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Structural and Optical Characterization of Spray Deposited Cadmium Sulphide Thin Film

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Abstract: Cadmium sulphide (CdS) thin film was prepared on glass substrate by chemical spray pyrolysis technique using the precursor solutions of cadmium chloride (CdCl2) and thiourea [(NH2)2CS] at the substrate temperature of 573 K.X ray diffraction analysis revealed the polycrystalline nature and the preferential orientation growth of CdS compound having hexagonal structure along (002) plane. The size of the cadmium sulphide crystallite with nano dimension was determined using the Full Width Half Maximum value of the Bragg peak. The surface morphology had been observed on the surface of this film using scanning electron microscope. The optical absorption and transmittance spectra have been recorded for these films in the wavelength range 400–800 nm. The optical band gap energy is found to be 2.42 eV with direct allowed band-to-band transition for film deposited at 573 K. The functional group is identified using FTIR spectra.
Keywords: Thin Film, Crystallite Size, Band Gap, Absorption, Transmittance.

1 Introduction

Thin films are well known for their applications in many technological based industries as materials for many semiconducting devices CdS and CdSe are suitable candidates used in manufacturing of light dependent resistors sensitive to visible and near infrared light. It can be combined with other layers for use in certain types of solar cells in thin film form. Also it is the first semiconductor materials to be used for thin-film transistors [1]. The interest in compound semiconductors for thin-film transistors largely demanded after the emergence of amorphous in current technology. The films of Cadmium Sulfide has been used for piezoelectric and have been used as transducers which can operate at frequencies in the Giga Hertz region [2-3]. It can also be used for electronic goods, displays of light emitting diodes, liquid crystal display, optical coating, luminance, magnetic and optical data storage, antistatic coatings, hard surface coatings, pigments. CdS thin films are regarded as one of the most promising materials for hetero junction thin film solar cells with optical band gap of 2.4 eV has been used as the window material together with several semiconductors such as Cadmium Telluride [4], Cu_2S [5], InP [6] and $CuInSe_2$ [7] with 14 to 16% efficiency [8].The yellow colored inorganic compound CdS and it occurs in nature with two different crystal structures as the rare minerals greenockite and hawleyite, butis more prevalent as an impurity substituent in the similarly structured zinc ores sphalerite and wurtzite, which are the major economic sources of cadmium. The compound that is easy for isolation and purification is the key component for the chosen system [9]. Chalcogenide semiconductor thin films are being intensively investigated for low-cost photovoltaic and optoelectronic applications. Cadmium sulfide is commonly used as *n*-type semiconducting layer for hetero junction thin films solar cells. Multilayered CdS films can be employed in the manufacture of the optoelectronic devices [10].

Chemical deposition of thin films has advantage as a low deposition cost technique to realize economic and large area devices on various aspects of chemically deposited thin films. The growth mechanism has an experimental advantage of varying the parameter such as deposition rate, composition and temperature [11].The deposition of CdS film has been explored by various techniques, such as thermal evaporation [12], sputtering [13], molecular beam epitaxy [14], spray pyrolysis [15],

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chemical bath deposition [16].Chemical spray pyrolysis technique is a method of growing thin films of certain materials on a glass substrate and it has been identified as a low cost process suitable for the preparation of large area thin films. In this paper, it is intended to prepare cadmium sulphide thin film on glass substrate at suitable thermal energy using the precursors consists of cadmium chloride and thiourea.

