

Structural and Optical Properties of CdS Thin films for the Solar Cell Applications

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Abstract: Solar energy has the potential of becoming a renewable energy alternative to fossils fuels. The thin film technologies reduce the amount of material required in forming the active material of solar cell. CdS being a wide band gap material and with better lattice matching properties made it suitable option for solar cell applications. CdS thin films have been prepared by spray pyrolysis technique. The spraying solution consists of an aqueous solution of cadmium chloride [CdCl₂·2H₂O], Thioacetamide [TAA], ammonia as complexing agent and N, N-Dimethylformamide [N, N-DMF] as a solvent. These CdS thin films are fabricated by spray pyrolysis to maintain parameters such as air pressure 15 Kg/cm³, solution flow rate of 2.5 Kg/cm³, nozzle to substrate distance of 20 cm and of different substrate temperatures like 250°C, 300°C and 350°C. The structural properties of CdS thin films have been investigated by X-Ray Diffraction (XRD) & Atomic Force Microscope (AFM) and the optical properties were observed by UV – Vis Spectrometer (UV-Vis).

Keywords: CdS thin films, Spray pyrolysis, XRD, AFM, UV-Vis

1. Introduction

The fabrication of thin films in nano size is important because of their potential applications in the various fields like solar energy conversions and optoelectronic devices due to their low production cost. The films can be fabricated by multi-layers and multi-compounds on the different substrates of different sizes and shapes. There are a number of physical and chemical ways to preparing thin films, like chemical vapor deposition, chemical bath deposition [1], electro deposition [2], RF-sputtering [3], pulsed laser deposition, thermal evaporation, ion-beam sputtering, vacuum deposition, spin coating technique [4], co-precipitation, sol-gel [5, 6], successive ionic layer adsorption and reaction method [7], spray pyrolysis [8] etc. Spray pyrolysis is a technique used to fabricate thin films, thick films and ceramic coatings. Compared with other above mentioned techniques spray pyrolysis is very simple, fast, low-cost method and get uniform deposition of the films [9, 10]. This spray pyrolysis technique, depends on the parameters like air pressure, solution flow rate and nozzle to substrate distance etc., this controls the film deposition [11]. The CdS thin films are II-VI semiconductor nanocrystal materials, it is having wide band gap of 2.42 eV [12]. Due to these reason it has been use as a window material to fabricate the solar cells [13]. Present work deals with fabrication of CdS thin films by Spray Pyrolysis technique at different substrate temperatures like 250°C, 300°C and 350°C. These thin films were characterized by XRD, AFM and UV-Visible absorption spectrometers.

2. Experimental Details

Cadmium Sulfide (CdS) thin films were fabricated by spray pyrolysis technique, dissolving the precursor materials Cadmium Chloride [CdCl₂·2H₂O] and Thioacetamide [CH₃CSNH₂] in the molar ratio of 1:2 in double distilled water along with the complexing agent triethanolamine

(TEA) of 0.1M, which is chosen to stabilize the grain size. The amount of solution was made together as 50 ml. The spray pyrolysis setup consists of a substrate heater, spray gun, air compressor, solution reservoir and a gas exhaust unit. The heating of the substrate was performed using a ceramic heating plate with electrical heating wires. Optically plane cleaned glass plates was placed over the hot plate. The aqueous solution was then sprayed on the preheated glass substrate maintained at different temperatures 250°C, 300°C and 350°C by conventional chemical spray pyrolysis technique to obtain homogeneous thin films.

2.1 Solution Preparation

The precursor solution used for Cadmium sulphide thin films was obtained by dissolving the salts of cadmium chloride and Thioacetamide in the molar ratio of 1:2 in double distilled water, ammonia as complexing agent and N, N-DMF as a solvent were added drop by drop. The amount of solution was made to 50 ml.

2.2 Spray Process

The spray pyrolysis setup consists of a substrate heater, spray gun, air compressor, solution reservoir and a gas exhaust unit. The heating of the substrate was performed using a ceramic heating plate with electrical heating wires. Optically plane cleaned glass plates was placed over the hot plate. The aqueous solution was then sprayed on the preheated glass substrate maintained at different temperatures 250°C, 300°C and 350°C by conventional chemical spray pyrolysis technique to obtain homogeneous thin films.

