International Journal of Engineering Research-Online
A Peer Reviewed International Journal
Articles available online http://www.ijoer.in

Vol.3., S3, 2015

NCERFM-2015

ISSN: 2321-7758

CHARACTERIZATION OF CdSe THIN FILMS PREPARED BY VACUUM THERMAL EVAPORATION TECHNIQUE FOR SOLAR CELL APPLICATIONS

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ABSTRACT

Cadmium Selenide (CdSe) thin films of thickness 300 nm have been deposited onto pre cleaned glass substrates by thermal evaporation technique under a high vacuum of $2x10^{-5}$mbar. The pristine and annealed films are characterized for structural, morphological and optical properties. X-ray diffraction (XRD) studies revealed that the films are polycrystalline in nature with cubic structure. Atomic Force Microscopy analysis shows uniform deposition of the film over the entire substrate surface. The optical transmission spectra for as prepared and annealed CdSe films were studied and estimated the band gaps. The variation of the optical band gap with annealing temperature has been investigated and discussed. With increase in annealing temperature the optical band gap of these films found to decrease.

Keywords: Thin film, Thermal evaporation, XRD, AFM.

1. INTRODUCTION

Cadmium Selenide is a promising material of II–VI compound semiconductors and used in thin film devices due to its large absorption coefficient, optical band gap (1.74eV)and high photo sensitivity [1–2]. CdSe is used in many applications because of its outstanding properties, including deodorizing [3], defogging [4], light emitting diodes[5], field emitters[6] and hybrid solar cell applications [7]. The CdSe thin films can be prepared by a number of deposition techniques like electro deposition, chemical vapor deposition, chemical bath deposition, spray pyrolysis, thermal evaporation, sputtering, electron beam evaporation, molecular beam epitaxy and successive ionic layer adsorption and reaction method(SILAR) [8-16].

The CdSe thin film sample on ITO was assembled as devices for BJH solar cells by Yan'ge Zhang et al [17]. Annealing effects on the photo response properties of CdSe nano crystalline thin films was reported by Shiyun Lou et al [18] under laser illumination by Kelvin probe force microscopy and this work revealed that the work function of the annealed CdSe nano crystalline films changed more rapidly than that of the non-annealed film in air at room temperature. Assembly of CdSe onto mesoporous TiO_2 films induced by a self-assembled monolayer for quantum dot-sensitized solar cell applications was carried out by Lai-Wan Chong [19]. The relationship between refractive index-energy gap and the film thickness effect on the characteristic parameters of CdSe thin films was reported by Yunus Akaltun et al [20], the crystalline and surface properties of the films improved with increasing film thickness. The work of R.B. Kale et al [21] revealed that after annealing of CdSe thin films the meta stable nano crystalline cubic phase transformed into stable polycrystalline hexagonal phase. The influence of annealing in nitrogen atmosphere on the properties of CdSe thin films deposited by chemical bath deposition (CBD) was reported by S. Erat et al [22] and they concluded that a transition from meta stable nano crystalline cubic to stable polycrystalline hexagonal phase has been observed after annealing. The effect of annealing on the properties of CdSe thin films in $Ar+Se_2$ atmosphere was studied by O. Portillo Moreno et al [23].

This paper presents the effect of air annealing on structural, optical and morphological properties of CdSe thin films which were prepared by thermal evaporation technique. The investigation of structural, optical and morphological properties of as deposited and annealed CdSe thin films was done by X-ray diffraction, UV-

VIS spectroscopy and atomic force microscopy respectively. The crystalline parameters like inter-planar spacing, crystallite size and strain are calculated. From the optical results the energy gaps of as deposited and annealed CdSe thin films were investigated and discussed.

2. Experimental:

2.1. Preparation of CdSe thin films

The CdSe powder of purity 99.999% was procured from Balzers Company, USA. Commercially available glass slides was washed using detergent and deionised water followed by ultrasonic bath for 15 minutes. The CdSe thin films of thickness 300 nm were deposited onto the substrates employing thermal evaporation technique at a substrate temperature of 100^{o}C. Total pressure in the chamber was kept at 2X10^{-5}mbar and the distance between source and substrate was 10 cm. These deposited CdSe thin films were subjected to air annealing at temperatures 200^{o}C, 300^{o}C and 400^{o}C for one hour in a furnace.

2.2. Characterization of CdSe thin films

The structural properties of as deposited and annealed CdSe thin films were characterized employing X-ray diffraction using CuK$_{\alpha}$ (λ=1.54 Å) in the 2ϴ range from 20^{o} to 80^{o}. The morphological studies were carried out using atomic force microscopy and the scanning process was taken in an area of 500 nm x 500 nm employing contact mode. The optical properties of CdSe thin films were determined by using UV-VIS spectrophotometer at room temperature in the wavelength range 200-900 nm and the energy gaps of as deposited and annealed CdSe thin films were also calculated.

