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Structural and Optical Properties of Zinc Doped CdS Thin Films

Karunathi U.*, Pabahar S., Sikanth S., Karunkaran R.T.
Department of Physics, Government Arts College, India
*E-mail: karunanitiu30@gmail.com

Abstract

In this paper, different aspects and facts concerned with the synthesis of thin films of lead chalcogenides along with its opto-electro-structural properties is presented. The polycrystalline thin films were put onto chemically clean and optically plane glass substrates by chemical bath deposition technique from aqueous solutions of Cadmium chloride, Zinc acetate, thiourea, triethanolamine and ammonia. X-ray diffraction analysis has been used for the structural characterization. It indicates that the crystallized layers are cubic in form. By using Scherrer's formula and the data obtained from the XRD studies,the grain size was calculated as 16.5 nm. The band gap energy estimated for Zinc- doped CdS thin films is 2.95 eV.

Keywords: Zinc doped CdS, X-ray diffraction, Scherrer's formula, Cadmium chloride, Solar cells

1 Introduction

A layer or multiple layers of atoms of a particular substance whose thickness falls within the range of 10 nm and 1μm can be defined as a thin film. The interest in thin films raised from the wide range of use and application in electronic equipments and devices. These films have been used in various fields such as of manufacturing (p-n) junctions, rectifiers, mirrors with two types ordinary and thermally, reflected and antireflected coating, photograph, integrated circuits, and optical communications as light emitting diodes, detectors solar cells, etc. This leads to study of optical and electronic properties of thin films. Semiconductors differ from insulators only in the width of the forbidden band (Eg). An insulator has a forbidden gap is so wide that very few electrons cross it at room temperature, whereas a semiconductor possesses a narrow gap which allows a considerable amount of electrons to the conduction band. At room temperature the semiconductors have conductivity in the range of (10^{-8}-10^{3}) $\Omega^{-1}cm^{-1}$. Cadmium sulphide is a direct band gap semiconductor of about 2.4 eV. It is found near the photon energy of maximum solar radiation spectrum, it causes absorption in the short wavelength side, and has a high absorption coefficient (10^{5} cm^{-1})

within the solar radiation to generate carriers across the band gap with wavelength less than (0.520 mm). The refractive index of CdS is 2.3, 2.26 and dielectric constant 8.64. Cadmium-sulphide is a suitable material for fabricating a photovoltaic p-n junction comprising of a p-type CGS and CIS. CdS is naturally n-type with a close lattice match to CIS and possessing a wide optical band-gap (Anbarasi, Nagarethinam, & Balu, 2015; Hashim, Habeeb, & Ghanim, 2013; Ravangave & Biradar, 2013). It is usually used as a very suitable window layers which are prepared as thin as possible to avoid optical transition losses.

Numerous film deposition methods such as Thermal Evaporation in Vacuum Deposition, Sputtering technique, Chemical Vapor Deposition, Pulse Laser Deposition, Thermal Pyrolysis Deposition and Chemical bath deposition have been employed for preparing II-VI compound. Amongst the techniques, Chemical Bath Deposition (CBD) facilitates continuous coverage of rough surfaces with minimal costs and thickness and hence is considered as one of the prominent techniques for film synthesis. In contrast to other deposition techniques, CBD Zinc dopped CdS thin films exhibit a congruent growth on the glass substrate. Congruent growth is vital as it allows depositing of a uniform CdS film on a substrate with the required thickness (Agbo, Nweke, Nwofe, & Ukwu, 2014; Theivasanthi & Alagar, 2011). On the contrary, in the absence of congruent growth, the film thickness may indicate pronounced local variations (Brindha & Devi, 2016; Ezema, Hile, Ezugwu, Osuji, & Asogwa, 2010; Lozada-Morales, Rubı́n-Falfán, Zelaya-Angel, & Ramı́rez-Bon, 1998).

The Zinc dopped CdS thin films grown at improved preparative parameters were characterized by means of the ensuing techniques. A Philips PW-1710, X-ray diffractometer using Cu Ka radiation with wavelength 1.542 Å was used to obtain the diffraction patterns. X-ray diffraction patterns were studied to find the structural information of Zinc dopped CdS thin films. A UV-Vis-NIR spectrophotometer model Hitachi-330 was used to do the optical film absorption studies in the wavelength range of 100-1000 nm.

