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OPTICAL, STRUCTURAL AND MORPHOLOGICAL PROPERTIES OF THIN FILM CdS USING SPRAY PYROLYSIS METHOD

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Abstract: In the present work, cadmium sulphide (CdS) thin film was deposited on microscopic glass slide using equimolar concentration of cadmium chloride (CdCl₂.H₂O) and thiourea (CS(NH₂)₂). Spray pyrolysis method was used to prepare the film at 375°C. Spray pyrolysis is a simple, inexpensive, chemical method for the preparation of good quality thin films. The film was investigated for structural, optical and morphological properties using X-ray diffractometer, UV-Vis Spectroscopy and FESEM respectively. The synthesised film showed polycrystalline structure with hexagonal phase oriented along (101) reflection plane. The optical study revealed the average optical transmission of deposited film (45%) and calculated band gap value (2.49 eV). Morphological studies described the formation of dense, uniform thin film with small capsules of CdS grains. Uniform, adherent, thin film CdS is of great interest to study for optoelectronic and sensors applications.

Keywords: CdS, Spray pyrolysis, XRD, band gap

1. INTRODUCTION

Polycrystalline thin films are fascinating in scientific research and industries. These materials are largely used in sensors, optoelectronic devices, detectors and biomedical applications. Cadmium sulphide (CdS) is a binary chalcogenide II-VI group semiconductor material with n type conductivity, high optical transmission and tunable wide band gap. These characteristics lead the material in many applications, especially solar cells [1], photosensors [2], gas sensors[3] etc. There are various thin film deposition techniques used to prepare uniform, adherent polycrystalline CdS thin film, it includes chemical vapour deposition [4], sputtering [5], pulsed laser deposition [6], SILAR [7], electrochemical deposition[8], chemical bath deposition [9] and chemical spray pyrolysis [10]. Among these methods, chemical spray pyrolysis is most suitable technique for thin film deposition due to its various features like simple and low cost technique, does not require vacuum and high quality substrate and/or target which makes it capable to deposit large area thin film for industrial applications [11].

In the present work, cadmium sulphide (CdS) thin film is deposited using spray pyrolysis technique. The prepared thin film was characterised using XRD, UV-Visible spectrometer and FESEM to study structural, optical and morphological properties.

2. EXPERIMENTAL DETAILS

2.1. CLEANING OF SUBSTRATE

Substrate cleaning is an initial step to approach good quality thin films of high uniformity and excellent adherence. In the present work soda lime glass substrates (76x25x1mm) has been used to deposit CdS thin film. Initially, slide was washed three to four times with soap solution. The washed slide was subjected to chromic acid solution for 24 hours. In the last, the slide was removed from chromic acid solution and washed three to four times with distilled water.

2.2. PREPARATION OF CdS THIN FILMS

Cadmium chloride (CdCl₂.H₂O) and thiourea (CS(NH₂)₂) were used in the present work to prepare CdS thin film. Molar concentrations of both precursors were kept same viz. 0.05M in 50ml double distilled water. The precursor solution was mixed using magnetic stirrer for 10 minutes and later it was filled in the spray gun. Fig. 1 showed schematic diagram of spray pyrolysis system. The heater was set to 375°C, deposition temperature. The carrier gas (air) was adjusted to 20 lpm. Nozzle to substrate distance was 26cm.



Fig 1. Schematic diagram of chemical spray pyrolysis system for deposition of CdS thin film ad deposition temperature 375°C

In the present work, the precursor solution was sprayed with flow rate of 5ml per minute to the hot glass substrate. The deposition was carried out for 10 minutes. Finally, the prepared CdS thin film was cooled to room temperature in the heating system and then different characterizations were carried out to study the prepared film.

2.3 THIN FILM CdS CHARACTERIZATIONS

X-rav diffractometer (Bruker D8 Advance. Germany), Cu Ka_c line (λ =1.54056 Å) was used to record X-ray diffraction pattern of as deposited CdS thin film for angle 2θ ranging from 20° to 80° . The analysis of diffraction pattern explores various structural information of CdS thin film such as crystalline phase, grain size and texture coefficient. UV-visible spectrophotometer Shimadzu UV-1800 was used to study the optical properties of CdS thin film such as transmittance and optical band gap. The wavelength of spectrum used to study optical properties was 300-1000nm. The FE-SEM images were recorded using Hitachi-4800 with operating voltage 10 kV to study the surface morphology of the films.

