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STRUCTURAL AND OPTICAL CHARACTERIZATION STUDIES OF CHEMICALLY SYNTHESIZED CADMIUM SELENIDE THIN FILMS.

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The Cadmium Selenide (CdSe) films have been prepared on glass substrate at room temperature by chemical bath deposition techniques. Structure of thin films was chararacterized by x-ray diffraction (XRD). X-ray diffraction study indicates that the grown films are polycrystalline with hexagonal structure. The optical properties were investigated in the wavelength range of 0.36-1.10μm. The band gap energy and type of optical transition were determined from optical absorbance data and the value was found to be from 1.70-1.80eV.

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Keywords: Thin films, CdSe, chemical bath deposition, film characterization.

1. Introduction

Cadmium Selenide (CdSe) is the most extensively studied material due to its strong size-tunable properties and possible applications (Covin *et al*, 1994). Cadmium selenide, a group 11-VI compound semiconductor has been considered as an important candidate for opto-electronics and solar cell application. The deposition and characterization of CdSe films have been reported in recent years. Its properties depend largely on preparation method. In this paper, we report the deposition, structural and optical properties of CdSe thin films onto glass substrate using chemical bath deposition technique from an aqueous solution containing cadmium trioxo nitrate (v) and selenium trioxosulphate (v).

2. Experimental details

Thin films of CdSe, were deposited by chemical bath deposition technique on a glass substrate at room temperature. Prior to deposition, the substrate were degreased in trioxonitrate (v), washed with detergent, rinsed in distilled water and dried in air. The precursors used were $Cd(NO_3)_2$, as the cadmium source, $SeSO_3$ as the selenide source, TEA acted as the complexing agent and NH_3 was used to provide the alkaline medium needed for maximum growth and to increase the film adherence respectively. For deposition, 5ml of 1M $Cd(NO_3)_2$ was complexed with 5ml of 0.5M TEA. To this, 2ml of 0.1M $SeSO_3$ was added slowly to the reaction mixture. The pH of the reaction bath was adjusted to 10.2 by addition of (5ml) ammonia and the volume was made up to 50ml with distilled water. The cleaned glass substrate was vertically immersed into the chemical bath with the help of the synthetic foam. The reaction mechanism for the growth is represented as follows:

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$Cd(N0_3)_2 + TEA \rightleftharpoons [Cd\ (TEA)]^{2+} + 2N0_3^-$

$[Cd(TEA)]^{2+} \rightleftharpoons Cd^{2+} + TEA$

$SeS0_3 + 0H^- \rightleftharpoons HSe^- + H_20$

$HSe^- + 0H^- \rightleftharpoons Se^{2-} + H_20$

$Cd^{2+} + Se^{2-} \rightleftharpoons CdSe \downarrow$

The films were deposited at different deposition time (15-28hrs) on pre-cleaned substrates. The substrates coated with CdSe thin films were removed, rinsed with distilled water, and dried in air.

The structural properties of thin films were investigated by X-ray diffraction (XRD) using CuK_α (λ=1.5406 Å) radiation. The optical absorption of the films was measured using Janway 6405 UV-VIS spectrophotometer in the wavelength range of 0.36-1.10µm.

3. Results and discussion

3.1 Structural analysis of Cadmium Selenide film.

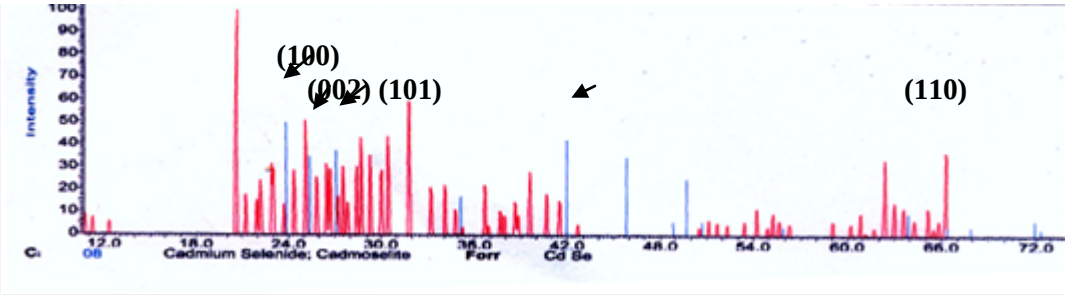

Fig.1 X-ray diffraction of CdSe selenide film.