2 Materials and Methods

The CdS thin film deposition is founded on the Cd^{2+} and S^{2-} ions reaction in deionised water solution. Chemical baths used for the Zinc doped CdS thin film deposition consist of Cadmium chloride (Merk 99%), thiourea (Nice 99%), Zinc acetate (Nice 99%), triethanolamine (Nice 99%) and ammonia. By adding ammonia the pH of the solution can be adjusted. Thin film deposition is done at a temperature of 80 °C. 1:1 molar proportions of Cadmium chloride, Zinc acetate and thiourea 1:1 is used. At a pH value of 12, deposition is performed. The time periods are varied from 30 to 60 min and the substrates are placed vertically in the bath. Thus deposition parameters such as dipping time, concentration of ions in the bath and temperature have been optimized.

3 Results and Discussion

3.1 X-ray diffraction studies

The XRD pattern of the Zinc doped CdS thin films on glass substrate is shown in the Figure 1. The peak position (2θ) values comparison of American Standard for Testing Materials (ASTM) card (03-0932) with XRD spectra data suggests that film have cubic structure and exhibit polycrystalline structure. The XRD pattern shows prominent peaks at 2θ values of 26.60, 44.30 and 52.03 which could be scattering indexed from (111), (220) and (311) planes respectively of cubic Zinc doped CdS thin films. It is clear from the table A1 that the standard values and the data obtained in this work closely resemble each other.

The diffraction peaks shape specifies that the product is well crystallized. The XRD pattern shows no impurity phase. The XRD pattern results clearly indicate high intensity and litle broad reflections due to good crystallinity observed in the film. Scherrer's eqution was used to calculate the average crystallite size of Zinc doped CdS. Scherrer's formula is represented as follows Equation 1.

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

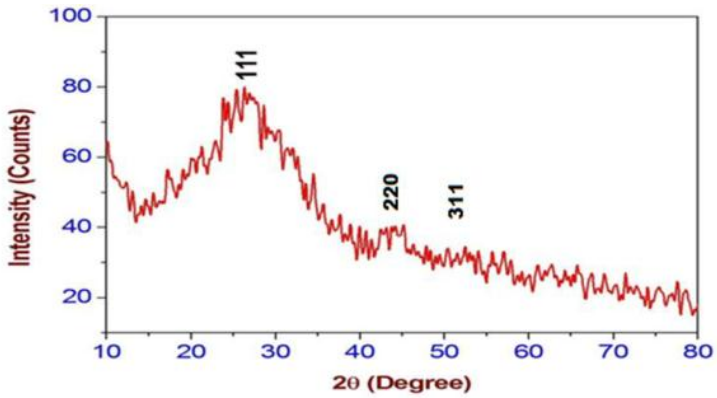

Figure 1. X-ray Diffraction spectra of Zinc doped CdS thin films prepared at pH 12 (60 minutes)

where D represents the crystallite size, λ is denotes the wavelength of the X-rays (1.5406 Å), β is the full width at half maximum and θ is the diffraction peak angle. The average sample particle size is found to be 16.65 nm. Based on the Scherrer equation, the diffraction peak broadening is in accordance with the small grain sizes (Agbo et al., 2014; Theivasanthi & Alagar, 2011). Table 1 shows the calculated and standard θ and D values for corresponding diffraction angles of predominant peaks. The values are found to be in close association with the standard values of Zinc dopped cadmium Sulphide.

Table 1. Comparison between experimental and standard XRD data for Zinc doped CdS thin films

Standart JCPDS			**Experimental values**		
HK1	**d-spacing**	**2θ (Degrees)**	**HK1**	**d-spacing**	**2θ (Degrees)**
111	3.16	28.21	111	3.24	28.41
220	1.93	47.05	220	1.88	47.47
311	1.64	56.03	311	1.62	56.56

3.2 Optical studies

Optical absorption and transmittance spectra of CdS thin films measured as a function of the wavelength of incident photons for pH 12 at deposition time period 60minutes are presented in Figure 2 and Figure 3. Between the wavelength of 600-1100nm transmittance is high with a gradual fall near the fundamental absorption region. The films show an optical transmittance of 70-80 % in the 600-800 nm range which is high enough for photovoltaic application. The spectrum (Figure 3) reveals that the deposited film has low absorbance in the VIS/NIR region. On the other hand it is high in the UV region. Hence absorbance of the film is inversely proportional to wavelength and directly proportional to photon energy. It can be positively concluded that the material is of highly absorbing in nature.