3. RESULTS AND DISCUSSION:

3.1 X-RAY DIFFRACTION STUDIES:

X-ray diffraction is generally used to study structural properties of synthesised material in the form of powder or thin film. Fig. 2 shows the X-ray diffractogram of CdS thin film deposited at 375°C. The multiple Bragg's diffraction peaks recorded in Fig. 2 confirm the polycrystalline phase of as deposited CdS thin film. The Bragg peaks of high intensity were recorded at Bragg's angles, 2θ = 24.97, 26.79, 28.21 43.87and 52.153 whereas additional weak peaks were located at 2θ = 36.77, 48.03, 52.94, 66.92, 69.66 and 71.1 and 75.83. The X-ray diffraction data of as deposited CdS thin film was in good agreement with JCPDC card-80-0006 which confirmed hexagonal phase of CdS thin film. The different planes of orientation of as deposited film at different Bragg angles were reported in table 1. High deposition temperature caused more number of planes of reflections in CdS thin film with significantly high intensity of corresponding peaks. [12,13].



Fig 2. X²ray diffraction pattern of CdS thin film at 20 (deg) deposition temperature375°C

Grain size (D) of as deposited CdS thin film was calculated using Debye Scherrer's formula stated in equation (1)

$$D = \frac{0.9\lambda}{\beta\cos\theta}$$
(1)

Where, λ is the wavelength of incident X-ray

radiation (λ =1.54A°), β is the full width at half maximum (FWHM) of the respective diffraction peak in radian and θ is the Bragg diffraction angle.

Table 1 X-ray diffraction data of spray-depositedCdS thin film at substrate temperature 375°C

2θ (deg)	(hkl) plane	d (°A)
24.97	100	3.56178
26.79	002	3.323793
28.21	101	3.159627
36.77	102	2.44134
43.87	110	2.061279
48.03	103	1.892004
52.05	112	1.754933
52.94	201	1.727506
58.54	202	1.574881
66.92	203	1.39656
69.66	210	1.348173
71.1	211	1.324359
75.83	105	1.253068

Grain size of CdS for three high intense diffraction peaks were mentioned in Table 2 and the average grain size was found to be 30.21nm. The obtained value explores the formation of nano sized CdS particles.

Table 2 Grain size and texture coefficients of spray-deposited CdS thin film at substrate temperature 375°C

20 (deg)	D(nm)	TC(hkl)	
24.97	3.56178	1.429	
28.21	3.159627	0.9889	
43.87	2.061279	1.7127	

Texture coefficient provides the quantitative investigation of degree of preferred orientation of plane of reflections. The texture coefficient can be calculated using relation (2).

$$TC_{hkl} = \frac{\frac{I_{hkl}}{I_{ohkl}}}{\frac{1}{N} \left[\sum_{N} \frac{I_{hkl}}{I_{ohkl}} \right]}$$
(2)

Where, I(hkl) is the measured intensity of the corresponding diffraction peak in X-ray diffraction pattern, Io(hkl) is the standard intensity in JCPDS cards and N is the number of diffractions peaks corresponding to reflection planes.

The obtained texture coefficient of strongest diffraction peaks corresponds to (100), (101) and (110) reflection planes were mentioned in Table 2 which were either close to 1 or greater than 1 indicating strong orientation of CdS particles along these planes [14].

3.2 UV-VISIBLE SPECTROSCOPY STUDIES:



Fig 3. UV-Visible spectrum f optical transmission of CdS thin film at deposition temperature 375°C

UV-Visible spectroscopy is an important characterisation to study optical properties of CdS thin film.

The UV-visible spectrum in Fig. 3 shows optical transmittance of CdS thin film in NIR and Visible

region. The recorded spectrum showed low transmittance due to high thickness of deposited CdS thin film. However, surface roughness of thin film also greatly attributes to the optical transmission of thin film. Surface roughness causes surface scattering due to overgrowth of crystal grains at the surface of film [15]. The obtained optical transmission spectrum shows sharp fall at wavelength 500nm [16]. The fall edge is extrapolated to find optical band gap which was 2.47eV and it is in good agreement with reported values and higher than that of bulk CdS, 2.4eV. [17]. 3.3. FIELD **EMISSION** SCANNING

ELECTRON MICROSCOPY STUDIES:

FESEM micrograph of CdS thin film deposited at 375°C is shown in Fig 4.



Fig 4. *FESEM micrograph of CdS thin film at deposition temperature375°C*

The surface morphology showed uniform and dense distribution of tiny capsule like CdS particles with less number of voids. These CdS capsules lead to formation of cluster of leaf like structure due to agglomeration [18].

4. CONCLUSIONS

Cadmium sulphide (CdS) thin film was prepared using chemical spray pyrolysis method at substrate temperature 375°C. The yellowish deposited film was uniform and adherent. The as deposited film showed polycrystalline hexagonal phase. The calculated grain size of CdS thin film described the formation of nanosize particles. These nanosize particles were highly oriented along (100),(101) and (110) reflection planes with large value of texture coefficient. Optical studies of CdS thin film informed the average optical transmission 45% for wavelength below 500nm. The calculated optical band gap was 2.47eV. FESEM micrograph image explained distribution of clusters of CdS particles throughout the surface and film was covered with leaf like structure and less voids. The as deposited films showed great potential towards thin photosensors and optical devices such as solar cells.

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