2 Experimental Details

The spray pyrolysis technique is a simple technology in which an ionic solution containing the constituent elements of a compound in the form of soluble salts is sprayed onto over heated glass substrate using a stream of clean, dry air. The CdS thin film was prepared by spraying an aqueous solution of cadmium chloride and thiourea on glass substrate. The precursor solutions were sprayed at the substrate temperature of 573 K. The other deposition parameters like solution flow rate, carrier gas pressure and nozzle to substrate distance were kept as 4 ml per minute, 0.6 kg/cm^2 and 25 cm respectively. After deposition of these films, it was allowed to cool to room temperature, cleaned with distilled water, dried and then stored in a dessicator. The colour of the deposited thin film is light yellow and adheres to the substrate. The atomization of the chemical solution into a spray of fine droplets is effected by the spray nozzle, with the help of compressed air as carrier gas. The substrate is glass having 2.5 cm x 1.5 cm x 0.1 cm, and is placed in a fitted socket at the surface of a substrate heater when sprayed. The heater is a cylindrical stainless steel block furnace electrically controlled to an accuracy of ±3ºC. The X-ray diffraction (XRD) pattern of the film was recorded with a JEOL Pa X-ray diffractometer operating with a 0.1540 nm monochromatized Cu kα radiation at 40 kV and 30 mA. Transmission and absorption coefficient spectra of the prepared sample were measured by normal incidence oflight, using a double beam UV-3101 Shimadzus pectrophotometer in the wavelength range 400 to 800 nm. Functional group analysis was determined using Perkin Elmer Spectrophotometer in the frequency range 400-4000 cm^{-1}.

3 Results and Discussions

3.1 Structural Characteristics

Figure 1 shows the XRD diffraction profile of the spray pyrolysised CdS thin film with the substrate temperature of 573K. The diffracted Bragg peaks at the 2θ positions were obtained 13.802˚, 23.183˚ and 28.108˚. But the crystallanity with the preferential orientation growth of film having hexagonal structure along (002) plane diffracted with single prominent Bragg peak at the 2θ position is 28.108˚ (JCPDS card no. 27-0060). The interplanar spacing corresponding to this peak is determined to be 3.174 A˚ on the substrate plane.

Authors Battisha et al. [15], Laukaitis et al. [18], Mathew et al. [19] and Ashour et al. [20], using spray pyrolysis and different techniques [17], obtained a single phase of hexagonal phase of CdS thin films. The crystallite size can be determined from the (002) diffraction line using the Scherrer formula [21]:

$$\text{Crystallite size} = K\lambda / \beta \cos\theta$$

where β is the full width at half maximum (FWHM) of the peak corrected for instrumental broadening: λ is the wavelength of the X-ray, and K is the Scherrer constant (0.9), which generally depends on the crystallite shape. The crystallite size was calculated in this spray pyrolysised film for the prominent peak is 57 nm. These crystallite size are similar to those obtained by Mahmoud et al. [12].

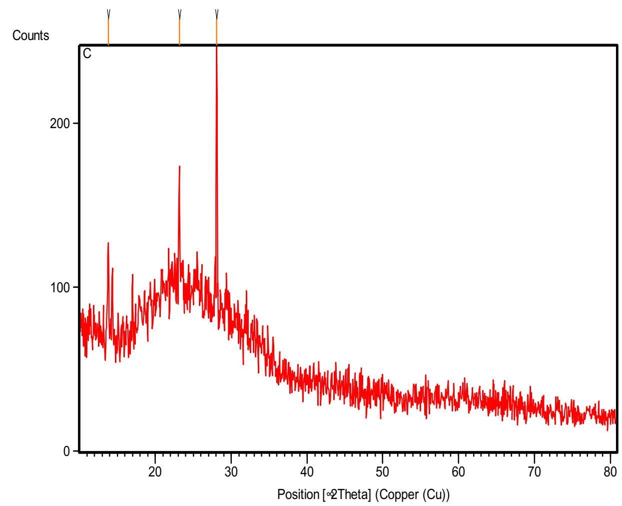

Fig.1: XRD pattern of CdS thin film at 573 K.

3.2 Morphology Characterization

The surface morphology of the thin film deposited at this substrate temperature was studied and analyzed by photographing the scanning electron microscope image with magnification 40k as shown in Figure. 2. It is seen from the random and spherical shaped grains and good adhered to the substrate.

3.3 Optical Properties

To study the optical properties of the materials, the optical absorption spectra of this spray pyrolysised CdS thin film is recorded in the wavelength range 400–800 nm as shown in Figure. 3. Hence the optical transmittance (T) with respect to wavelength of spray pyrolysised CdS thin film in the above wavelength range at substrate temperature is calculated and plotted as shown in Figure 4.

