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Structural and Optical Properties of Cd_{0.4}Se_{0.6} Thin Films Prepared by CBD

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Abstract: Cd_{0.4}Se_{0.6} thin films have been prepared on a glass substrate by chemical bath deposition (CBD) technique. AFM and X-ray analysis were utilized to investigate the effect of thickness variation on surface morphology and crystallinity. The optical properties of thin films were also investigated as a function of film thickness, which was noticed to be improved with the increasing of film thickness. This could be attributed to the fact that films thinner than 400 nm are under strain which decreases as the film thickness increases.

Keywords: CBD, thin films, optical properties, structural properties

1. INTRODUCTION

Cadmium selenide thin films are considered as a promising semiconductor material for the development of many interesting applications such as nanosensors, biomedical imaging device, lasers, photo electrode, nanotransistor, charge coupling device, light amplifiers, gas sensor, electro photography, photo detector photo conductor and gamma ray detector [1-13].

A variety methods have been used to prepare CdSe thin films, including, thermal evaporation, successive ionic layer adsorption and reaction (SILAR), physical vapour deposition, sputtering electrodeposition, chemical bath deposition and thermal evaporation [14-21]. The aim of the present work is to prepare CdSe thin film by Chemical bath deposition technique and to study their structural and optical properties

2. EXPERIMENTAL DETAILS

Cd_{0.4}Se_{0.6} were prepared by chemical bath deposition. For the deposition of CdSe thin film cadmium chloride CdCl₂ as a Cd²⁺ and sodium selenosulphate Na₂SeSO₃ as Se²⁻ (this solution is unstable and therefore it must be prepared prior to thin film deposition process). While the malonic acid is used as a complexing agent to give cadmium malonate. Which used to slow and uniform the deposition of CdSe thin films. It's worthy to note that the PH value plays an important role in the chemical deposition of CdSe thin films. The final PH was around 7.5.

CdSe was deposited on a glass substrate. Prior to deposition The substrates were boiled in chromic acid for

one hour, washed with soap, rinsed in acetone, and cleaned with ultrasonic bath containing re-distilled water.

The substrate was vertically immersed in the reaction bath and kept for 24 h at room temperature. The substrate was then removed, washed with distilled water for several times, dried naturally and kept in glass desiccator over anhydrous CaCl₂. The resultant film was found to be homogeneous.

The thickness of the film was estimated by gravimetric method. Crystallographic study was carried out using X-ray diffractometer (Shimadzu- XRD600) with CuK_α radiation in the range 20-60°. The surface images were taken by atomic force microscopy (Angstrom AA 3000 scanning probe microscope).

Transmittance measurements have been carried out with a (Shimadzu UV- probe) spectrophotometer in the wavelength range (350-700) nm.

3. RESULTS AND DISCUSSION

Fig. 1 (a) and (b) illustrates the XRD patterns of CdSe thin films with 300 nm and 450 nm respectively. The films exhibited the preferred 100 orientations due to the minimal surface energy in the CdSe hexagonal polycrystalline structure [22]. Two peaks were observed in Fig. 1 (a), (100) and (002) while three peaks noticed from Fig. 1 (b), (100) (002) and (110).

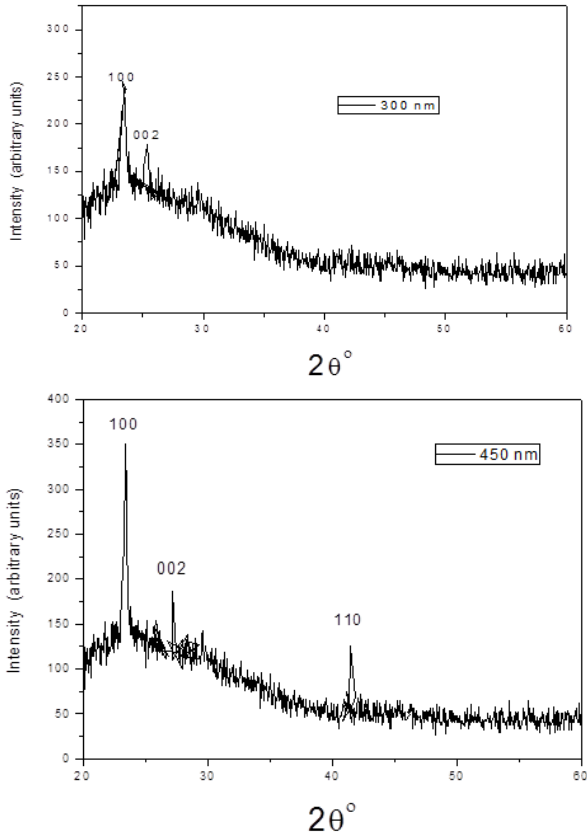


Fig. 1 XRD spectra for the as deposited thin films.

