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SINGLE CRYSTAL CADMIUM SULFIDE THIN FILMS PREPARED BY THERMAL EVAPORATION TECHNIQUE

M. M. KAREEM[a*], S. J. MEZHER[b], A. A. BEDDAI[b]
[a]*College of Education, University of Garmian, Kalar, Iraqi Kurdistan*
[b]*Materials Techniques Engineering Department, Middle Technical University*

In this work, highly crystalline CdS thin films are deposited on glass substrates by thermal evaporation technique (TET). XRD analysis revealed single crystalline structure with a significant peak along 002 orientation against $2\theta=26.62^{o}$ and average grain size 64 nm. Optical properties analysis showed that CdS thin films prepared by TET have direct band gap with energy gap (E_g=2.35 eV). Field emission scanning electron microscope (FESEM) image depicted grains with Gaussian distribution and grain size compatible with that calculated from XRD analysis. Atomic force microscopy showed that CdS thin films prepared by TET have smooth surface with surface roughness Sq=0.322 nm. These properties have important applications in optoelectronic devices.

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1. Introduction

In the last two decades there has been a remarkable interest in semiconducting thin films because of their important applications in optoelectronic devices. In that respect, CdS thin films has been the subject of intensive research because of its intermediate bandgap, high absorption coefficient, reasonable conversion efficiency, stability and low cost [1-3]. Many techniques [4-8] have been used to deposit CdS thin films into various substrates with preferred optical properties. Among these TET, spray pyrolysis, chemical bath deposition, and sputtering. Single crystal structure of CdS is known to be more suitable for optoelectronic devices because that structure in particular has sharp absorption edge and well-defined band gap [9]. However, it is not easy to obtain single crystal thin films from. In this work, we report the ability of thermal evaporation to yield single crystal cadmium sulfide.

2. Experimental details

In this research work, CdS thin films were deposited by TET from a resistivity-heated tungsten-boat containing high-purity CdS powder. The vacuum system (Edwards Co.) having a diffusion pump sustaining low pressure about 10^{-6} Torr. The substrates which used in the experiments were carefully cleaned microscope slides. The slides were already cut to smaller pieces of area 2x2 cm^2. Then they were immersed in Acetone (propane) and exposed to ultrasonic bath for 10 min. The glass slides were also rinsed ultrasonically in distilled water for 10 min. and in ethanol alcohol for another 10 min. The glass substrates were ultrasonically rinsed again in distilled water and finally have been dried using pure nitrogen gas. The glass slides were put in a bell jar to be used as substrates for CdS films.

* Corresponding author: mahmood.mohammed@garmian.edu.krd

3. Result and discussion

The X-ray diffraction pattern of CdS thin film is shown in Fig. 1. The spectrum was found by scanning 2θ in the range 10– 80°.

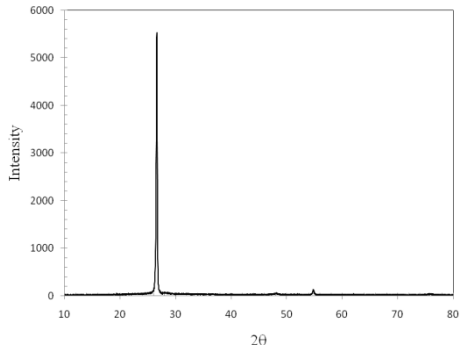

Fig. 1. XRD for CdS thin film prepared by thermal evaporation technique.

We can see from the diffraction patterns that the peak intensity increases abruptly at 2θ=26.62 and the peak sharpness indicates the structure is single crystal. The intense peak corresponds to the CdS hexagonal plane (002) with only one phase. Table 1 below abbreviates the results of XRD analysis.

(hkl)	2θ(deg)	FWHM(deg)	Grain size D(nm)	Micro-strain ($x10^{-4}$)	Dislocation $(\mu m)^{-2}$
(002)	26.62	0.2096	40.66	39	605

The particle size could be obtained using Scherer formula [10]:

$$D = \frac{K\lambda}{\beta_{2\theta}\cos\theta} \tag{1}$$

where K is a constant often approximated to 0.94, ($\lambda = 1.54$ Å) is the X-ray wavelength, 2θ the Bragg angle and $\beta_{2\theta}$ is the FWHM of the diffraction peak. A grain size value of 38 nm crystallite size has been estimated from (002) diffraction peak for CdS films deposited by TET. The dislocation density $\delta = 1/D^2$ and microstrain $\varepsilon = \beta_{2\theta}\cos\theta/4\sin\theta$ were calculated in Table (1) following reference [15]. These results give lattice constant a=4.16 Å and c= 6.689 Å. The table also indicates that the CdS films deposited by TET are under tensile strain of about $6.89x10^{-4}$ along the (002). As a comparison, the lattice constants (a and c) for strain-free CdS powders are respectively 4.16 and 6.756 Å [11].

