittance spectra of the Zn0.5Cd0.5S films in the visible region for the different thickness films are shown in the Fig.2. It reveals that the transmittance decreases with the increase of film thickness. Fig.3 shows the Absorbance Spectra of Zn0.5Cd0.5S thin films for various thickness are in the range of 350-1200nm ,the absorbance increases with the increasing of film thickness. Absorption coefficient (α) associated with the strong absorption region of the films was calculated from absorbance (A) and the film thickness (t) using the relation : $\alpha = 2.3026\ A/t$. Absorption coefficient of the Zn0.5Cd0.5S films for the different thickness films increases with thickness as shown in Fig.4.

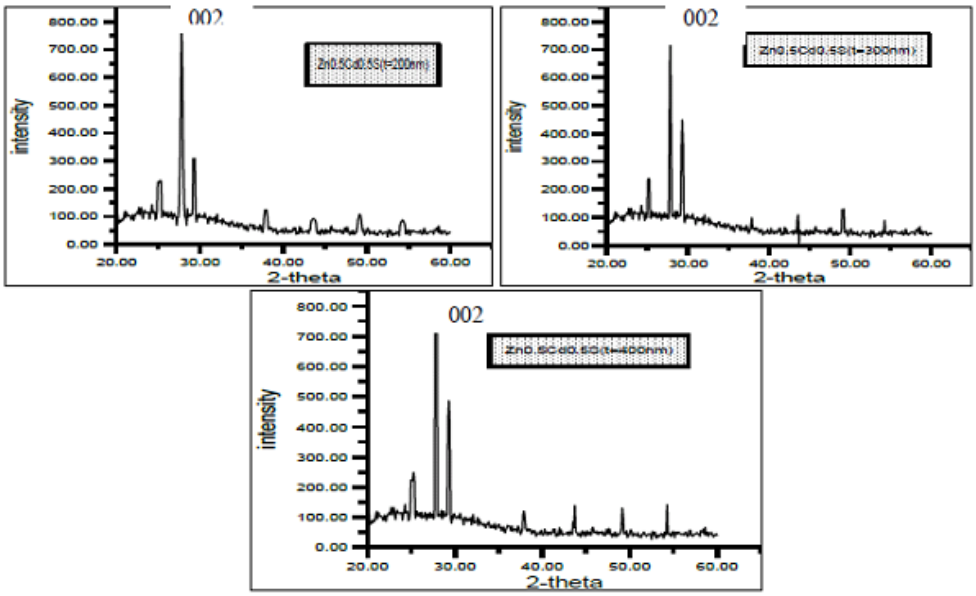

Figure 1: X-ray diffractograms of $Zn_{0.5}Cd_{0.5}S$ thin film for different thickness.

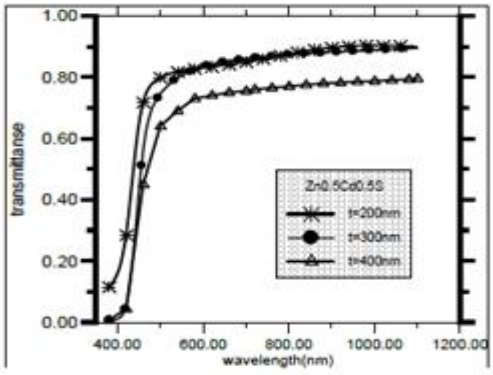

Figure 2: transmittance spectra of th of $Zn_{0.5}Cd_{0.5}S$ films for the different thickness**.**

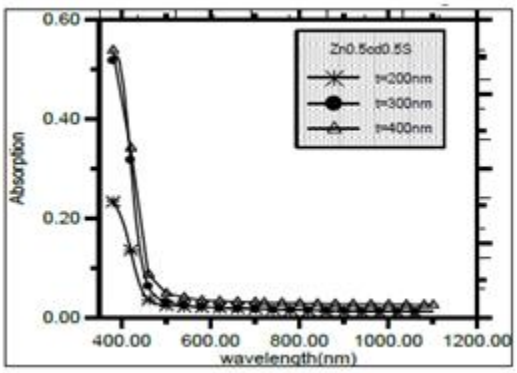

Figure 3: Absorbance spectra of $Zn_{0.5}Cd_{0.5}S$ films for the various thickness.

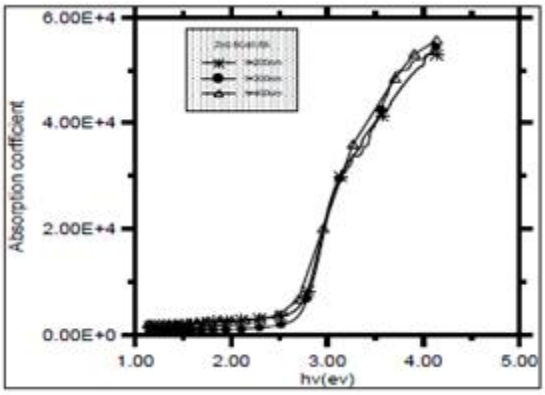

Figure 4: Absorbance coefficient of $Zn_{0.5}Cd_{0.5}S$ films for the various thickness.

