

Structural and Optical Characteristics of CdSe Thin Films Prepared by Chemical Bath Deposition Technique

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Cadmium selenide thin films were deposited on glass substrate using chemical bath technique for different bath temperatures 313K, 333K and 353K. Polycrystalline nature of the material was confirmed by X-ray diffraction technique and various structural parameters were calculated. The optical properties were revealed by UV-Visible transmittance spectra and the band gap energy was determined.

Keywords: Thin films, CdSe, X-ray diffraction, Scanning electron microscopy, Optical properties

Received: 2 September 2009, **Revised:** 28 September 2009, **Accepted:** 5 October 2009

1. Introduction

The II-VI binary semiconducting compounds belonging to the cadmium chalcogenide family (CdS, CdSe, CdTe) are considered to be very important materials for photovoltaic applications [1-3]. CdSe is a promising photovoltaic material because of its high absorption coefficient and nearly optimum band gap energy for the efficient absorption of light and conversion into electrical power [4]. CdSe has been extensively investigated for its potential applications in photoelectrochemical (PEC) solar cell, optoelectronic devices and gamma ray detectors [5-7]. CdSe is an important material for the development of various modern technologies of solid state devices such as high efficiency thin film transistors and light emitting diodes. Other areas of successful applications include photo-detectors, light amplifiers, lasers, gas sensors, large-screen liquid crystal display and photoluminescence response [8]. Semiconductor devices based on CdSe thin films strongly depend on the structural and optical properties of the films obtained from various experimental conditions. A direct band gap range of 1.65 eV-1.84 eV has been reported for CdSe by various authors [9-10] and its photosensitivity gives it an edge over other semiconducting materials.

Several physical and chemical techniques are available for the growth of CdSe thin films. CdSe thin films have been deposited using different techniques such as electrodeposition [11-12], molecular beam epitaxy [13], spray pyrolysis [14], successive ionic layer adsorption and reaction method [15], vacuum deposition and chemical bath deposition [16]. Among these methods chemical bath deposition has several overriding advantages with other techniques such as uniform film deposition, control of thickness, precise maintenance of deposition temperature, low cost [17-18]. The deposition parameters are usually optimized to obtain specularly reflecting films with a good adherence to the substrate [19-21].

In the present investigation, chemical bath deposition of cadmium selenide thin films has been reported. Structural characterization from XRD, EDAX and optical characterization from UV-Vis were carried out.

2. Experiment

Chemical bath deposition technique was adopted for the preparation of cadmium selenide (CdSe) thin films. The chemicals used for the preparation were analytical grade cadmium

acetate (99%), selenium powder (99.5%) and sodium sulphite (98%).

The reaction mixture was prepared by adding ammonia (NH₃) solution in 0.1 M of cadmium acetate [(CH₃COO)₂Cd.2H₂O] till a pH of 11 is attained. To the precursor cadmium acetate-ammonia solution, 5ml of freshly prepared sodium selenosulphite (Na₂SeSO₃) diluted with 5ml of distilled water was added drop by drop under continuous gentle stirring using magnetic stirrer at about 80±1rpm. Sodium selenosulphite was prepared by refluxing 4gm of selenium powder with 12gm of anhydrous sodium sulphite (Na₂SO₃) in 50ml of double distilled demineralised water for 4 hours at 80±0.5°C. Thoroughly cleaned glass substrates were vertically immersed at the centre of the reaction bath.

The deposition of the film was carried out at bath temperatures 313K, 333K and 353K. The bath temperature was controlled using a digital thermostat connected with Pt-100 thermocouple. The colourless bath turned orange in colour and then to orange-red as time progressed. The time of deposition was optimized as 130min. After deposition, the substrates were rinsed in distilled water and dried. The films were then annealed in air at a temperature of 553K for 15min. During annealing the colour of the film changed from orange to red then to dark brown. Films prepared by this method were uniform, well adherent to the substrate, smooth and reflecting.