2.3 Parameters to be considered for Spray Pyrolysis

(a) Type of salt: water soluble, (b) Air pressure: 15 Kg/cm³, (c) Deposition spray rate: 2.5 Kg/cm³, (d) Substrate temperature: 250°C, 300°C & 350°C, (e) Nozzle to substrate

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distance: 20 Cm, (f) Spray time: 5 Sec, (g) Repeated cycles: 2 minutes, (h) Peristaltic pump rate: 50 rpm.

3. Characterization Techniques

Crystal structure and grain size was calculated from XRD results of Bruker D8 advanced using $\text{CuK}\alpha$ radiation, surface morphology of CdS thin films were estimated from AFM image using A100 AFM Version 11.1 and the band gap is measured from Systronics UV – Vis spectrometer 2202.

4. Result and Discussions

4.1 Structural Properties

The X-ray diffraction patterns of the CdS thin films at different substrate temperatures were shown in figure.1

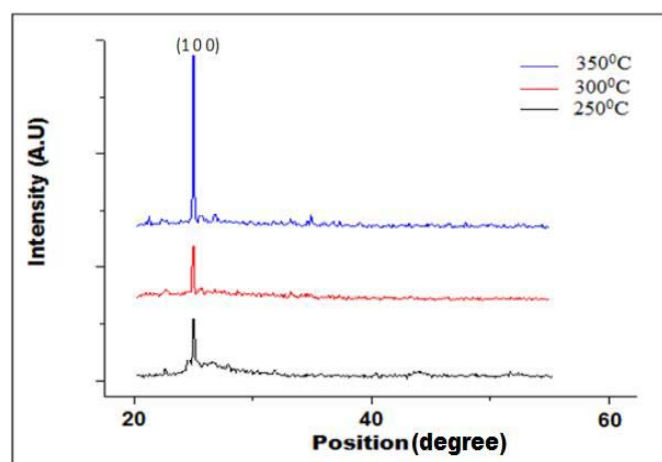


Figure 1: XRD pattern of CdS thin films at different substrate temperatures

They are polycrystalline hexagonal structures. Film formations have a single peak represented at 25° with planes oriented in (1 0 0) direction and it has good agreement with standard X-ray diffraction data which was reported in JCPDS card number 02 – 0549. The grain size of CdS thin films were measured using Debye-Scherrer's formula as shown below

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

where D is the average grain size of the thin film, λ is the wavelength of the radiation, β is the full width at half maximum (FWHM) of the peak, θ is the Bragg's angle.

The obtained average grain size was 11 nm, 18 nm and 22 nm for 250°C, 300°C and 350°C respectively. The peaks became sharper by increasing the substrate temperature which indicates that as the average grain size decreases. Temperature increases the quality of the film [14, 15].

The AFM images of CdS thin films fabricated by spray pyrolysis process at different substrate temperatures 250°C, 300°C and 350°C as shown in figures 2a, 2b and 2c respectively.