From Fig. 1 (a) and (b) it can be clearly observed that the intensity of the film increases with thickness and, the full width at half maximum FWHM was decreased from 0.5° to 0.3° .

the crystallite size of the thin films was calculated by XRD pattern using Debye Scherer's equation [23]:

$$D = \frac{0.9 \lambda}{\beta \cos \theta} \quad (1)$$

Where D is the crystallite size, (λ) is the X-ray wavelength used, (β) is the full width at half maximum intensity in radians, and (θ) is Bragg's angle.

The grain size values were found to be 17 nm and 23 nm for 300 nm and 400 nm thickness respectively.

The dislocation density (δ) was also calculated in the present work in order to have more information on the amount of defect by using the following formula [24]:

$$\delta = \frac{1}{D^2} \quad (2)$$

The values of dislocation density were found to be 0.00346 and 0.00189 for 300 nm and 450 nm thickness respectively.

Large D , small (β) and (δ) refer to better crystallization, which indicate that 450 film thickness have a better order of crystallinity than 300 nm film thickness.

The surface morphology of the deposited CdSe thin films on glass substrates were studied using atomic force microscope (AFM) shown in Fig. 2 (a) and (b), which shows the dependence of surface roughness on the thickness. The surface roughness for 300 nm thickness was found to be 2.7 nm while for 450 nm, the surface roughness increase to 3.98 nm. The increase of roughness with film thickness is due to the increase in grain size as it has noticed from XRD measurements.

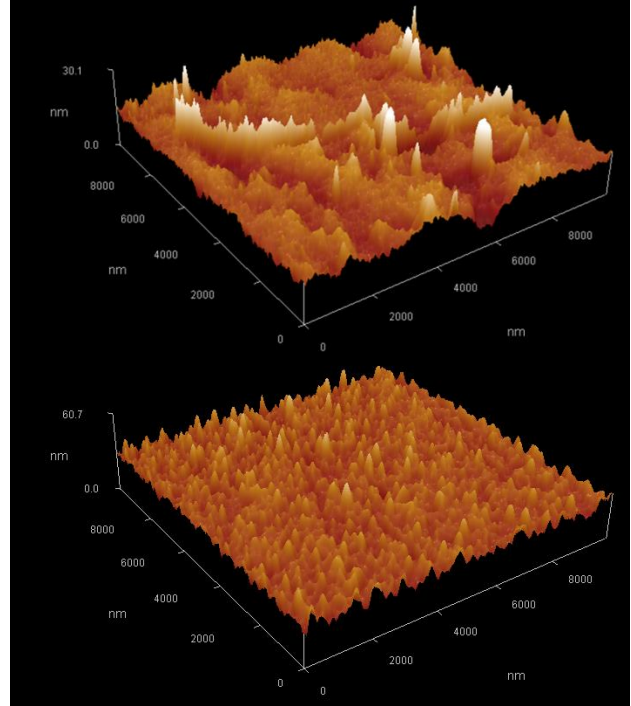


Fig. (2) The AFM micrographs for the as deposited thin films. The room temperature transmittance of CdSe thin films deposited for different thickness is shown in Fig (3). It can be noticed that the threshold of optical absorption is shifted toward long wavelength as the thickness increase (red shift).

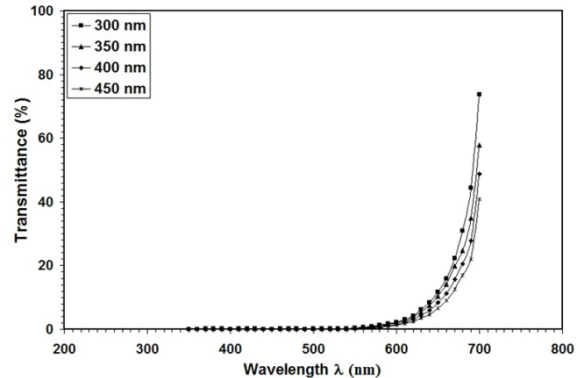


Fig. (3) Transmittance for the as deposited thin films. The absorption coefficient (α) of the film is related to their optical energy gap E_g by the relation [25]:

$$(\alpha h\nu)^2 = A (h\nu - E_g) \quad (3)$$

Where A is a constant and ($h\nu$) is the incident photon energy.

