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EFFECT OF PRECURSORS ON THE STRUCTURAL AND OPTICAL PROPERTIES OF SPRAY PYROLYSIS COATED CDS THIN FILMS

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Abstract: **Pure Cadmium Sulphide (CdS) thin films have been coated on glass substrate at 400°C by spray pyrolysis (SP) technique using different precursors (Cadmium nitrate-A, Cadmium acetate-B and Cadmium chloride-C). Pure CdS thin films were characterized by various techniques such as X-ray diffraction, SEM and optical studies. X-ray diffraction measurements show that CdS thin films belong to the cubic crystal structure with preferential orientation along (1 1 1) direction. The average crystallite size (D) of CdS thin films with different precursors are 48 nm (A), 29 nm (B) and 27 nm (C) respectively. The average dislocation density (δ) and stacking fault (SF) of CdS thin films are 5.93x10^{15} lines/m^2 (A), 13.71x10^{15} lines/m^2 (B), 16.73x10^{15} lines/m^2 (C) and 0.7996 Å (A), 1.3367 Å (B), 1.3325 Å (C). The surface morphology of the thin films was determined by scanning electron microscopy (SEM). The optical energy band gap of thin films is 2.43 eV (A), 2.31 eV (B) and 2.16 eV (C). The luminescence spectrum shows a strong emission peak at 518 nm (A), 521 nm (B), 525 nm (C). We can postulate that our fabricated CdS thin films will be useful for optoelectronic devices.**

Index Terms: **CdS thin films, Spray pyrolysis, Structural and Optical studies.**

I. INTRODUCTION

Cadmium sulphide (CdS) has long been the most studied one of the II–VI compounds of the chalcogenide family with a direct bandgap of 2.4eV and large absorption coefficient of the order of 4 x 10^{-4} cm^{-1}. CdS thin films have unique physical and chemical properties when compared with those of the corresponding bulk material due to the quantum confinement effect. CdS has great potential applications such as gas sensors, photo-detectors, solar cells, piezo-electric transducers, light emitting diodes, transparent UV protection films, biological systems (drug delivery and bio-imaging) etc.[1]. CdS thin films can be produced by many processes like chemical bath deposition[2], vacuum evaporation[3] and SILAR method[4]. The spray pyrolysis technique has a few advantages when compared with other methods. It is simple, basic set-up is not expensive and flexible for process modifications. It is used for the preparation of a large number of semiconducting and insulating thin films[5]. In view of enormous application of CdS films in various technologies we have prepared and characterised CdS films by spray pyrolysis method. Moreover, in order to enhance the purity, we have chosen the different precursors systematically studied the change in behaviour of CdS thin films based on the structural, optical properties.

II. EXPERIMENTAL

Spray pyrolysis method consists mainly of spraying solution on heated substrate. For film preparation 0.5 M of different precursors (Cadmium nitrate-A, Cadmium acetate-B and Cadmium chloride-C) and 1 M sodium sulphide dissolved in double distilled water. These mixed solutions were ready to make thin films. Well cleaned substrates were placed on the heater and the distance between the tip of the nozzle and surface of the substrate was maintained at 18 cm. A constant flow rate, 3ml/min was maintained for all the samples to be deposited on substrates maintained at 400°C. Before supplying the compressed air the heater was allow to heat the

substrate to attain the required temperature. When compressed air along with the precursor solution was passed through the nozzle at constant pressure, finely formed aerosol descended to reach the reactor zone where the film was deposited on the heated substrate to produce CdS thin films.

X-ray diffraction analysis was performed using X ray Diffractometer (Shimadzu X-600) in order to study the crystal structure of the spray pyrolysis thin films. The surface morphology was recorded using scanning electron microscope SEM (JEOL 2 – JSM 6000). Optical transmission spectra of all films were obtained using UV-VIS spectrophotometer (UV Vis NIR JASCO V-670). The luminescence studies were carried out using Fluoromax 4 spectrophotometer.