At intermediate temperature (333K), the ions get sufficient time to condense on the substrate surface and therefore large amount of material gets deposited on the substrate giving maximum layer thickness. At relatively higher temperatures, more and more ions are released but all the ions do not get chance to adsorb on the substrate surface, they settle down at the bottom of the reaction container decreasing the film thickness [22].

The CdSe films were structurally characterized by X-ray powder diffraction using a JEOL JDX services instrument with CuK_α radiation (λ=1.5406Å). The microstructures of these samples were characterized using Hitachi S-3400 equipped with an EDAX spectrometer. The optical properties of CdSe films were measured using UV-Vis spectrophotometer (JASCO V-530 dual beam).

3. Results and discussion

The structural elucidation of CdSe film for the bath temperatures 333K and 353K are presented in Fig. (1) with the diffraction 2θ from

20 to 70°C. The observed *d* spacing and the respective prominent peaks correspond to reflections from (111), (220) and (311) planes which coincide well with JCPDS data [23]. Therefore it has been concluded that the deposited CdSe thin films are polycrystalline in nature with cubic structure. The lattice parameter (*a*) for cubic structure is determined using the relation

$$a = d\sqrt{h^2 + k^2 + l^2} \quad (1)$$

where, *d* is the spacing between the planes in the atomic lattice, *hkl* are the Miller indices

The grain size (*D*) for CdSe thin films are calculated using Scherrer's formula

$$D = \frac{k\lambda}{\beta \cos \theta} \quad (2)$$

where, the constant *k* is the shape factor, taken as 0.94, λ is the wavelength of X-rays (1.5406Å for CuK_α), θ is the Bragg's angle and β is the full width at half maximum

The dislocation density (*δ*) has been evaluated from Williamson and Smallman's formula $\delta = 1/D^2$ (lines/m²). The micro strain (*ε*) is obtained using the relation $\epsilon = \beta \cos \theta / 4$.

All these parameters are calculated and presented in Table (1).

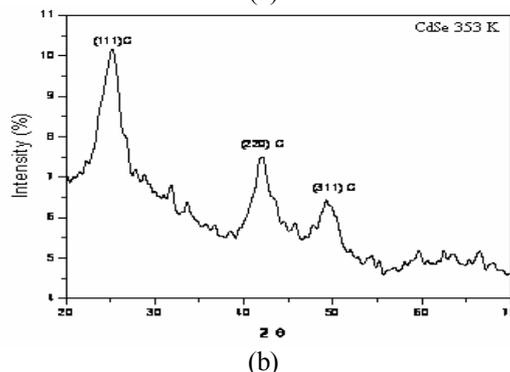
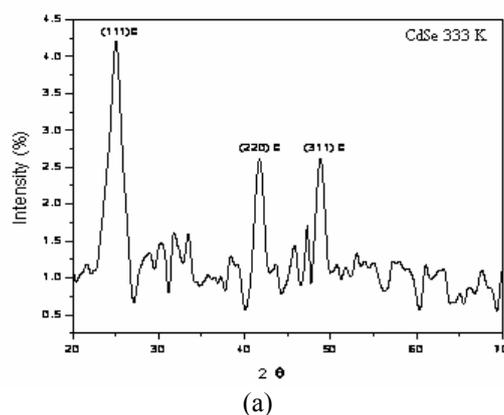


Fig. (1) (a) XRD pattern of CdSe thin film (333K), (b) XRD pattern of CdSe thin film (353K)

Table (1) Structural Parameters of CdSe Thin Film

Material (temp. in K)	2 θ (deg)	d (spacing) Å	(β) FWHM	(hkl)	Lattice (a) Å	Grain Size(D) nm	density (δ) $\times 10^{15}$ lines/m ²	Micro strain (ϵ) $\times 10^{-3}$
	25.3436	3.51438	1.170	111	6.0870	7.2701	18.9193	4.9798
CdSe (333K)	42.1084	2.11360	1.160	220	5.9781	7.6660	17.0160	4.7226
	49.8257	1.8286	1.152	311	6.0647	7.9430	15.8499	4.5579
	25.2062	3.53030	1.152	111	6.1146	7.3818	18.3516	4.9045
CdSe (353K)	42.0122	2.14887	1.152	220	6.0779	7.7167	16.7930	4.6916
	49.6925	1.8046	1.142	311	5.9851	8.0082	15.5927	4.5208