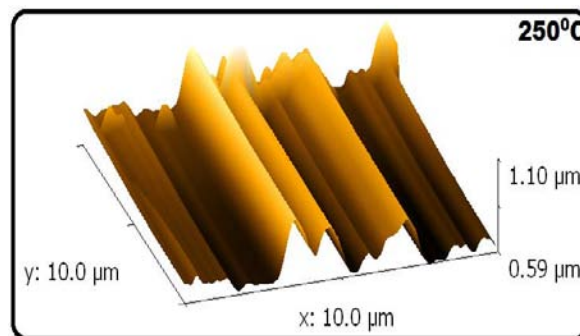


Figure 2a: AFM image of CdS thin films at substrate temperature 250°C

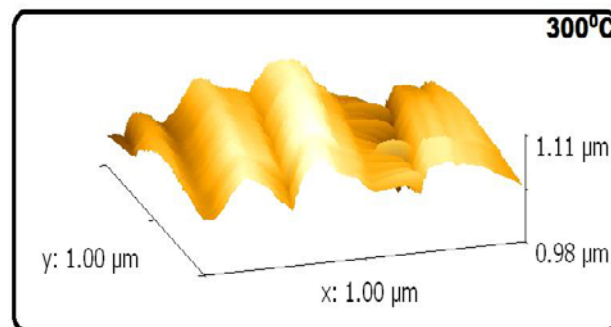


Figure 2b: AFM image of CdS thin films at substrate temperature 300°C

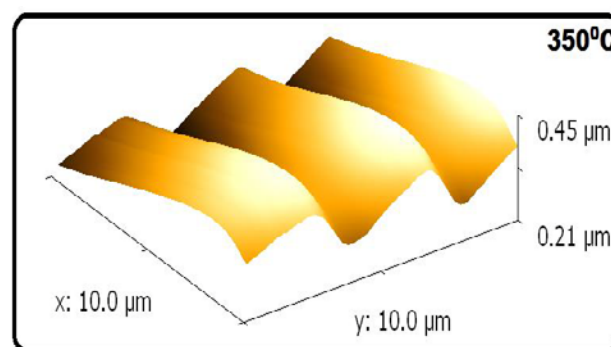


Figure 2c: AFM image of CdS thin films at substrate temperature 350°C

The film obtained at substrate temperature of 250°C shows that it has dense structure with un-even distribution of particles. At substrate temperature of 300°C the film exhibits rough surface and strips like structures. The image at 350°C substrate temperature possess that the film is homogeneous and plain, showing without any cracks. This film connected with continuous grains and the structure looks like a smooth roof. The root mean square (rms) surface roughness of the films obtained as 300 nm to 600 nm ranges for different substrate temperatures 250°C, 300°C and 350°C [16].

The elemental percentages of CdS thin films at different substrate temperatures obtained from EDX pattern is shown in figure 3.

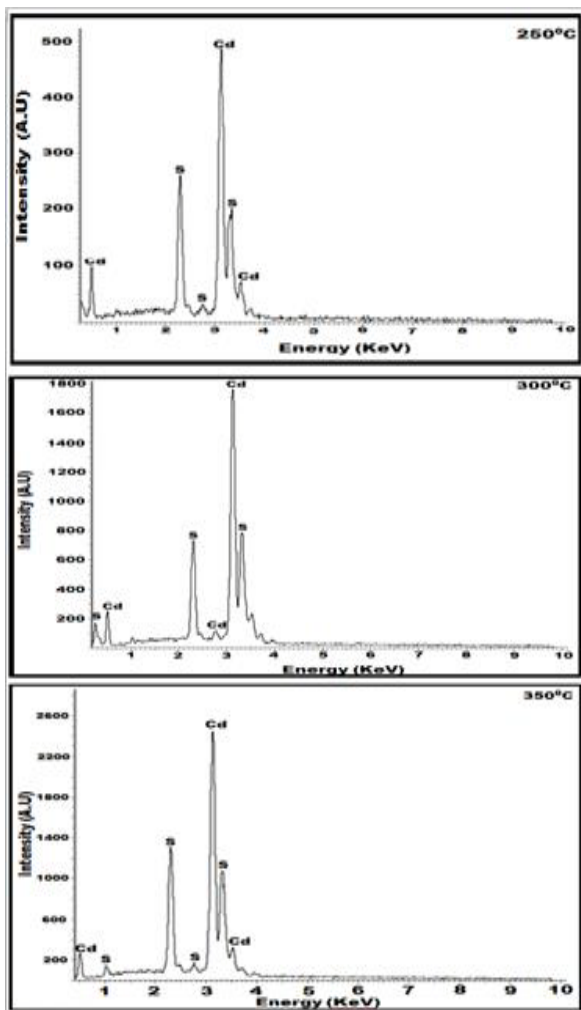


Figure 3: EDX Spectrum of CdS thin films at different substrate

The table shows that the weight percentages of Cadmium and Sulphur elements. It has been observed that when the substrate temperature increased, the weight percentage of sulphur also increased which is shown in figure 3. and table 1.

