Effect of Substrate Temperature on the Structural Surface Morphological and Optical Properties Of nanostractured CdS Thin Films

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Abstract :

In this study, the effect of substrate temperature on structural, morphological and optical properties of CdS thin films deposited by spray pyrolysis is investigated. XRD analysis revealed that the deposited CdS films are polcrystalline in nature with perferential orientation of (100)(002)(101)(220) (311) plane. The grain size increases as deposition temperature increases. Atomic Force Microscopy(AFM) investigation showed that the deposited film contains columnar growth and the average grain size were (125.75nm, 104.45nm) and the root mean square of roughness were (7.01 nm, 8.35 nm) at Ts=300°C and 400°C respectively. The optical properties of nanostructure CdS films are strong depedence on substrate temperature. The band gap(Eg) of the CdS films deposited at T_s=300,350 and 400°C was found to be (2.38 ,2.44 ,2.41 eV) respectively.

1. Introduction

The use of thin film polycrystalline semiconductors have attracted much interest in an expanding variety of applications in various electronic and optoelectronic devices The technological interest in polycrystalline based devices are mainly caused by their low production cost [1] . Cadmium Sulfide films are compound semiconductors with a wide range of potential applications. This material have exist in cubic or hexagonal forms and are wide- direct-band gap semiconductors [2]. Among the II-VI semiconductors , CdS polycrystalline thin films is a representative material with many applications such as large area electronic devices and solar cells, it has a wide direct band gap (2.42 eV) so has been used as a window material together with several semiconductors such as CdTe ,Cu2S and CuInSe2. Also the interest in CdS thin films stems from its piezoelectric properties and potential laser applications.[3,4,5] Many techniques have been reported in deposition of CdS thin films. These include evaporation, sputtering, spray pyrolysis, molecular beam epitaxy (MBE) technique, photochemical deposition, successive ionic layer adsorption and reaction (SILAR) method [6,7]. In all of these deposition methods there are some problems in each of them, for example , it is difficult to obtain a stiochiometric CdS thin films by evaporation technique and a high substrate temperature is required in spray deposition [8]. Thin films of CdS had been extensively It is found that,the physical properties depend on the preparation technique [9,10]. In this work the morphologyical ,structure and optical properties of polycrystalline nanostructured CdS films were investigated as a function of substrate temperature.

2. Experimental

The chemical spray pyrolysis technique is a simple technology in which an ionic solution containing the constituent elements of a compound in the form of soluble salts is sprayed onto heated substrates using a stream of clean, and dry air [11]. The apparatus we used for our sprayed process is diagrammed in figure 1. The CdS thin films were prepared by spraying of an aqueous solution of cadmium chloride ($CdCl_2$) and thiourea [$(NH_2)_2CS$] on glass substrate kept at temperature of 300, 350 and 400 °C. The spray rate was optimized to 3 ml/min through the nozzle to ensures a uniform film thickness. Glass substrates of 2.5 cm x 2.5 cm, are placed in a fitted socket at the surface of a substrate heater when sprayed.The heater used was a hot plate with controller. The substrate temperature was varied, while other spraying parameters were kept constant.

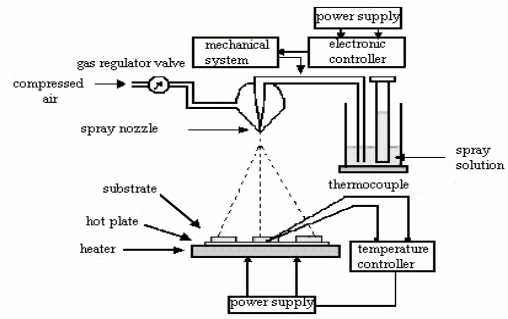

Figure 1. Schematic diagram of the chemical spray pyrolysis system.

The X-ray diffraction (XRD) analysis of the films were recorded with a SHIMADZU 6000X-ray diffractometer operating at λ=1.541874 A° using Cu k_α source radiation at 40 kV and 30 mA with angle range 10-80. Atomic Force Microscopy AFM (AA 3000 SPM User"s Manual) was used to study the surface morphology of the film.The force applied by the tip was carefully adjusted to avoid any noticeable tip induced damage during scanning. The AFM topography data were used to calculate the average roughness and grain size.Transmission spectra T and Optical energy gap Eg of the deposited films were measured by normal incidence of light, using a double beam UV-VIS spectrophotometer model Cintra-5-GBC, in the wavelength range 300- 1000 nm, using a blank substrate as a reference.