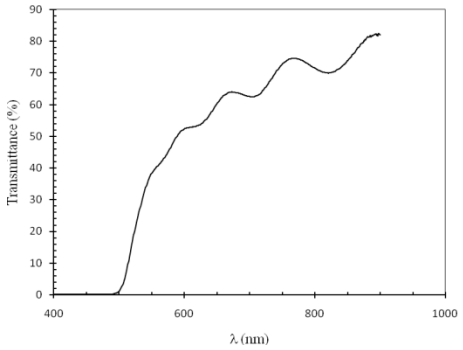

Fig. 2. The transmittance for CdS films prepared by TET.

Fig. 2 shows transmittance spectrum of CdS obtained in the wavelength range (400−900) nm. The spectrum reveals high optical transmission values above 600 nm. The dents in the transmission curve are due to interference fringes [12, 13]. Fig. 2 shows the $(\alpha h\nu)^2 - h\nu$ plot for CdS films, where α is the absorption coefficient, h is Plank's constant and ν is the frequency of the incident light. The band gap E_g of CdS has been obtained by extension of the linear part of $(\alpha h\nu)^2$ to intercept with $h\nu$ -axis. The optical band gaps of the films is calculated using the well-known relation for direct transition

$$\alpha h\nu = A(h\nu - E_g)^{1/2} \tag{1}$$

where A is a constant, $h\nu$ is the photon energy. The E_g value calculated from the extrapolation method is 2.36 eV. This illustrates that band gap of CdS is direct. The energy gap of the films is slightly larger than its bulk counterpart of 2.46 eV [14].

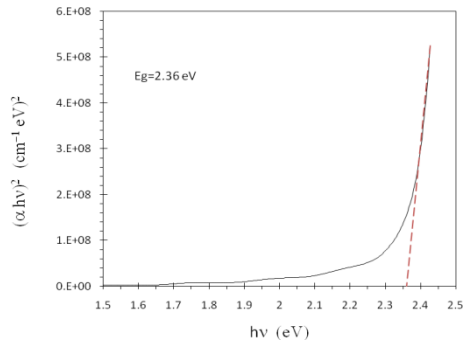

Fig. 3. The plot of $(\alpha h\nu)^2$ *against* $h\nu$ *for CdS films prepared by TET.*

This discrepancy can be attributed to quantum size effects [16]. The cut-off wavelength can be calculated by using Plank's law: $\lambda(nm) = 1240 / E_g(eV)$ which give cut-off wavelength 525 nm.

The surface morphology of CdS thin films imaged by AFM technique and shown in Fig. 4. The Sa and Sq roughness were respectively 0.279 and 0.322 nm. The surface morphology tends to be smooth with low roughness.

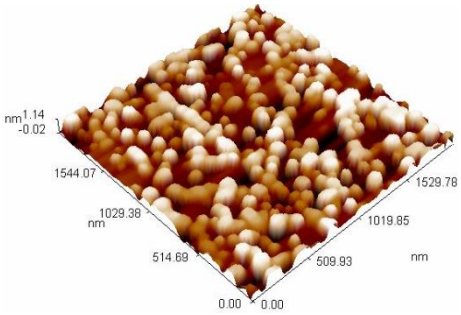

Fig. 4. AFM image for CdS thin film prepared by thermal evaporation technique.

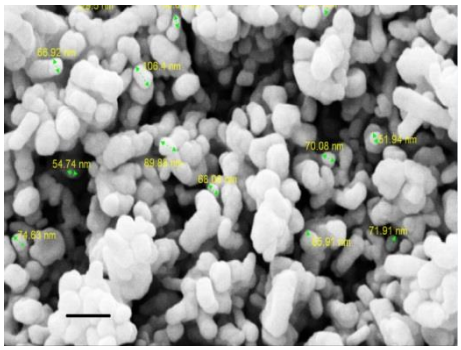

Fig. 5. FE-SEM image for CdS thin film prepared by thermal evaporation technique.

The obtained FE-SEM images show that all the CdS thin films prepared by TET consist of grains with average grain size in the nano-size order. This is compatible with AFM analyses in Fig. (4). FE-SEM images for CdS thin films fig(5) shows average nanoparticle size of 74.05 nm. The length of black bar is 200 nm. The shapes of CdS nano-grains are similar to that obtained by [17].

4. Conclusions

In this study, we report the formation of single crystal cadmium sulfide using thermal evaporation technique. X-ray diffraction pattern showed a single peak which is corresponding to hexagonal closed packed structure. The AFM and FE-SEM confirmed the formation of CdS nano-grains which is compatible with that estimated by Scherer equation. CdS thin film showed direct energy gape of 2.36 eV.

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