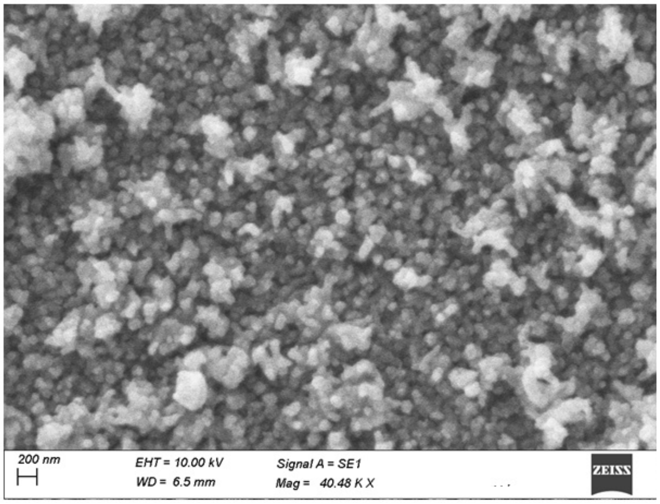

Fig. 2: SEM image of CdS thin film at 573 K.

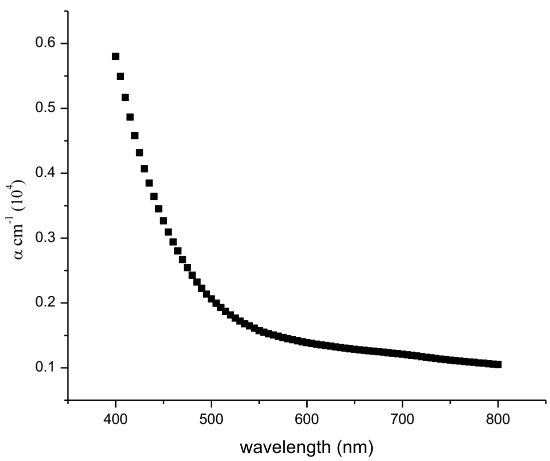

Fig.3: Absorbance coefficient of CdS thin film at 573 K.

A typical optical transmission spectrum of this film in generally, the optical transmission of CdS film depends on the thickness because of the increase in diffuse scattering from the adsorbed colloids, especially when the film is deposited in the presence of heavy homogeneous reaction.

The optical transmission of this film below the band edge of CdS film ranged from 70 to 80%, this suggests that minimization of the homogenous reaction improves the optical transmission below the band edge [22].

In the high photon energy region, the energy dependence of the absorption coefficient $\alpha \geq 10^4$ cm^{-1} suggests the occurrence of direct optical transition, which is investigated by the relation.