Fig.1 is the x-ray diffractogram of cadmium selenide thin film prepared at a substrate temperature of 300k. It reveals the existence of (100), (002), (101) and (110) planes of reflections of hexagonal structure with composition CdSe. The presence of large number of peaks indicates that the films are polycrystalline in nature. The lattice constants from the XRD were found to be 4.299Å and c=7.01Å from which the grain size (D), dislocation density (δ), and micro strain (ε) were calculated. The results of all other peaks and their relative planes are presented in table 3.1. Using the following expressions, the grain size,

$$D = \frac{k\lambda}{\beta \cos\theta,}$$ (Klug and Alexander, 1974 and Gomez *et al*, 1999)

micro strain, $\varepsilon = \frac{\beta \cos\theta}{4}$ (Lifshin, E. 1999) and dislocation density,

$$\delta = \frac{15 X \varepsilon}{\alpha x D}$$

where K = 0.9 which varies from (h k l) and crystallite shape
θ = diffracting angle, β is the full width half maximum (FWHM)
λ= wavelength of x-ray and α is the lattice constant.

Table 1: The structural parameters of CdSe film and thicknesses.

Thickness, t (μm)	h k l	2θ (deg)	(rad.)	d Measured (Å)	d standard (Å)	FWHM (rad.)	α (Å)	Grain size D (Å)	Dislocation density δ $X10^{-2}$	Strain ε $X10^{-2}$
1.31	100	23.90	0.417	3.76	3.72	O.362	4.299	3.91	7.88	8.85
	002	25.35	0.442	3.51	3.51	0.362		3.93	7.97	8.83
	101	27.08	0.473	3.29	3.29	0.380		3.76	8.71	9.23
	110	41.96	0.732	2.15	2.15	0.384		3.88	8.25	8.98
1.46	100	23.97	0.418	3.766	3.72	0.362	4.299	3.92	7.88	8.85
	101	29.15	0.509	3.06	3.29	0.380		3.77	8.51	9.20
	102	35.90	0.627	2.64	2.55	0.382		3.82	8.29	9.08
	110	40.21	0.702	2.24	2.15	0.384		3.84	8.20	9.03

The results from table 1 show that the grain size (D) increases with increase in film thickness but the dislocation density (δ), and the microstrain (ε) are found to decrease with increase in film thickness. The comparisons of the observed d values with the standard d clearly indicate the formation of the hexagonal phase of CdSe. This compares well with the result reported by Kale and Lokhande (2005) for CdSe film. Kissinger *et al*, (2010) obtained a film of orientation (002), (101), (110) and (103) planes of reflections of CdSe prepared by Electron Beam Evaporated technique. Osuji R.U (2002) reported the XRD pattern showing only (111) and (110) planes.

3.2 Optical properties of CdSe films.

The thicknesses of the deposited films were determined by the optical method as was described by Theye (1985). Fig.1 shows the variation of thickness with deposition time.