Table 1: Elemental Compositions Of Cds Thin Films At Different Substrate Temperatures

Elements	Weight Percentages at 250°C (%)	Weight Percentages at 300°C (%)	Weight Percentages at 350°C (%)
Cd	54.65	53.68	51.04
S	45.35	46.32	48.96
Total	100.00	100.00	100.00

4.2 Structural Properties

The optical absorption spectra of the films deposited on glass substrate were studied in the range of 300 – 1100 nm wavelength. The variation of absorbance (A) and transmittance (%) with wavelength for the thin films under study are shown in fig. 4 and fig. 5 respectively. The films show high absorption in entire UV region and a part of visible region. The absorbance was uniform for most of visible region and lower absorbance in infrared region as shown in figure 4.

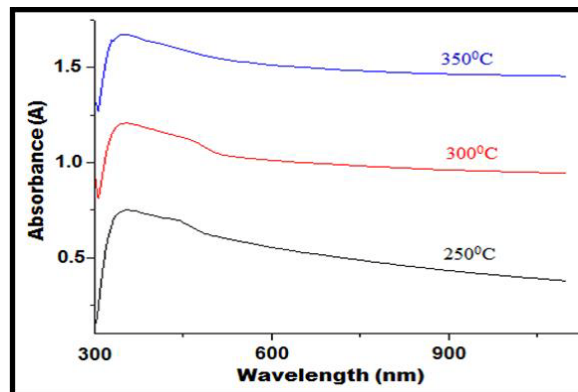


Figure 4: UV-Visible absorption spectrum of CdS thin films for different substrate temperatures

The transmission spectra show that the films transmit well in the visible and infrared region. The transmittance of the films increases gradually with wavelength in the visible region of the spectrum as shown in fig.5.

The absorption co-efficient (α) of CdS thin films were measured using the equation

$$\alpha = \frac{4\pi K}{\lambda} \quad (2)$$

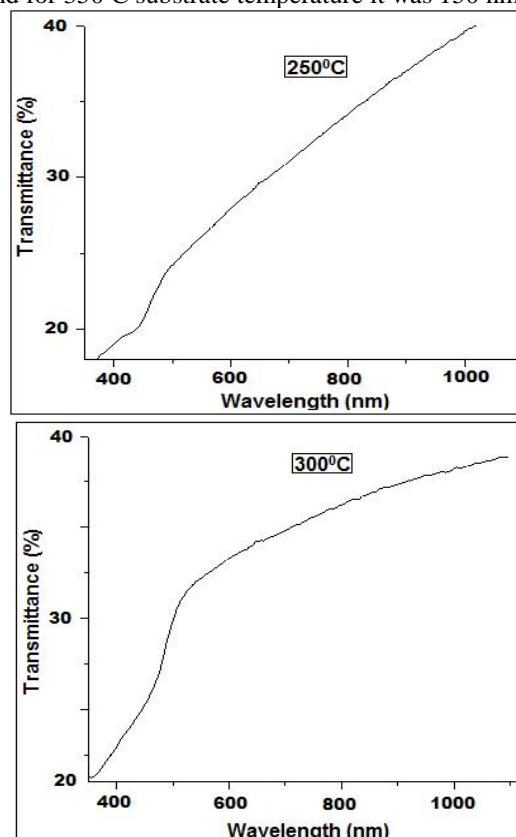
where K is absorbance and λ is wavelength.

The thickness of the films have been measured using below equation

$$t = \frac{2.303 A}{\alpha} \quad (3)$$

where A is absorbance, α is absorption co-efficient.

The calculated thickness for 250°C substrate temperature was 118 nm, whereas for 300°C substrate temperature was 132 nm and for 350°C substrate temperature it was 150 nm.