$$(\alpha h\nu)^n = k\,(h\nu - E_g)$$

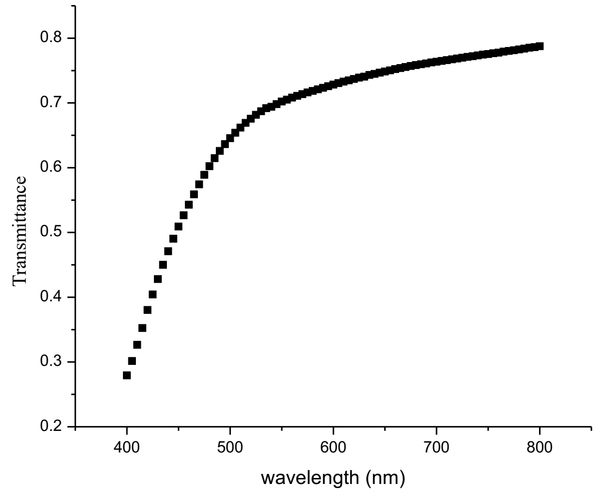

Fig.4: Transmittance spectra of CdS thin film at 573 K

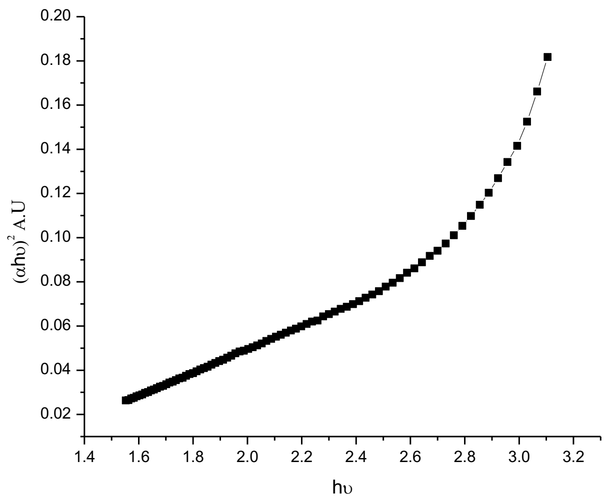

Fig. 5: $(\alpha h\nu)^2$versus hν plot for CdS thin film at573 K.

Where k is the proportionality constant, Eg is the optical band gap and n = 2 for a direct allowed transition. The band gap estimation of cadmium sulphide thin film achieved by plotting $(\alpha h\nu)^2$ as a function of (hν) as shown in Fig. 5.The plot yields a straight line which indicates a good fit, extrapolation of the straight line to $(\alpha h\nu)^2 = 0$ gives the optical direct band gap value 2.42 eV for this substrate temperature.

3.4 FTIR Analysis

The FTIR spectroscopy studies were effectively used to identify the functional groups present in the synthesized compound and to determine the molecular structure. In order to analyze qualitatively the presence of the functional groups in FTIR spectra was in the range 400–4000 cm^{-1}.The characteristic vibrational frequencies of the functional groups have been presented in Fig 6.

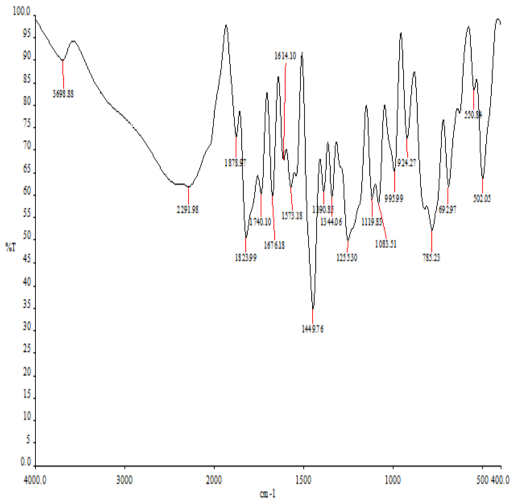

Fig. 6: FTIR spectra of CdS thin film at 573 K.

The absorption bond at 3698 cm^{-1} indicates the presence of N–H symmetric stretching mode. The absorption band at 1614 cm^{-1} shows the presence of NH_2 in the bending mode. The C–N stretching vibrations at 1083 cm^{-1} are shifted to the higher frequency of 1119 cm^{-1}. The increase in frequency may be attributed to a strong double bond character of the carbon to nitrogen bond on complex formation and the single bond character of the carbon to sulfur bond [22]. The formation of an S–Cd bond is expected to increase the contribution to the highly polar character of the structure of the thiourea molecule. The band found in CdS at1449 cm^{-1} corresponds to the N–C–N vibrations. The same type of vibrational analysis was done by reported literatures [23-25].

4 Conclusions

Cadmium sulphide thin film was fabricated with nano dimensions had been deposited on to glass substrate by chemical spray pyrolysis using the precursor solutions of cadmium chloride and n–n dimethyl- thiourea at the substrate temperature of 573K.Polycrystalline nature of the film with hexagonal structure grown with preferential orientation of (002) miller plane and the surface morphology of this film with 40k was determined. The spray pyrolysised thin film shows direct allowed optical transition nature with a direct optical band gap value exhibited 2.42 eV. The functional group present in the synthesized compound and to determine the molecular structure. These results suggest that CdS thin film could be a potential candidate for opto- electronic as well as thin film solar cell devices.

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