3. Results and Discussion

3.1 Film structure

XRD were used to characterize the structural properties of CdS thin films. Diffractograms of CdS films prepared at different substrate temperatures

(300 and 400°C) are shown in Figure 2. The X-ray diffraction patterns of the CdS thin films reveald the films are mited of polycrystalline hexagonal (wurtzite) and cubic (zincblende) structure. The diffraction peak existed at 2θ =22.9°, 24.6°, 26.3°, 41.7°, 49.8° and the corresponds planes are crystallines (100) (002) hexagonal and the (220) (311) cubic planes [13,14].The degree of preferred orientation increased with the substrate temperature. It was observed that the increase of the substrate temperature increase the diffraction peak intensity of (002) plane which resulted in increase in grain size and good crystallinity of the films. The effect of substrate temperature on the grain size (GS) of the obtained phase was also investigated . If the broadening is due only to the effect of crystallite size, grain size can be simply determined from the (002) diffraction line using the Debye-Scherrer formula [15,16]:

$$Gs = \frac{K\lambda \text{ EMBED Equation. 3 }}{\beta \cos\theta} \quad (1)$$

where β is the full width at half maximum (FWHM) of the peak corrected for instrumental broadening: λ is the wavelength of the X-rays, and K is the Scherrer constant, which generally depends on the crystallite shape. Considering that the Scherrer constant K is equal to unity according to the widespread practice, and that the effect of residual macrostrain is negligible. the variation of grain size with substrate temperature is shown in figure.2. It shows, that as the substrate temperature changes from 300°C to 400°C, the grain size changes from 13.06nm to 29.75nm at constant growth rate.

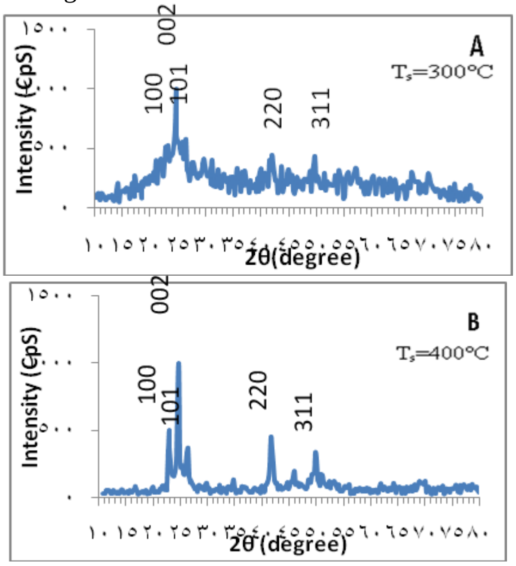

Figure 2. X-ray diffractograms of sprayed CdS films with different substrate temperatures , A-T_s=300°C, B-T_s=400°C.

The lattice constant (a) was calculated by using the relation[17]:

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

Table (1-1) The x-ray diffraction peak intensity of (002)(220) plane lattice constant of CdS films.

Thin Films	Lattice Parameter (nm)		Lattice Parameter (nm) (ASTM)
	T_s=300°C	T_s=400°C	
CdS(Hexagonal)	0.7236	0.72366	0.672
CdS(Cubic)	0.8624	0.86552	0.824

We can notice from Table(1-1) that the lattice constant of CdS films has been found to variation with increasing the substrate temperature.

3.2 Surface morphology

In order to investigate the morphology of CdS thin films deposited on glass, atomic force micrographs were recorded for 2 x 2 μm^2 regions. The average size and rms surface roughness measured for the CdS thin films, indicate that surfaces and cross-section of CdS layers, deposited at various substrate temperatures are given in figure 3. All the films show that the particles are closely bonded and no voids are observed.

Fig. 3a & 3b show cluster of particles with highly dense structure. The CdS thin films layer has the advanced surface and typical columnar structure with highly dense grains . Fig. 3a shows typical 2µm×2µm AFM images 2-D,3-D of CdS film deposited on glass at a substrate temperature of 300°C. It shows a homogeneous formation of film and with no voids observed in the structure. This means that the film is very dense structure with high packing density. The average grain size diameter of the CdS film was 125.75nm with an average roughness of 5.53nm and a root mean square roughness of 7.01nm.

Fig. 3b shows a typical 2µm×2µm AFM images 2-D,3-D of CdS film deposited on glass at a substrate temperature of 400°C. The average grain size diameter of the CdS film was 104.45nm with an average roughness of 8.35nm and a root mean square roughness of 10.7nm. Observed in Fig. 3a & 3b The increase of substrate temperature further from 300°C to 400°C gives the crystalline increment of the surface relief of CdS layer. In the increase of columnar structures grain size with decrease The average diameter . AFM images also revealed that CdS films become more uniform and dense with the increase of substrate temperature.The average grain size of the film, observed by AFM is larger than that calculated from XRD pattern. This may well be due to defects such as twins, and dislocations, etc., induced into the crystallites during the growth [18].

