Optical Properties Of Zn_xCd_{1-x}S Thin Films

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<u>Abstract</u>

Optical properties of $\mathbf{Zn}_x \mathbf{Cd}_{1-x} \mathbf{S}$ thin films prepared by using a fast thermal evaporation technique with different \mathbf{Zn} concentrations in the range $(0.0 \le x \le 1.0)$ have been investigated in room temperature. Optical transmission of films are recorded in the wavelength range 300-700 nm. Direct energy band gap to these films were determined by correlated between the optical absorption coefficient with the photon energy .Energy gaps values were in the range (2.4 - 3.5 eV).

Key words: ZnCdS thin films, optical properties thin films

1. Introduction

The average solar radiation reaching the earth surface AM1.5 is very rich in photon with an energy ranging from about (1.5 eV - 3 eV). [1]

Elements of II-VI group are attracting a great deal of attention because their potential abilities in the wide spectrum optoelectronic devises , high absorption coefficient , high efficiency of radiative recombination and nearly matching band gaps with the visible region of solar spectrum are the root causes of popularity of II-VI group semiconductors.[2,3]

Cadmium sulfide CdS is considered as a n-type direct semiconductor with room temperature band gap energy 2.42 eV. CdS films are regarded as one of the most promising materials for the hetrojunction of thin films solar cells, where 0.1 μ m of a CdS film absorbs 36% of the incident radiation with energy higher than 2.42 eV. [4,5] Zinc sulfide ZnS is a wide gap and direct transition semiconductor, so, it is an important devices materials for the detection, emission and modulation of visible and near ultra violet light, band gap of ZnS is 3.66 eV [4,6]

Thin films of $Zn_xCd_{1-x}S$ are known to have properties between those CdS and ZnS because of addition of ZnS [7]. The $Zn_x Cd_{1-x} S$ band structure has a large energy gap than CdS, this makes the material much more attractive for the fabrication of solar cells .[8]

 $Zn_xCd_{1-x}S$ thin films have been widely used as a wide band gap window material in hetrojunction photovoltaic solar cells and photoconductive devices. [9,10] In solar cell systems, where CdS films have been demonstrated to be effective, the replacement of CdS with the higher band gap ternary ZnCdS has led to decrease in window absorption losses, and has resulted in an increase in a short circuit current in solar cell.

This ternary compound is also potential useful as a window material for the fabrication pn junction without lattice mismatch in the devices base on quaternary materials like $CuIn_xG_1$. $_xSe_2$ or $CuIn(S_sSe_{1-x})_2$.[11]

ZnCdS thin films have been prepared by a Variety of techniques, which include spray chemical pyrolysis , evaporation, chemical bath deposition, dip technique, electro-deposition and organic chemical vapor deposition (MOCVD).[12,13]

2. Experimental

 $Zn_xCd_{1-x}S$ (0.0 $\leq x \leq 1.0$) thin films were deposited on thoroughly cleaned glass substrates by using a fast thermal evaporation technique from single boat .Varian 3117 system (made in Italy) used to preparation films . Both CdS and ZnS powder purity (99.999 %) product in (Balzers company) are evaporated from Mo boat .The vacuum chamber is evacuated to $5x10^{-5}$ torr . Substrate temperature was measured by a thermocouple (type K) directly onto the substrate holder and was controlled by a temperature controller type (CXTA 3000). At first the substrates are heated at 525 K for 15 min. to remove any moisture , then substrates temperature decreased to kept at 350 K during the evaporation .The evaporation rate was adjusted at a range of 40-45 nm/sec and films thickness were about approximately 400-450 nm .

To study the optical properties of films , the transmission has been recorded using single beam UV/VIS spectrophotometer type (Thermo spectronic 200-900 nm) in the transmission range 300-700 nm .

3. <u>Results and discussion</u>

 $\overline{Zn_xCd_{1-x}S}$ films are bright yellow orange and the yellowness increases with increasing zinc concentration where ZnS films are transparent in color.

Optical transmission measurements were used to determine the films bandgap.

Figure 1 shows the thin films – substrate system used for Optical measurements, where (t) is the film thickness and n, (n = n-ik) is the reflective and complex reflective index respectively, (k) its extinction coefficient.

The reflection coefficients R_1 , R_2 for two interfaces ,air-film and film – substrate are given by:[14]

$$R_{1} = \frac{(n-1)^{2} + k^{2}}{(n+1)^{2} - k^{2}} = 1 - T_{1} \qquad \dots \dots 1$$
$$R_{2} = \frac{(n-n_{s})^{2} + k^{2}}{(n+n_{s})^{2} + k^{2}} = 1 - T_{2} \qquad \dots \dots 2$$

Where

 n_s = reflective index for substrate.

