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The Effect of Cadmium Concentration (x) Variation on the Structural Properties of $Zn_{1-x}Cd_xS$ Thin Films

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Abstract

The $Zn_{1-x}Cd_xS$ alloys was prepared in evacuated quarts tubes by the method of melt quenching from element, the $Zn_{1-x}Cd_xS$ thin films prepared by thermal evaporation method and at different value of x, (x = 0.1, 0.2, 0.3, 0.4 and 0.5).

X-Ray diffraction technique was used to study the structure of this films and the effect of x value on it. X-ray diffraction analysis confirmed that these films are crystalline structure nature having faced centered cubic (f.c.c.), and lattice parameters are reported.

The preferential orientation is along [111] direction for all deposited films together. The lattice parameter, grain size, microstrain, dislocation density in the film are calculated and correlated with x.

Keywords: Structure Properties, Thin Films, $Zn_{1-x}Cd_xS$.

الخلاصة

تم تحضير سبائك $Zn_{1-x}Cd_xS$ بطريقة التبريد المفاجئة. ثم حضرت أغشية $Zn_{1-x}Cd_xS$ الرقيقة بطريقة التبخير الحراري لقيم مختلفة لـ (x = 0.1, 0.2, 0.3, 0.4 and 0.5).

أستخدمت تقنية حيود الأشعة السينية لدراسة تركيب تلك الأغشية وتأثير تغير قيمة (x) عليها. حيث أظهرت فحوصات الأشعة السينية أن جميع الأغشية المحضرة تمتلك تركيب بلوري مكعبي نوع متمركز الأوجه (f.c.c.) ، بالأضافة الى معرفة قيمة ثابت الشبيكة. تمتلك الأغشية المحضرة توجه تفضيلي بأتجاه [111].

تم حساب الثوابت التركيبية مثل(ثابت الشبيكة، حجم البلورة، المطاوعة المايكروية، كثافة الأنخلاعات) للأغشية المحضرة وحساب تاثير (x) عليها.

1- Introduction

There has been increasing interest in the electronic and optical properties of $Zn_{1-x}Cd_xS$ thin films. The reason being that the thin films of $Zn_{1-x}Cd_xS$ has properties in between those of CdS and ZnS [Reddy *et al.*, 1992 and Okoli *et al.*, 2006]. The $Zn_{1-x}Cd_xS$ thin film band structure has a larger energy gap than CdS. This makes the material much more attractive for the fabrication of solar cells. It has been widely used as a wide band gap window material in heterojunction photovoltaic solar cells [Basol 1984, and Reddy *et al.*, 1992] and in photoconductive devices [Torres and Gordillo, 1992]. $Zn_{1-x}Cd_xS$ thin films have been prepared by a variety of techniques, including spray pyrolysis [Chynoweth and Bube, 1980 and Mustafa and Yazici, 2004], ion beam deposition [Kuroyanagi, 1994], molecular beam epitaxial growth [Karasawa *et al*., 1991], and screen printing method [Kumar *et al*., 1998].

The structure parameters via the crystalline, crystal phase, lattice constant, and strain grain size, orientation etc. are strongly dependent on deposition parameters.

As in other large band gap semiconductor systems various methods have been used for the growth at $Zn_{1-x}Cd_xS$ thin film.

2- Experimental

$Zn_{1-x}Cd_xS$ thin films were deposited on highly clean glass substrates in a vacuum better than (10^{-5} torr) by using thermal evaporation method. Pure Zn, Cd, Se powder (99.99%) was used for deposition. The rate of deposition was (5 Å/sec) and the source to substrate distance was kept at (12 cm). The X-ray diffraction (XRD) patterns of the deposited films were recorded with the help x-ray diffractometer. Using CuKα radiation, the XRD patterns of all films were taken from (20^o to 60^o). In this paper, deposition of $Zn_{1-x}Cd_xS$ thin films at room temperature on glass substrates with different value for x.