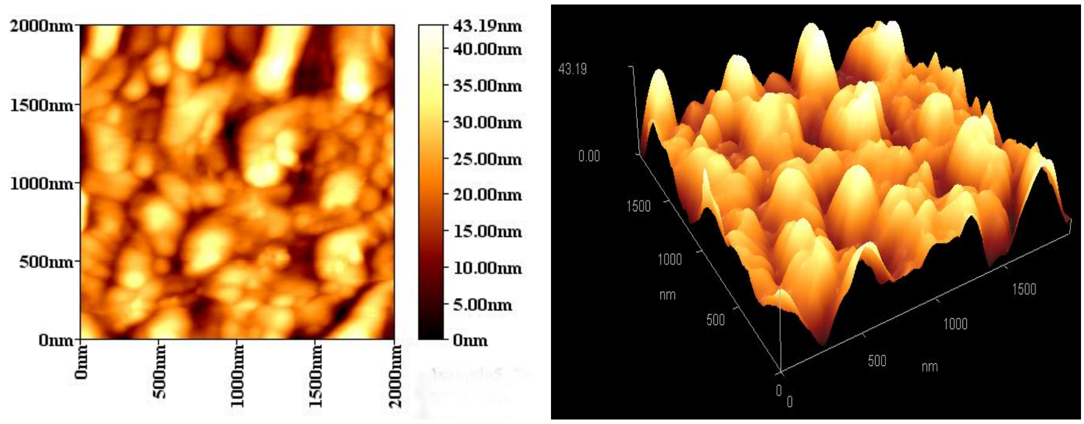

Figure 3a. AFM images morphology of CdS film at substrate temperature 300°C.

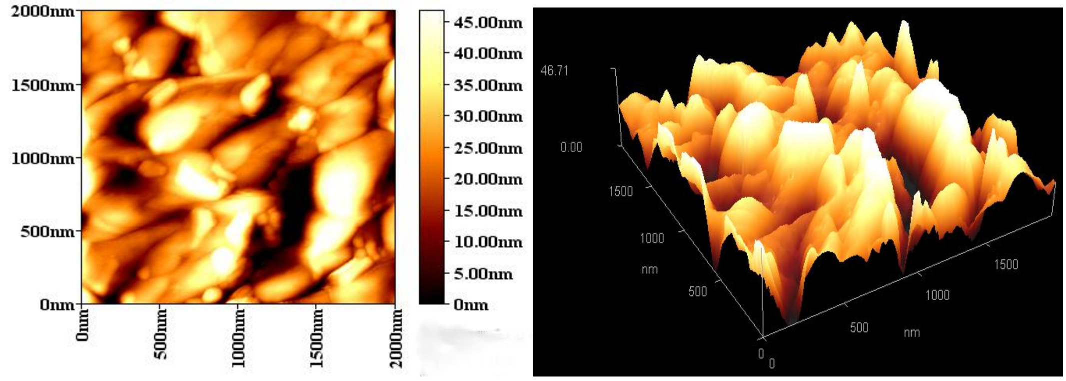

Figure 3b. AFM images morphology of CdS film at substrate temperature 400°C.

3.3 Optical properties

The optical properties of nanostructure CdS films are similar to those produced by other methods. Figure 4, shows the variation of optical transmission as a function of wavelength for the films prepared at different substrate temperatures with constant growth rate. The films fabricated at 300°C have a low optical transmission, and those prepared at higher temperatures have a higher transmission. This improvement can be attributed to either the decrease in thickness or the improvement in perfection and stoichiometry of the films [19]. This is easily interpreted as follows: the increase in substrate temperatures causes a decrease in the thickness of the films, so the transmittance increases according to Lambert's law[20]:

$$T = (1-R)\, e^{-\alpha t} \quad .. (3)$$

WhereT: transmittance , R: reflectance

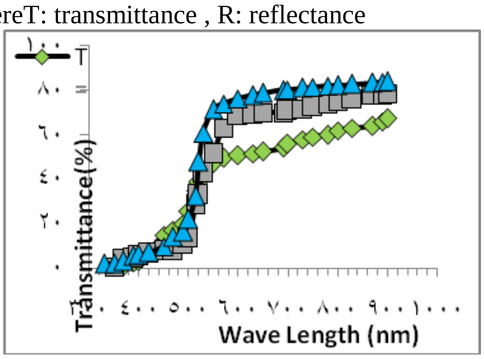

Figure 4. Transmittance vs. wavelength for CdS films sprayed at various substrate temperatures(Ts=300,350,400 °C) with the growth rate constant.