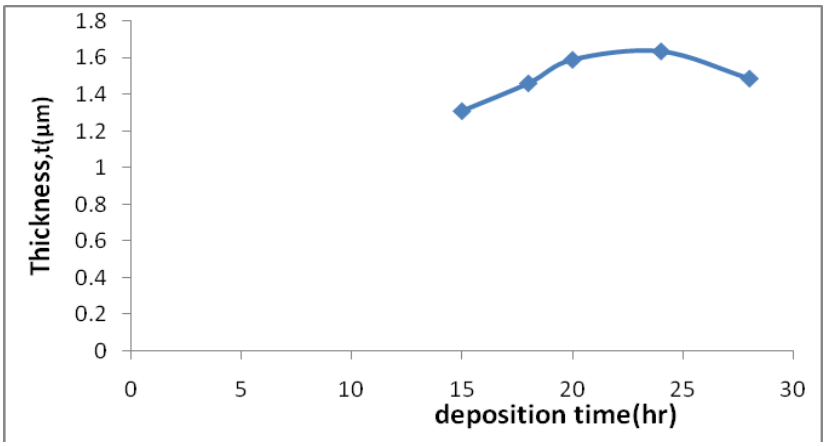

Fig. 2 Variation of thickness vs deposition time

Fig 3 & 4 show the spectral absorbance and transmittance of CdSe thin films deposited in this work. They show a decrease in absorption and an increase in transmission as the wavelength increases. The film has high absorbance in the ultraviolet region (0.35-0.40μm). The curve show a decay of absorbance as it enters the VIS-NIR regions of the electromagnetic spectrum. The value of absorbance ranged from 0.08 - 0.22 in UV- VIS regions and 0.05 – 0.10 in NIR region. This compares well with the reported result by Kale and Lokhande (2005) who obtained a high absorption in UV-NIR regions and a low absorption in IR region. Kissinger *et al*, (2010) revealed the optical absorption behavior of CdSe films prepared by Electron Beam Evaporation technique

which demonstrate good optical absorption at UV-VIS region. The high absorbance in the ultraviolet region (0.35-0.40μm) makes it suitable to form p-n junction solar cells with other suitable thin film materials for photovoltaic generation of electricity among others.