3. Results and discussion:

The X-ray diffraction patterns of as deposited and annealed CdSe thin films at temperatures 200^{o}C, 300^{o}C and 400^{o}C were presented in the Fig.1.

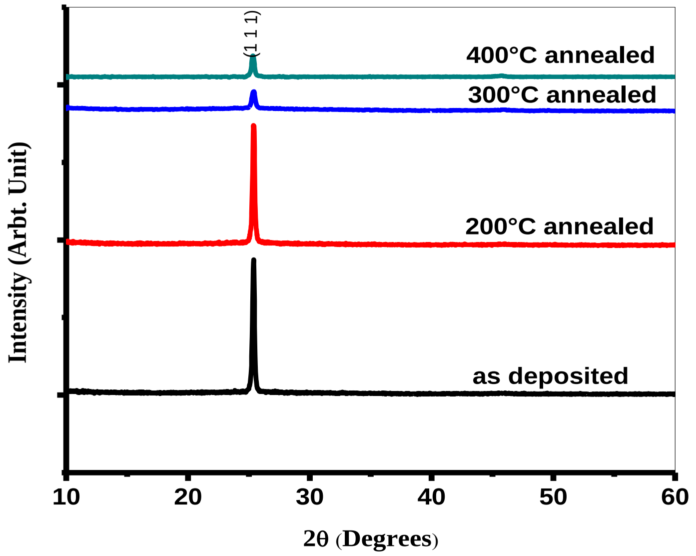

Fig.1. The XRD patterns of as deposited and annealed CdSe thin films.

From the XRD patterns of as deposited and annealed CdSe thin films it is cleared that the sharp diffraction peak at angular position 25.3^{o} and the prominent plane is observed corresponding to reflection (1 1 1), coincide well with the JCPDS data file[24]. The X-ray diffraction results confirmed that the as deposited and thermally annealed CdSe thin films were polycrystalline in nature with cubic structure. The intensity and sharpness of the prominent peak was decreased with annealing temperature owing to decrease in crystallinity. These results are well supported by the earlier work done by A. Purohith et al.[25]. The interplanar spacing (d) was calculated by Bragg's diffraction law and relation concerned [26, 27].

$$\alpha = d\sqrt{h^2 + k^2 + l^2}$$

Where *h, k and l* are miller indices.

The calculated values of interplanar spacing are presented in the Table.1.Due to annealing treatment the values in table.1. are slightly changed. The crystallite size of as deposited and annealed CdSe thin films is calculated by Debye Scherrer formula [28].

$$D_{hkl} = \frac{k\lambda}{\beta\ cos\theta}$$

Here, k is Scherrer constant given by 0.94, ϴ is Bragg's angle, λ is wavelength of X-ray used and the β is full width at half maxima (FWHM) of the peak intensity. The calculated crystallite size values are varied with different annealing temperatures due to variation in corresponding FWHM. The Strain (ε) in the CdSe thin films was calculated using the relation concerned [29].

$$\varepsilon = \frac{\beta}{4cos\theta}$$

As shown in the Table.1. the values of strain were varied with annealing temperature.

Table.1. Structural parameters of as deposited and annealed CdSe thin films.

CdSe Thin films	2θ	FWHM	Crystallite size (nm)	Strain (ε)	d-spacing (Å)
As deposited	25.3	0.384	22.16	0.0074	3.507
Annealed at 200°C	25.3	0.5760	14.77	0.0112	3.506
Annealed at 300°C	25.3	0.3149	27.02	0.0061	3.507
Annealed at 400°C	25.3	0.4723	18.01	0.0092	3.514

Optical properties of the deposited films have been studied from transmittance spectra measured by a UV–VIS spectrophotometer. The optical transmittance and absorbance spectra of as deposited and annealed CdSe thin films are presented in Fig.2. From the transmittance spectra we have also calculated the optical band gaps of as deposited and annealed CdSe thin films. The value of the optical band gap can be calculated using the fundamental absorption, which corresponds to electron excitation from the valance band to conduction band. The absorption coefficient α and the incident photon energy $h\nu$ are related by the equation [30].

$$(\alpha h\nu)^{1/n} = A(h\nu - E_g)$$

Where A is a constant, E_g is the band gap of the material and the exponent n depends on the type of transition. n=1/2, 2, 3/2 and 3 corresponding to allowed direct, allowed indirect, forbidden direct and forbidden indirect, respectively. Taking n=1/2, we have calculated the direct optical band gap from $(\alpha h\nu)^{1/n}$ vs. $h\nu$ plot (Fig.3.) by extrapolating the linear portion of the graph to $h\nu$ - axis. The intercept on the $h\nu$-axis determines the direct band gap and these are varied with annealing temperatures, this may be due to the variation in crystallite size of the films.