 $T_1 \& T_2$ = transmission coefficients for two interfaces.

For the film – substrate system, T (optical transmission for the film in the semi-infinite substrate approximation) its measure compared with the optical transmission of glass substrate . T&R are given by :[15]

$$T = \frac{T_1 T_2 \tau}{1 - 2\sqrt{R_1 R_2} \tau \cos \varphi + R_1 R_2 \tau^2} \qquad \dots 3$$

$$R = \frac{R_1 - 2\sqrt{R_1R_2}\tau\cos \varphi + R_2\tau^2}{1 - 2\sqrt{R_1R_2}\tau\cos \varphi + R_1R_2\tau^2} \qquad \dots \qquad 4$$

where

 $\tau = \exp(-\alpha t)$, $\alpha = 4\pi k/\lambda$ (absorption coefficient), $\phi = 4\pi n/\lambda$ if, $2nt = m\lambda$ (m is an integer)

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Fig.1 Schematic diagram film-substrate system

Percentage transmission (T%) as a function of wavelength (λ) for $\mathbf{Zn}_{\mathbf{x}}\mathbf{Cd}_{1-\mathbf{x}}\mathbf{S}$ films with different concentrations (x = 0.0, 0.2, 0.4, 0.6, 0.8, 1.0) are shown in fig.2.

Transmission values almost 100% for energies lower than the energy gap. The transmission edge shift towards a shorter wavelength with increasing **Zn** concentration following the expected increase in the energy gap. From the transmittance data, nearly at the fundamental absorption edge, the absorption coefficient (α) of films are calculated in the region of strong absorption using the relation: [14]

where (t) is thickness of the films

Using equation (5), the value of absorption coefficient (α) has been calculated [15].

Fig.3 shows the plot of (α) versus photon energy .Since the value of (α) is in the order of 10^4 cm⁻¹ and the absorption coefficient is measured at room temperature , the presence of excitation band is not likely to be possible . There for the absorption from band to band transition and it is only due to an allowed direct transition from the top of the valence band to the bottom of the conduction band at the center of the Brillouin zon [16,17].







Fig.3: absorption coefficient versus photon energy of films with different Zn concentration

For direct bandgap semiconductors , the energy gap (E_g) is determined through the relation : $\left[18\right]$

$$(\alpha h v) = A(h v - E_g)^{\frac{1}{2}} \qquad \dots \qquad 6$$

where (A) is a characteristic parameter independent of photon energy for respective transitions. $(\alpha h \upsilon)^2$ versus (hv) plots can be obtained as shown in fig.(4). Estimated energy-band gaps from the plots are explained in Table (1).





 Table(1): dependence of the energy gap on the Zn concentration

	E _{g.} (eV)		
х	Present work	Ref.4	Ref.8
0.0	2.4	2.41	2.4
0.2	2.5	2.56	2.66
0.4	2.86	-	2.72
0.6	3.04	-	3.15
0.8	3.2	-	-
1.0	3.5	3.48	-

In the present case of $\mathbf{Zn}_{x} \mathbf{Cd}_{1-x} \mathbf{S}$ thin films, \mathbf{E}_{g} value vary from 2.4 eV to 3.5 eV for x = 0.0 to 1.0.

Fig. 5 shows the variation of E_{g} with \mathbf{Zn} concentration .



Fig.5: Variation of Eg with different Zn concentration

conclusions

 $\overline{\mathbf{Zn}_{\mathbf{x}} \operatorname{Cd}_{1-\mathbf{x}}} \mathbf{S}$ thin films with a variation in $\overline{\mathbf{Zn}}$ concentration in the range $(0.0 \le x \le 1.0)$ were fabricated on the glass substrates heated to 350K by fast thermal evaporation technique . Increasing **Zn** concentration in films leads to a blue-shifted absorption edge.

The long wavelength optical transmission was found to be high enough for using these films in solar cells application. Increasing \mathbf{Zn} concentration in films leads to increasing the energy gap in these films.

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المستخلص

الخواص الضوئية لاغشية المركب Zn_xCd_{1-x}S الرقيقة المحضرة بتقنية التبخير الحراري السريع في الفراغ وبنسب مختلفة من العنصر Zn ضمن المدى (1.0 ≤ x ≤ 1.0) تمت دراستها في درجة حرارة الغرفة . تم تسجيل نتائج النفاذية الضوئية للاغشية المحضرة عند اطوال موجية في المدى mm 700-300 ومن ثم حسبت فجوة الطاقة المباشرة من خلال العلاقة بين معامل الامتصاص الضوئي وطاقة الفوتون الساقط . تراوحت قيم فجوة الطاقة ضمن المدى 3.5 - 2.4) eV)