The values of the direct optical band gap were determined by extrapolation the linear regions of the plots to zero absorption ($\alpha h\nu$)² = 0.

The obtained band gap of the deposited CdSe thin films can be estimated from Fig (4) (a), (b), (c) and (d) for different thicknesses.

The E_g value was found to decrease with the increasing of thickness. This result is in good agreement with the results obtained by XRD which shows that the average crystallite size is increased by thickness increasing which confirms the nano nature of the as grown thin film because in nanostructure there is an inverse relation between grain size with the value of the optical energy gap.

The decreased band gap of the films with thickness is due to improve in the crystalline nature of the film [26].

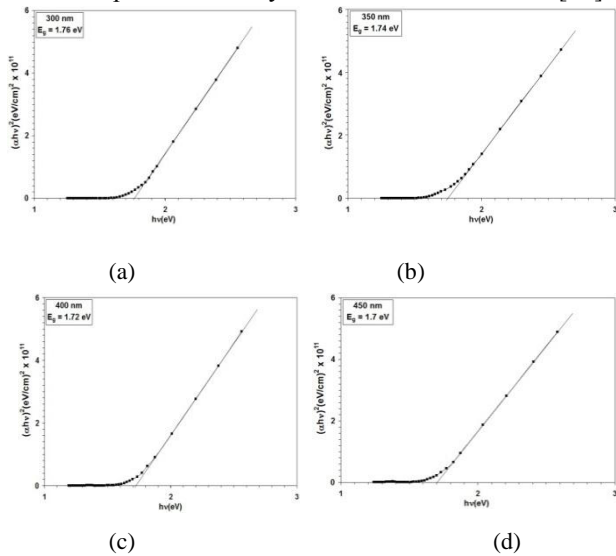


Fig. (4) The ($\alpha h\nu$)² for the as deposited thin films.

Optical response is most conveniently studied in terms of optical conductivity. The absorption coefficient α can be used to calculate the optical conductivity (σ) by using the relation [27]:

$$\sigma = \frac{\alpha n c}{4\pi} \quad (4)$$

Where (n) is the refractive index and (c) is the velocity of light. Fig (5) shows the variation of σ as a function of

photon energy for all the deposited films indicate that σ decrease as thickness increase.

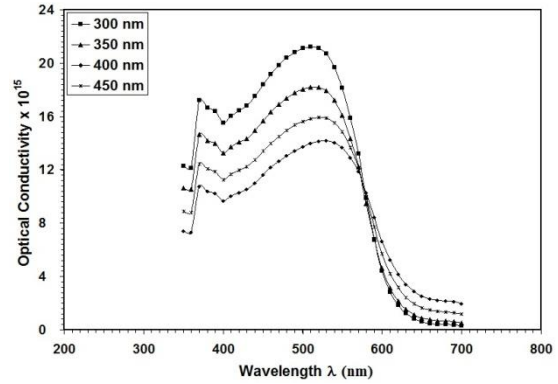


Fig. (5) Optical conductivity of the as deposited thin films. The classical skin depth can be defined as the distance at which the field amplitude drops of 1/e [28], and can be calculated by the following relation [29]:

$$\chi = \frac{\lambda}{2\pi k} \quad (5)$$

Where (λ) is the wavelength of the incident photon and k is the extinction coefficient.

Fig. (6) shows the variation of skin depth as a function of wavelength for CdSe thin film with different thicknesses, we can see from the Fig, at wavelengths greater than $\lambda_{cut-off}$, the absorption effect vanishes and the reduction in amplitude occurs after passing a large distance, in this case the skin depth will increase indicating that the skin depth is transmittance related.

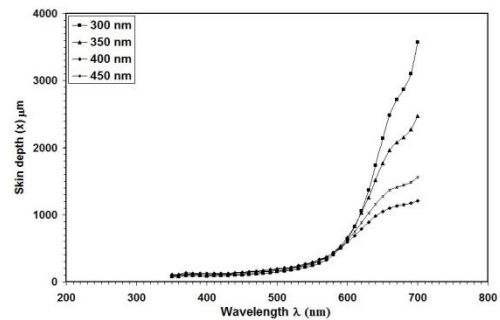


Fig. (6) Skin depth for the as deposited thin films.

4. CONCLUSIONS

Thin films of Cd_{0.4}Se_{0.6} have been prepared successfully by chemical bath deposition. The AFM image revealed that there was a gradual transition from vertical growth to lateral growth mode, which might be due to decrease in strain within film layers as the thin film thickness was increased. From XRD and AFM data one could conclude that these films have a nano structure, which was assured

by observed an inverse relation between the grain size and the optical energy gap.

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