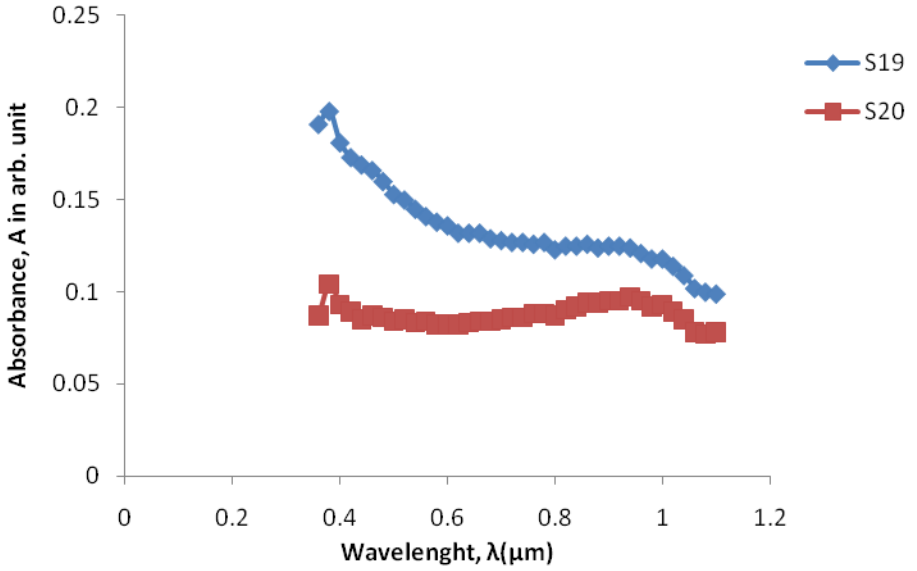

Fig 3. Spectral absorbance of CdSe for S_{19}& S_{20}

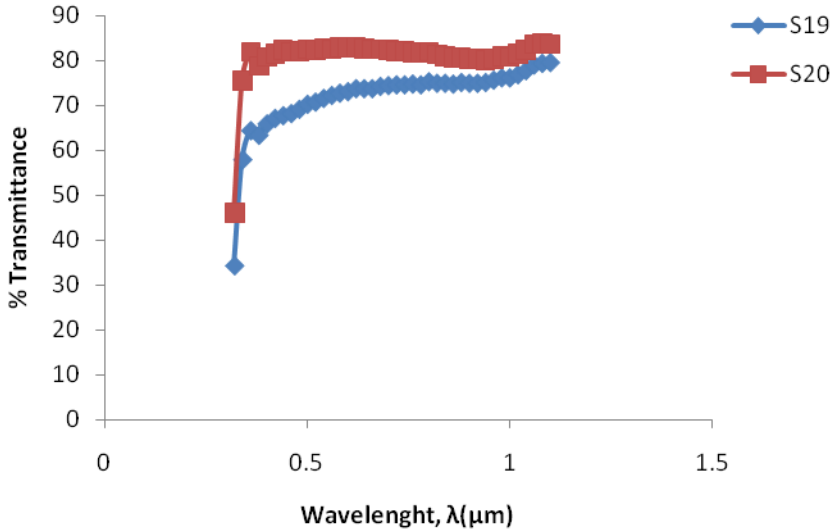

Fig. 4 Spectral transmittance of CdSe for S_{19} & S_{20}

The transmittance spectra in fig.4 showed a low transmittance below the wavelength of 400nm and a high transmittance of 70-80% in VIS-NIR regions. It compares well with Kissinger (2010) who revealed a very small transmission below the wavelength of about 400nm and a high transmittance in VIS-NIR regions. Kale and Lokhande (2005) reported a high percentage transmittance of 60. It is clearly seen from the optical spectra that the absorption and transmission edge shift towards a longer wavelength. The high transmittance makes the CdSe films efficient window materials.

The optical band gaps of the film were estimated from α^2 versus hυ curves shown in fig 5. The linear nature of the plot indicates the existence of the direct transition. The band gaps were determined by extrapolating the straight portion to the energy axis at $\alpha^2 = 0$. The band gap was found to be 1.70- 1.80eV. This compares well with the published results of Shreekanthan *et al*,

(2003) who reported a band gap of 1.89eV at room temperature. Osuji (2002) reported a band gap of 1.45- 1.98eV for CBD CdSe film. Kissinger reported *et al*, (2010) reported an energy gap ranging from 1.77-1.92eV for CdSe films prepared by Electron Beam Evaporation technique. From the results shown above, CdSe films have wide band gap and therefore could serve as good window layers for photo cells.

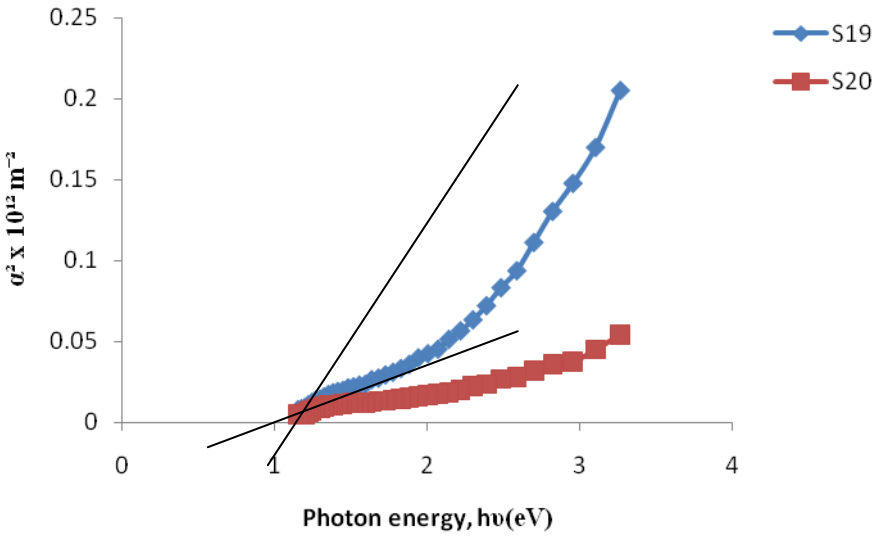

Fig 5. Plot of α^2 Vs hυ of CdSe for S_{19} & S_{20}

4 Conclusion

Cadmium selenide films have been successfully grown using chemical bath deposition technique. The deductions from the structural and optical characterization revealed that CdSe has hexagonal structure. The band gap ranged from 1.70-1.80eV. The films have high absorbance in the UV region and decays as the wavelength increased. It showed that CdSe films have high transmittance, and this makes the films suitable for use as aesthetic window.

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