3- Results and Discussion

It is observed that all $Zn_{1-x}Cd_xS$ thin films are polycrystalline having f.c.c. zincblende structure irrespective films. Fig.(1) represents the XRD patterns of six representative $Zn_{1-x}Cd_xS$ thin films having thickness 2500Å deposited at R.T. with different value for x.

All films show that the most preferred plane is [111], these are observed which establishes the single phase cubic structure of the films [Bedir *et al.*, 2005].

From Fig.(1) the diffraction pattern exhibits the heights of peaks are increased with the increase of the concentration of Cd in the films. This means that the crystallinlty of the films increased when the concentration of Cd increased.

The vacuum evaporated $Zn_{1-x}Cd_xS$ thin films cubic zincblende structure. It is confirmed by comparing the peak positions (2θ) of the XRD patterns of the films within standard X-ray powder diffraction data file. The lattice constant (a) for the cubic phase structure is determined by the relation [Warren, 1967]

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

While d is determined by the relation (Chopra, 1969 and James and Bailey, 2007):

$$n\lambda = 2d \sin\theta \quad \text{………………………………………............. (2)}$$

The lattice constant (a) then shows increasing tendency with increased the concentration of Cd, Fig.(2.a).

The change in lattice constant for the deposited thin film over the bulk clearly suggests that the film grains are strained and that may be owing to the change of nature and concentration of the native imperfections. The density of film is therefore expected to change in accordance with the change at lattice constant [Bedir *et al.*, 2002].

It is observed that the XRD patterns of all $Zn_{1-x}Cd_xS$ thin films show a preferred orientation along [111] plane. The [111] direction is the close-packing direction of the zincblende structure. The grain size of the deposited films is estimated using Scherer formula [Warren, 1967]:

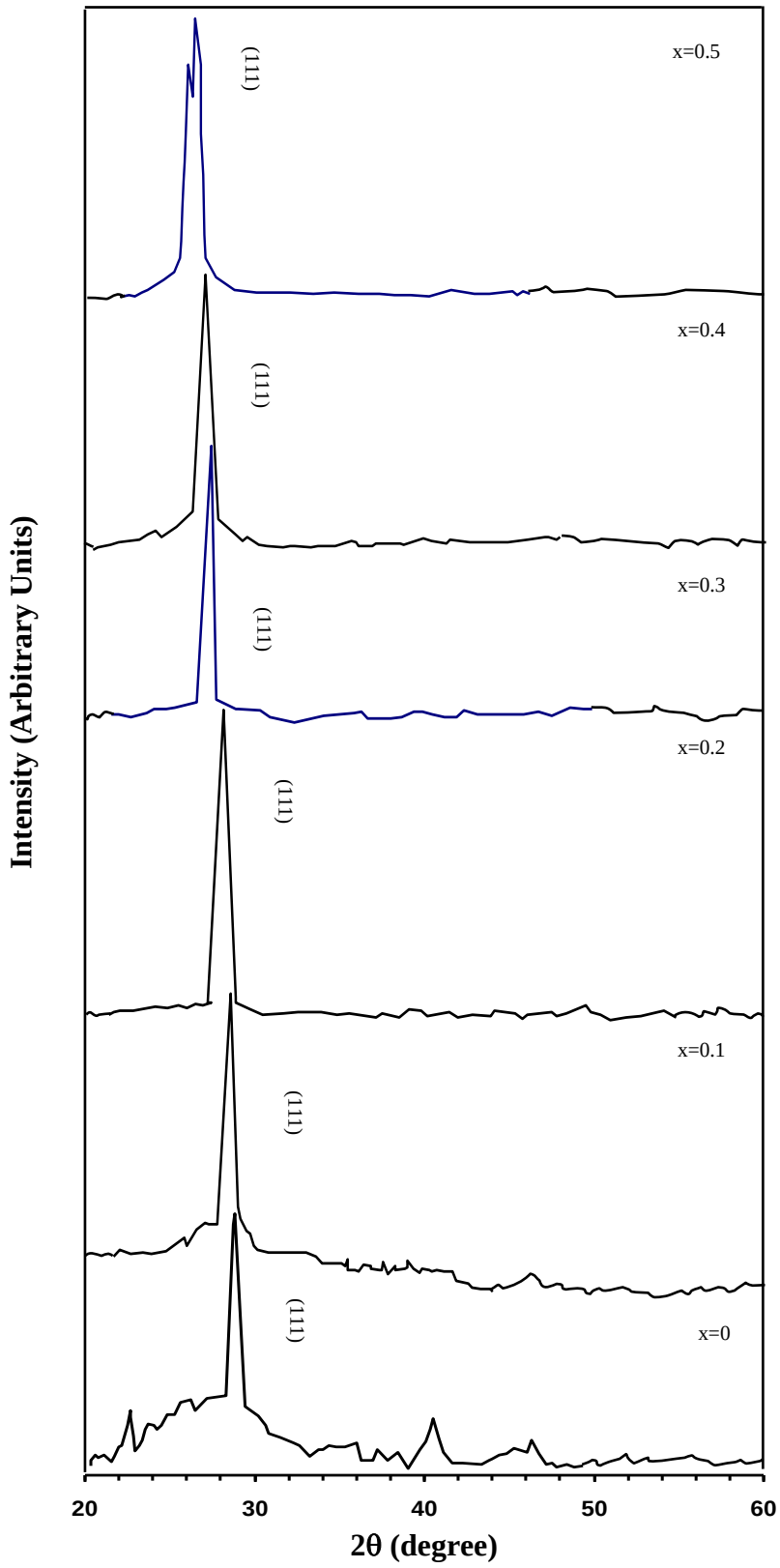

Figure (1): XRD traces for representative $Zn_{1-x}Cd_x S$ films.

$$D = k\lambda / \beta_{2\theta} \cos\theta \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

Where:

k: is taken as 0.94,

λ: the wave length of X-ray used and $\beta_{2\theta}$ the full width at half maximum of [111] peak of XRD pattern.

The grain size of the deposited films is small and decrease with increased concentration of Cd, as shown in Table (1). The change of grain size with the Cd concentration, is very prominent and this result agreement with find in other research [Bedir *et al.*, 2002].