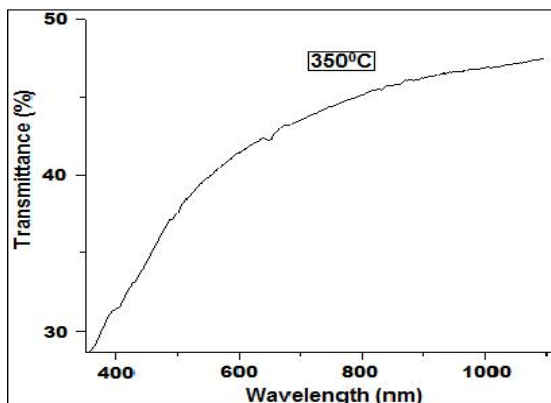


Figure 5: The transmittance as a function of wavelength for CdS thin films at different substrate temperatures

From the values mentioned above it can be inferred that as the substrate temperature increases the thickness of the film decreases [17]. The absorption spectra, which are the most direct and perhaps the simplest method for probing the band structure of semiconductors, were employed in the determination of the energy gap. The optical band gap was calculated using the Tauc-relation which is given by the formula

$$(\alpha h\nu) = A (h\nu - E_g)^n \quad (4)$$

Where A is absorbance, $h\nu$ is the photon energy, E_g is optical band gap of the material and α is the absorption coefficient, while 'n' depends on the nature of the transition. For direct transitions $n = 1/2$ or $n = 2/3$, whereas indirect transitions $n = 2$ or 3.

The direct band gap of the films were obtained from the linear portion of $(\alpha h\nu)^2$ versus $h\nu$ plot as shown in fig. 5. When $(\alpha h\nu)^2$ is plotted as a function of $(h\nu)$, the linear portion of the curve is extrapolated to $(\alpha h\nu)^2 = 0$.

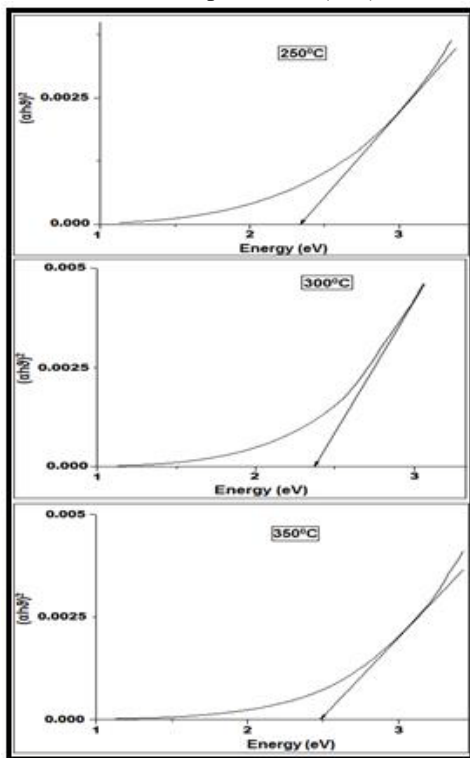


Figure 6: Photon energies of the CdS thin films at different substrate temperatures

The direct band gap values were calculated as 2.34 eV, 2.37 eV and 2.48 eV for CdS thin films at different substrate temperatures of 250°C, 300°C and 350°C respectively. This is a way of achieving band gap tuning in semiconductor materials and hence the development of new thin films for efficient photovoltaic application. It has been found that the energy band gaps of substrate temperature deposited thin films increased with substrate temperatures. As that substrate temperature increased, the sharp absorption edge was formed because the grain size increased as they became more crystalline. It was observed that the potential energy was less at lower absorption. Whereas the higher absorbance, higher the photon energy as shown in figure 6 [18].

5. Conclusions

The CdS thin films were successfully fabricated at different temperatures by Spray Pyrolysis technique. The structural properties were studied by XRD and AFM. XRD pattern shows that structure of the CdS thin films were in hexagonal phase. The average grain sizes were increased along with increasing of substrate temperatures. The AFM images of CdS thin films fabricated at different substrate temperatures shows that the smoothness and uniform thickness increased as the substrate temperature increased. The optical properties were examined by UV – Visible absorption spectrometry. The optical studies says that most of the films have high absorbance in the visible region of the spectrum and high transmittance in the near infrared region and therefore can be used as solar control device or selective absorber surface device. The band gap values were observed to increase as the absorbance decreased and substrate temperature increased. Tauc-relation showed that the band gaps were increases along with substrate temperatures.

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