The band gap *Eg* of CdS film was determined by analysing the optical data with the expression for the optical absorbance α and the photon energy hυ [19] using the relation ship[21]:

$$\alpha\, h\upsilon = k\, (h\upsilon_{1/2}\text{-}Eg)^{n} \quad \ldots(4)$$

where *k* is a constant, and *n* is also constant equal to one for a direct-gap material. As shown in Figure 5, the plot of $(\alpha h\upsilon)^2$ versus hυ was analysed using the above equation. Extrapolation of the linear portion of the plot to the energy axis yielded the values of band gap. It is noticed from figure.5 that increasing the depostion temperature resulted in an increase in the film band gap.

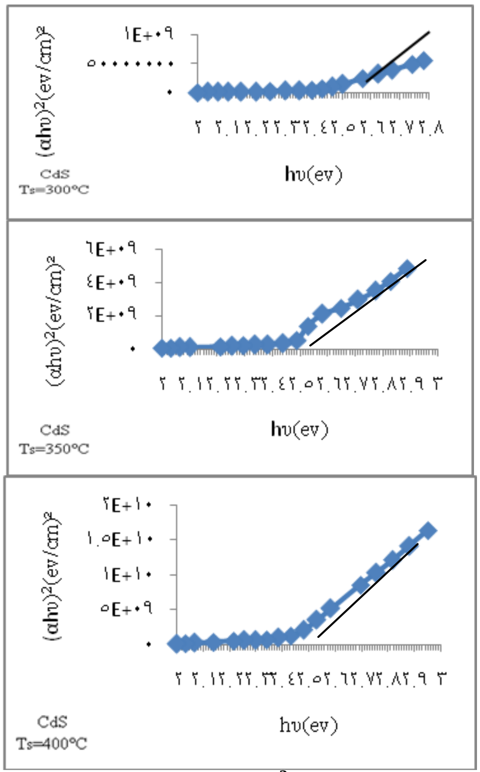

Figure 5. Variation of $(\alpha h\upsilon)^2$ with photon energy for films sprayed at various substrate temperatures.

4. Conclusion

In conclusion, we have investigated the effect of substrate temperature on the structural, surface morphology and optical properties of nanostructured CdS films deposited by spray pyrolysis technique. The films were deposited onto glass substrates at temperatures 300, 350 and 400 °C. It was found that the structural and optical properties of CdS films were sensitive to the substrate temperature. The crystallinity of films increased with the increase of substrate temperature, where the grain size becomes larger and it denser. The films became more uniform and dense with the increase of substrate temperature. Optical measurements, showed an increasing optical transmission with increasing substrate temperature as films thickness decreased with increased substrate temperature . The optical energy bandgap was sensitive to the variation of the substrate temperature Ts. The films exhibited a direct transition in the range 2.38 - 2.44 eV dependening on the substrate temperature. These results suggest that the method of spray pyrolysis for the deposition of CdS thin films should be further investigated for application towards the fabrication of heterojunctions photodetectors and solar cells.

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تأثير درجة حرارة القاعدة على الخصائص التركيبية والطبوغرافية السطحية والخواص البصرية لأغشية كبريتيد الكادميوم ذو تركيب نانو

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الملخص

تم دراسة تأثير درجة حرارة القاعدة على الخصائص التركيبية والطبوغرافيه السطحية والخواص البصرية لأغشية كبريتيد الكادميوم CdS المرسبة بتقنية الرش الكيميائي الحراري. ان تحليل XRD أوضح بأن أغشية CdS المرسبة ذات طبيعة متعددة البلورات وأتجاة مستوى بلوري (311) (220)(101)(002)(100) وان الحجم الحبيبي ازداد عند زيادة درجة حرارة الرش. وأوضحت نتائج مجهر القوه الذرية AFM تغير النماء البلوري للغشاء المرسب إذ وجد إن معدل الحجم الحبيبي (125.75nm, 104.45nm) وقيمة متوسط الجذر ألتربيعي للخشونة السطحية (7.01 nm, 8.35 nm) عند Ts=300°C,400°C على التوالي. أما الخواص البصرية لأغشية CdS ذات التركيب النانوي تعتمد بشكل كبير على درجة حرارة القاعدة. وجد فجوة الطاقة (Eg) لأغشية CdS المرسبة عند T_s=300,350,400°C تساوي (2.41 eV, 2.44, 2.38) على التوالي.