Fig shows that the value of absorption coefficient > 104 ,that means the type of transition is direct and allowed.

Fig.5 shows that the extinction coefficient (K) increases with increasing of film thickness. The extinction coefficients are calculated using the equation. K= 2.303 λ log (1/T) / 4πt The extinction coefficient (K) is directly related to the absorption of light. In the case of polycrystalline films, extra absorption of light occurs at the grain boundaries [14]. This leads to non-zero value of (K) for photon energies smaller than the fundamental absorption edge [15]. The optical band gab can be obtained by extra plotting the linear portion of the plot (αhγ)2 Versus hγ. From the plot, the variation of (αhγ)2 Versus photon energy for different thickness (200 nm, 300 nm, 400 nm) Zn0.5Cd0.5Sthin films are shown in Fig. 6.

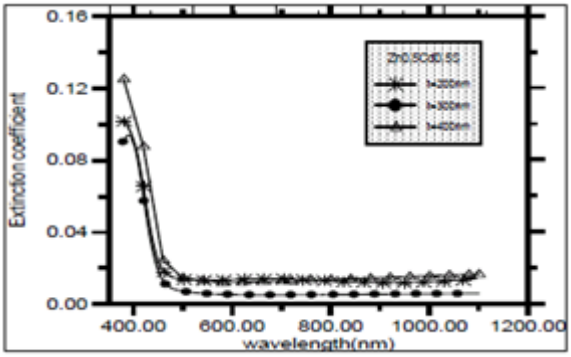

Figure 5: extinction coefficient of $Zn_{0.5}Cd_{0.5}S$ films for the various thickness.

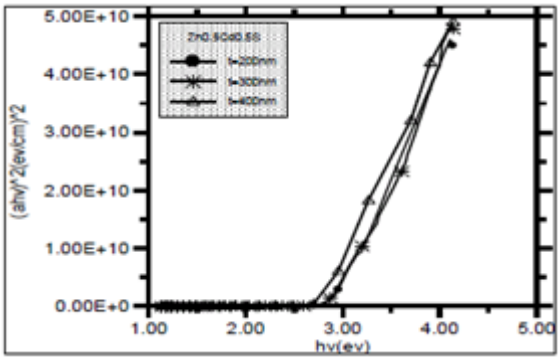

Figure 6: A plot of $(\alpha h\gamma)^2$ Vs. (hν) for $Zn_{0.5}Cd_{0.5}S$ thin films for the various thickness.

From these absorption peaks, the direct and allowed band gap energy is evaluated from the plot (αhγ)2 Versus hγ as shown in table 4.

Table 4: Variation of energy gap with thickness.

Band gap energy (eV)	Thickness nm
2.85	200
2.8	300
2.7	400

The observed decrease in the band gap energy with increases in thickness is due to the changes in the barrier height to the size of the grain in crystalline film and large density of dislocation. Real dielectric Constant (ε1) and imaginary part(ε2) are increases with the increase of thickness (t)of the films are shown in Fig. 7,8 respectively. (ε1) and (ε2) are calculated using the equations: $\varepsilon_1=n_0^2-K_0^2$ & $\varepsilon_2=2n_0K_0$, where n_0 is refractive index .

4. Conclusions

Zn0.5Cd0.5Sthin films prepared by spray pyrolysis are polycrystalline nature with hexagonal structure. The transmittance and absorbance spectra in the range of 350-1200nm has been taken by using UV .visible spectrometer. In absorbance spectra, the material has a high absorbing nature. The observed band gap energy is inversely dependent on film thickness.

Extinction coefficient, real dielectric Constant and imaginary part are increases with the ncrease of thickness.

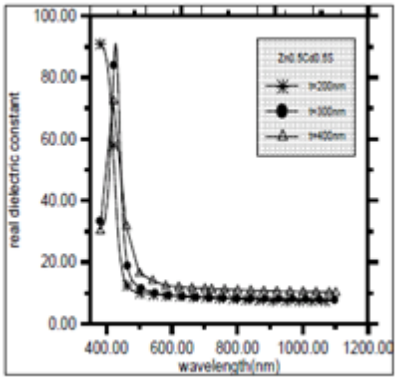

Figure 7: Real Dielectric Constant of $Zn_{0.5}Cd_{0.5}S$ thin films for the various thickness.

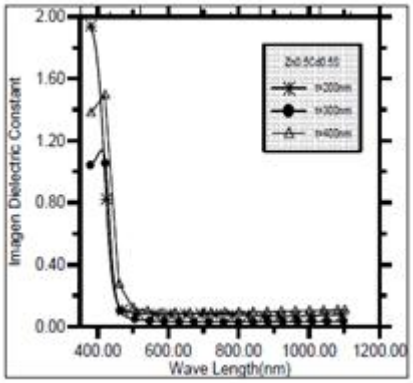

Figure 8: Emagen Dielectric Constant of $Zn_{0.5}Cd_{0.5}S$ thin films for the various thickness.

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