The quantitative analysis of CdSe films prepared at bath temperature 333K is shown in Fig. (2). The EDAX pattern confirms the presence of cadmium and selenide compounds. The average atomic percentage ratio of CdSe was found to be 19.57:3.78 showing that the sample was cadmium rich. Presence of silicon in EDAX is due to the silicon content in glass substrate, since Na₂SeSO₃ was used as a source of selenium, a small amount of sodium is present in the film where as sulphur escapes as H₂S or SO₂.

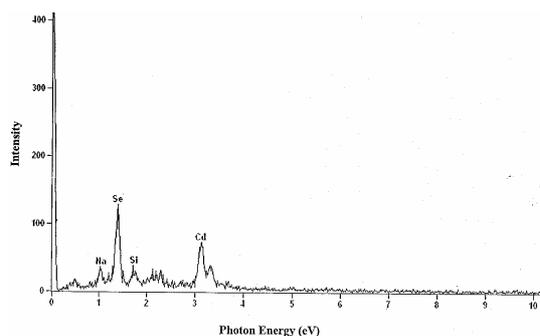


Fig. (2) Energy Dispersive X-ray analysis of CdSe thin film (333 K)

The optical transmittance spectra of CdSe thin film is recorded as a function of wavelength in the range 400-1200 nm as shown in Fig. (3). The CdSe material deposited on the glass substrate showed a transmittance of ~60 % for 313 K and is found to decrease as temperature increases along with the film thickness which shows the improvement in crystallinity. A typical plot of $(\alpha h\nu)^2$ with photon energy $h\nu$ for CdSe thin film is shown in Fig. (4). The band gap energy is obtained by extrapolating the straight line portion of the graph to zero absorption coefficient. The intercept on the $h\nu$ axis gives the value of band gap energy. It was found to be 2.12eV, 1.75eV and 1.52eV at bath temperatures 313K, 333K and 353K respectively. The direct band gap energy was found to decrease as temperature increases along with film thickness [16]. These changes are attributed to the crystallite size - dependent properties of the band gap energy.

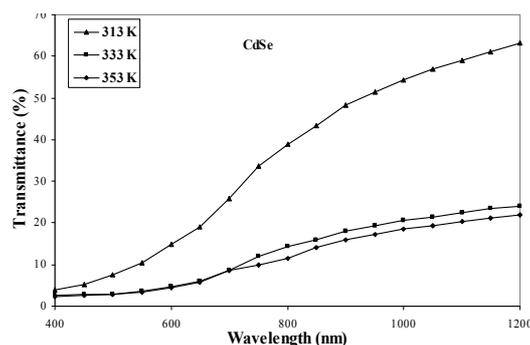


Fig. (3) Transmittance of CdSe

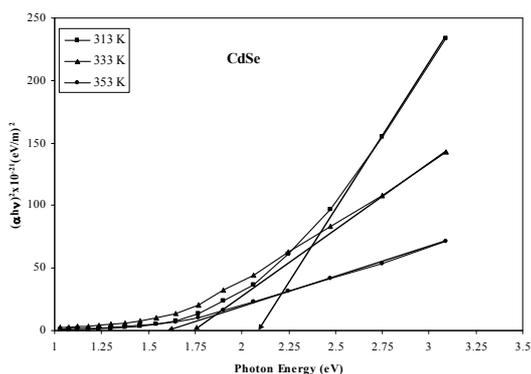


Fig. (4) Band gap energy of CdSe

4. Conclusions

CdSe thin films were deposited onto glass substrate by simple economical chemical bath deposition technique at bath temperatures 313K, 333K and 353K. XRD pattern confirms the cubic structure of CdSe thin film. SEM analysis revealed the presence of spherical shaped clusters of size 1.11 μ m. The presence of Cd and Se elements were confirmed from EDAX analysis. From the optical analysis the band gap energy was found to lie in the range 2.12eV - 1.52eV.

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