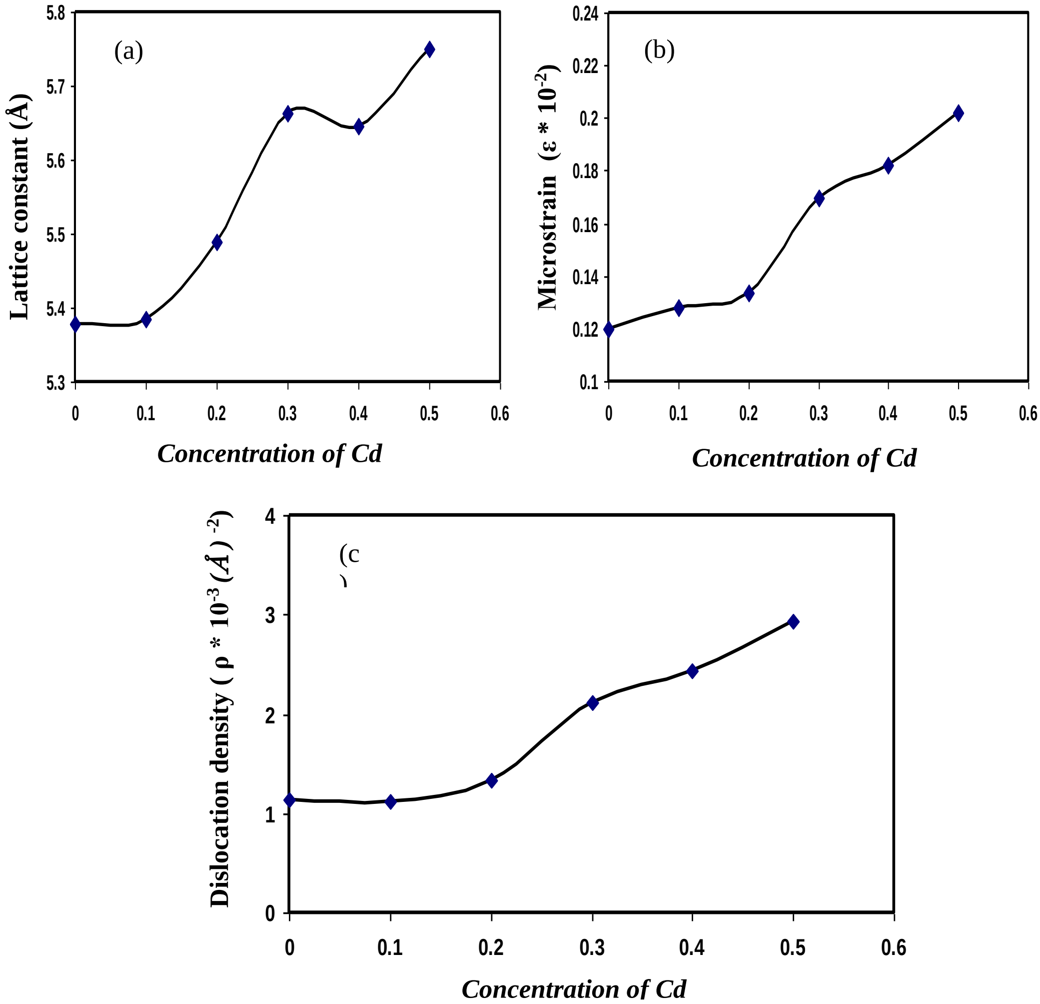

Figure (2): Variation of (a) lattice constant, (b) microstrain ε, (c) Dislocation density ρ with Concentration of Cd, in $Zn_{1-x}Cd_xSe$ films.

The microstrain (ϵ) developed in the $Zn_{1-x}Cd_xS$ thin film is calculated from the relation [Chopra, 1969]

$$\epsilon = (\beta_{2\theta} \cos\theta) / 4 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)$$

A dislocation is an imperfection in a crystal associated with the misregistry of the lattice in one part of the crystal with that in another part. Unlike vacancies and interstitial atoms dislocations are not equilibrium imperfections. i.e. thermodynamic considerations are insufficient to account for their existence in the observed densities.

In fact the growth mechanism involving dislocation is a matter at importance. In the present study, the dislocation density for cubic thin films is estimated from using the relation [Bedir *et al*., 2002]:

$$\rho = 15 \in / aD \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (5)$$

It is observed that microstrain (ε) and dislocation density (ρ) exhibit increasing with x. (fig. 2b and c), the increase of ε and ρ with x due to decrease of grain size.

Table (1): Structural parameters of thermally evaporated $Zn_{1-x}Cd_xS$ thin films.

x	2Θ (degree)	d (Å)	[hkl]	a (Å)	D(Å)	$\varepsilon x10^{-2}$	$\rho x10^{-3}$(Å) $^{-2}$
0	28.73	3.103	111	5.379	298	0.1200	1.129
0.1	28.67	3.103	111	5.384	281	0.1283	1.126
0.2	28.10	3.170	111	5.490	271	0.1333	1.342
0.3	27.50	3.270	111	5.663	212	0.1699	2.113
0.4	27.30	3.260	111	5.646	198	0.1822	2.437
0.5	26.80	3.320	111	5.750	179	0.2018	2.936

4-Conclusions

All thermally evaporated $Zn_{1-x}Cd_xS$ thin films at thickness 2500Å, deposited at R.T. with range of (x=0.1-0.5) are polycrystalline having f.c.c Zincblende type structure. Each films shows a preferred orientation along [111] plane for films.

The grain size of the deposited films has significant dependence on x value. Also all the other parameters that we calculated are change with increasing of the concentration of Cd in the films. We can see from the fig.(2a, b ,c)and Table(1) that the lattice constant , microstrain and dislocation density increase approximately with increasing of concentration of Cd for all ratio.

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