III. RESULTS AND DISCUSSION

A. Structural studies

The spray pyrolysed thin films were smooth, well adhered and visually transparent. Fig. 1 show the X-ray diffraction patterns for different precursors CdS thin films prepared on glass substrates at 300°C. These films show a preferential growth along the (1 1 1) direction and the other peaks associated with the (1 1 1), (2 2 0) and (3 1 1) plane are also observed with JCPDS Card No. 65-2887. The obtained diffraction peaks correspond to the cubic structure of CdS showing a polycrystalline nature. The determined lattice constant for CdS thin films are given in **(Table 1)**. The crystallite size of the sample was determined by using the Scherrer's formula,

$$\mathbf{D = K\,\lambda / \beta \cos\theta} \quad (1)$$

Where D is the crystallite size, λ is the wavelength, β is the full width at half maximum of diffraction peak measured in radians and θ is the Bragg's angle.

Dislocations are the imperfections in a crystal and associate with the mis-registry of the lattice in one part of the crystal with respect to another part. Unlike vacancies and interstitial atoms, dislocations are not equilibrium imperfections. In fact, the growth mechanism involving dislocations is a matter of importance. The dislocation densities of thin films are given by the Williamson and smallman's relation[6].

$$\mathbf{\delta = n / D^2} \quad (2)$$

Where **δ** is dislocation density, n is a factor which equals unity, giving minimum dislocation density and D is the crystallite size. The dislocation density values are represented in **(Table 1)**.

The stacking faults probability (α) is the fraction of layers undergoing stacking sequence faults in a given crystal and therefore one fault is expected to be observed in 1/α layer. The existence of stacking faults gives rise to a shift in a peak position of different reflection planes with respect to ideal position of fault free sample. The relation between stacking faults probability (α) with peak shift β is given by

$$\mathbf{\alpha} = \left[\frac{2\pi^2}{45(3tan\theta)^{1/2}}\right] \boldsymbol{\beta} \quad (3)$$

Where α is the stacking fault and β is full width half maximum. The stacking fault values are presented in **(Table 1)**.

B. Morphological studies

The surface morphology of the prepared CdS thin films was observed through SEM image analysis (Fig.2). Images showed that the morphology of the deposited CdS thin films was markedly affected by the different starting precursors (Cadmium nitrate, Cadmium acetate and Cadmium chloride).

C. Optical studies

The value of the optical band gap can be calculated using the fundamental absorption, which corresponds to electron excitation from the valence band to the conduction band. The absorption coefficient α and incident photon energy (hν) are related by the equation[7]

$$\mathbf{(\alpha h\nu)^{1/n} = A(h\nu - Eg)} \quad (4)$$

Where A is a constant, Eg is the bandgap of the material and the exponent n depends on the type of transition. Tag plot between $(\alpha h\nu)^2$ and energy are plotted and the linear portion of the graph is extrapolated to met the energy axis to determined the energy band gap as shown in Fig. 3. Depending on the doping concentration of the films the direct band gap values are 2.43 eV (A), 2.31 eV (B) and 2.16 eV (C).

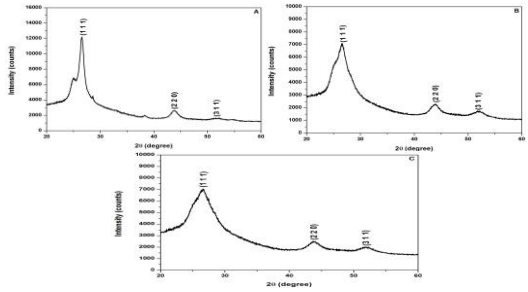


Fig. 1. XRD pattern of CdS thin films

TABLE 1: Structural Parameters of CdS thin films:

Sample	Crystallite Size (D)	Dislocation density (δ) (x10^{14} lines/m^2)	Stacking fault (Å)	Lattice parameter (Å)
A	65.71 50.29 29.47	2.3159 3.9540 11.514	0.6301 0.6796 1.0891	5.8590
B	21.20 39.58 28.28	22.249 6.3833 12.503	2.012 0.8636 1.1336	5.8431
C	18.21 35.06 28.99	30.156 8.1353 11.898	2.3397 0.6827 0.9751	5.8300