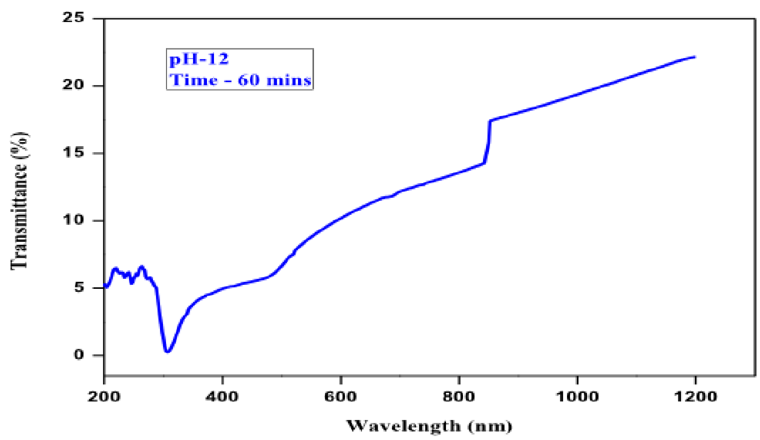

Figure 2. Transmittance Spectrum of CdS thin films prepared at pH 12 (60 minutes)

The Figure 3 indicates a high absorbance in the visible region between (300 to 400 nm) and a respective decrease in absorbance as the wavelength increases along the near infrared region. The decrease in absorbance in the near infra red region depicts high transmittance near the infra-red region of the spectrum for the Zinc doped CdS thin films. Figure B3 shows the optical transition energies (energy band gap) of prepared sample. The band gap energy could be estimated using the formula $Eg = hc / \lambda$, where h and c are the Planck's constant and velocity of light, respectively, and the calculated value for sample Zinc- doped CdS thin films is 2.95eV. However, the obtained value is at the green part of the solar spectrum, noticing that the synthesized film structure have a very good application prospect in the field of photovoltaic conversion. The previous report also says that the micrometer or sumicrometer sized particles posses enhanced scattering effect for visible light which is rather useful for photovoltaic applications (Wu et al., 2012).

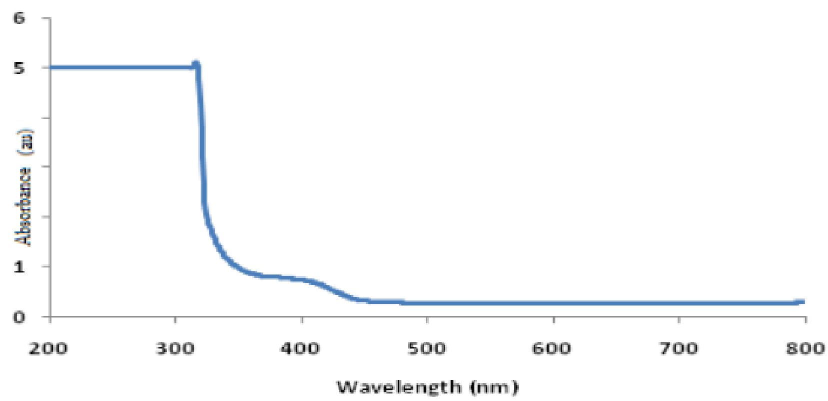

Figure 3. UV Visible absorbance Spectra of Zinc doped CdS thin films prepared at pH 12 (60 minutes)

The higher calculated values of the band gap are presumably due to the quantum size effect. Particularly, it is well known that the optical band gap of thin film materials, which are characterized by a length scale less than 10 nm, is higher than that of bulk material. As the molar concentration increases, the absorption edge shifts gradually towards longer wavelength and shifts the band gap. The energy band gap increase is mainly due to sp-d exchange interaction between the band electrons and the localized d-electrons of Zn^{2+} ions doped for CdS ions. The energy band gap measurement of sample is performed at room temperature owing to band gap is higher than that of bulk CdS samples. The earlier this researchers reported that the band gap of undoped and Zn substituted CdS samples are greater than that of bulk CdS due to the above room temperature (Lozada-Morales et al., 1998; Ravangave & Biradar, 2013). It reflects good experimental results which were expected. The increase of energy band gap is mainly due to sp-d exchange interaction between the band electrons and the localized d electrons of Zn^{2+} ions doped for CdS ions.

4 Conclusion

The Zinc doped CdS thin films have been deposited on glass substrates by chemical bath deposition route. Structural characterization performed using X-ray diffraction analysis indicates that the layers are crystallized in the cubic structure. The crystallite size calculated from the data obtained from the XRD studies, using the Scherrer's formula was 16.5 nm. The lattice parameters calculated are in good agreement with the standard data confirming that the Zinc doped CdS films are cubic in structure. Energy gap of zinc doped cadmium sulphide thin film is 2.95eV. These CdS thin film characteristics make them a suitable candidate for different optoelectronic and device applications.

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