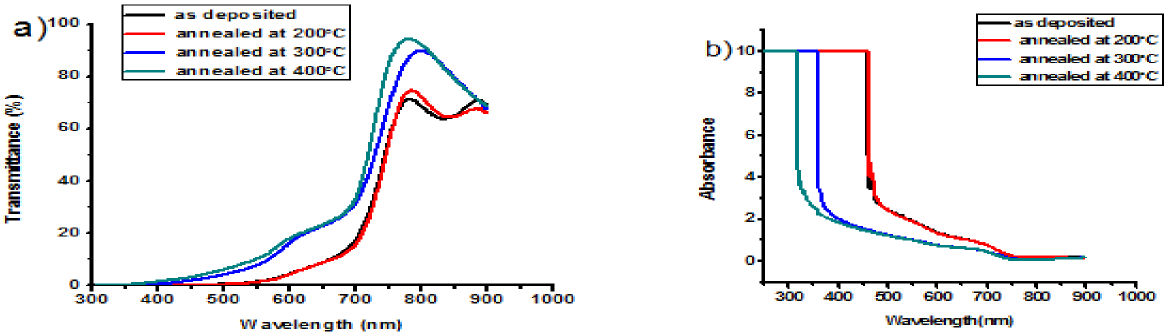

Fig.2. Optical a) transmittance and b) absorbance spectra of as deposited and annealed CdSe thin films.

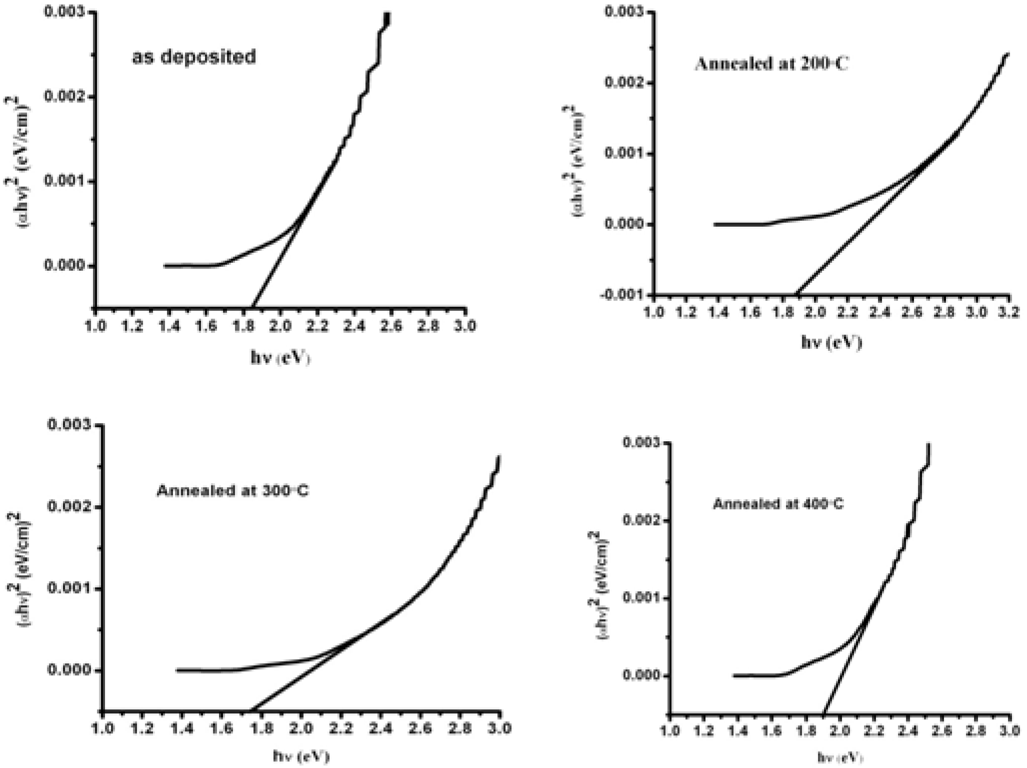

Fig. 3. Plots of $(\alpha h\nu)^2$ vs. $h\nu$ of as deposited and annealed CdSe thin films.