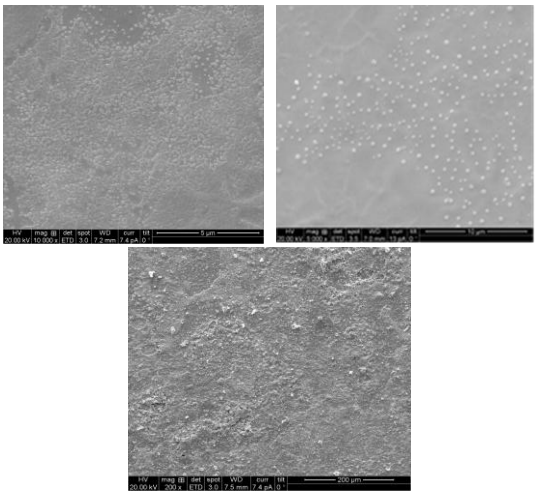
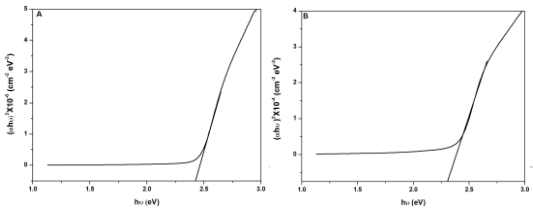


Fig. 2. SEM images of CdS thin films (A, B, C)



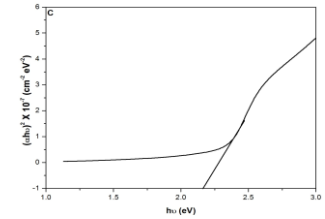


Fig. 3. Optical energy bandgap values of CdS thin films

D. Luminescence studies

Fig. 4 shows the fluorescence spectra of CdS thin films. During the characterization, Xenon lamp source at 370 nm as an exciton wavelength is used. The luminescence is originates from the recombination of surface states. In the spectra, the peak at 518 (A), 521 (B) and 525 nm (C) corresponds to emission of near band edge exitionic peak. The emission peaks 518, 521, 525 nm represents the green emission. The optical band gap measured to be 2.39 (A), 2.38 (B) and 2.36 eV (C) so it can be used in optoelectronic devices.

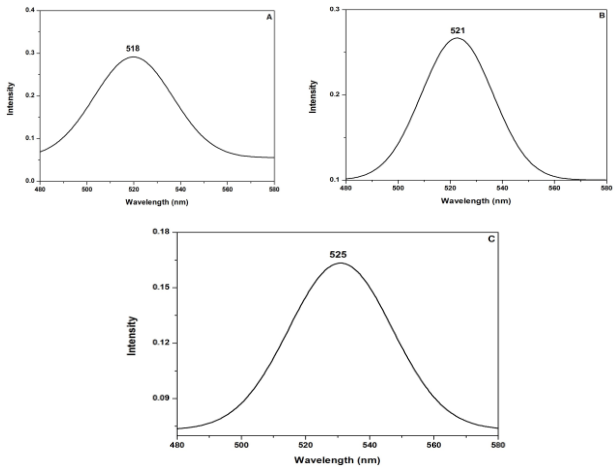


Fig. 4. Luminescence spectra of CdS thin films

IV. CONCLUSION

The CdS thin films were successfully deposited on glass substrate using spray pyrolysis technique. The films were characterized for structural and optical properties. The cubic phase of CdS thin film is observed by XRD analysis. From the SEM images

shows uniform thin film of CdS. Luminescence spectrum shows the emission at 518-525 nm. The optical band gap is measured to be 2.36-2.39 eV. And thus CdS thin films have good characteristic to be used as a window layer for photovoltaic applications.

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