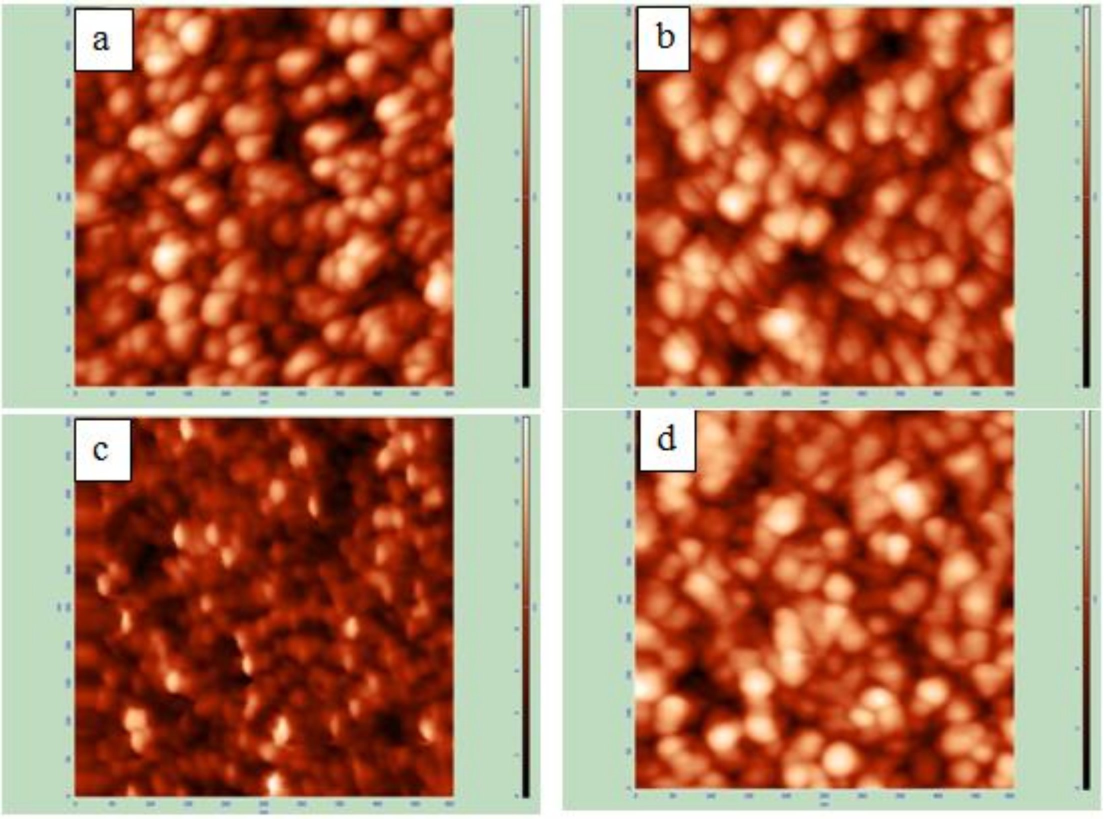

Fig.4. 2-D micrographs of CdSe (a)-As deposited, (b) Annealed at 200˚C, (c) Annealed at 300˚C, (d) Annealed at 400˚C.

To find the surface morphology of thin films the atomic force microscopy (AFM) is a unique method, the two dimensional images of as deposited and annealed CdSe thin films are presented in Fig.4. The scanning process is done in an area of 500 nm x 500 nm in contact mode.

From the results of AFM it has been observed that the surface morphology and roughness improved with annealing in air atmosphere which may be attributed to improvement in porosity of the films due to structural disorder. The root mean square roughness of the films is varied with annealing temperature. These results are in good agreement with the previous work, 'Effect of air annealing on structural, optical, morphological and electrical properties of thermally evaporated CdSe thin films' [25].

4. Conclusions:

In summary, the influence of air annealing on the structural, optical and morphological properties of the thermally evaporated CdSe thin films was investigated. The thin films were deposited on glass substrates and subjected to annealing at temperatures 200°C, 300°C and 400°C in the air atmosphere. The as deposited and thermally annealed CdSe thin films were characterized for structural, morphological, optical properties. The X-ray diffraction pattern shows that the films have cubic phase with preferred orientation (1 1 1). The structural parameters like interplanar spacing, crystallite size and strain were calculated and found to be varied with annealing temperature. The energy gap values of as deposited and annealed CdSe thin films were calculated from the transmittance spectra and found to vary with annealing temperature. The atomic force microscopy (AFM) shows that the surface morphology and roughness are improved with annealing temperature which may attributed to improvement in porosity.

5. Acknowledgement:

The author NJB would like to thank the Head, dept. of Physics, Osmania University for providing experimental facility to carry out the above work. The author acknowledges the Department of Science and Technology (DST), New Delhi, India for providing financial assistance in the form of DST INSPIRE JRF during the research. One of the authors (MVRR) thanks UGC (UPE - FAR), OU, for providing financial assistance to carry out this work.

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