The effect of doping ratio of Cu on the structural properties of CdSe Films

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Abstract

Films of CdSe have been prepared by evaporation technique with thickness 1µm. Doping with Cu was achieved using annealing under argon atmosphere . The Structure properties of these films are investigated by X-ray diffraction analysis. The effect of Cu doping on the orientation , relative intensity, grain size and the lattice constant has been studied. The pure CdSe films have been found consist of amorphous structure with very small peak at (002) plane. The films were polycrystalline for doped CdSe with (1&2wt%) Cu contents and with lattice constant (a=3.741,c=7.096)A°, and it has better crystallinty as the Cu contents increased to (3&5wt%) Cu. The reflections from [(002), (102). (110), (112), and (201)]planes are more prominent referring to hexagonal unit cell. Therefore the crystal structure of CdSe:Cu films are hexagonal at Cu content (pure, 1&2wt%) with a sharpness and also in the hexagonal form at (3&5wt%).The crystalline size were found to depend on concentration of doping materials, and it is varied between (20.3-81.4)nm and increased with Cu content.

1-Introduction

The optical and electrical properties, as well as its good chemical and mechanical stability, recommends cadmium selenide(CdSe) as a semiconductor well studied for optoelectronic applications, such as photo detection or solar energy conversion[1], this procedure provides materials such as a CdTe, CdSe and CdS which are used in solar cells, and the second method is chemically spray[1]. In recent years much attention has been shown in semiconducting II-VI compounds because of their optoelectronic properties and applications. Cadmium selenide is an important number of this group of binary compounds. It has a direct intrinsic band gap of 1.74 eV which make it an interesting material for various applications. This material has grown in bulk single crystalline form and has been used as in efficient photoconductor. CdS and CdSe films which are grown by evaporation technique has been used as gas sensors for detection of oxygen[2]. Al-Ani et ai[3] has studied the structure properties of CdSe with various heating substrate. They found that the grain size was increased as the substrate temperature increased. Also the same authors[4] have prepared CdSe:Cu by vacuum evaporation technique. Mahmoud et al [5] and Narayaandass et al[6] has prepared CdSe film by hot wall deposition technique onto glass substrate, they studied the X-ray diffraction and found that the films exhibit preferential orientation along the (103) plane and changes to the(002) plane as the thickness increased. However, according to our knowledge no detailed studies have been report on the structural parameters such as lattice constant, crystalline size(D) and dislocation density of the film materials. The evaluation of the

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material for application is complete and meaning full only when it is structure and composition are precisely known and related to it is electronic properties. The purpose of this work is to study the structure of the CdSe:Cu films at different content of Cu.

2-Experimental:

Cadmium selenide thin films (CdSe) were prepared by thermal evaporation onto glass substrate of a stoichiometric powder of the compound (chemical purity 99.9999%), in a residual air pressure of 10^{-6}Torr with thickness 1μm from molybdenum boat using BALZERS COATIN UNIT. Doped with copper (1,2,3 &5wt%) by chemical diffusion have been achieved. The electrodes were Aluminum vacuum deposited. The structure of CdSe:Cu films has been examined by X-ray diffraction type Siemens D0500 with CuKα wavelength(λ=1,5405A°). The scanning angle has varied in the range(20°-60°) with speed 2/cm/min. current 20mA and voltage 40kV. Computer programs calculate the lattice constants.

The inter planer distance $d_{(hkl)}$ for different planes was measured by using Braggs law[7,8]:

$$2d \sin\theta = n \lambda \quad \text{-----------------------------} (1)$$

Where n is the reflection order, λ is the x-ray wavelength and θ is the diffraction angle. By comparing these d-values with (ASTM) cards for FCC of CdSe:Cu films. The CdSe:Cu grain size dimension (D) can be evaluated from diffraction line broadening using Scherrer equation[9,10]:

$$D = K \lambda / \beta \cos\theta \quad \text{---------------------------} (2)$$

Where K is the shape factor which takes value about(0.9), β is the line broadening which equal to:

$$\beta = B - b \quad \text{-----------------------------------} (3)$$

where B is the width of the CdSe diffraction line at half maximum intensity and b is the instrument effect estimated from the broadening of the substrate diffraction line and will take zero then the equation (2) becomes:

$$D = 0.9 \lambda / \beta \cos\theta \quad \text{-------------------------} (4)$$

3-Results and Discussion:

Fig.(1) shows the X-ray diffraction for pure CdSe film and doped with different copper concentration(1,2,3 &5wt%) which annealed at temperatures 623K with vacuum annealing under argon atmosphere, it could be inferred that these films are amorphous structure when it is pure with very small peak at (002) plane, while it was shown that the films are polycrystalline at orientation [(002),(102)] for films doped with 1%Cu and the orientation are [(002), (102). (110), (112), and (201)] for films doped with 2%Cu which indicate that the structure was hexagonal according to ASTM cards when CdSe was doped with Cu content(1&2wt%), while the better crystallinty appear for the films with doping (3 &5wt%) and there is only reflection from (002) plane appear which indicates a crystal growing on this plane and the structure was hexagonal unit cell(see Table(1)). Spanulescu et al[11] and Moore et al[12]

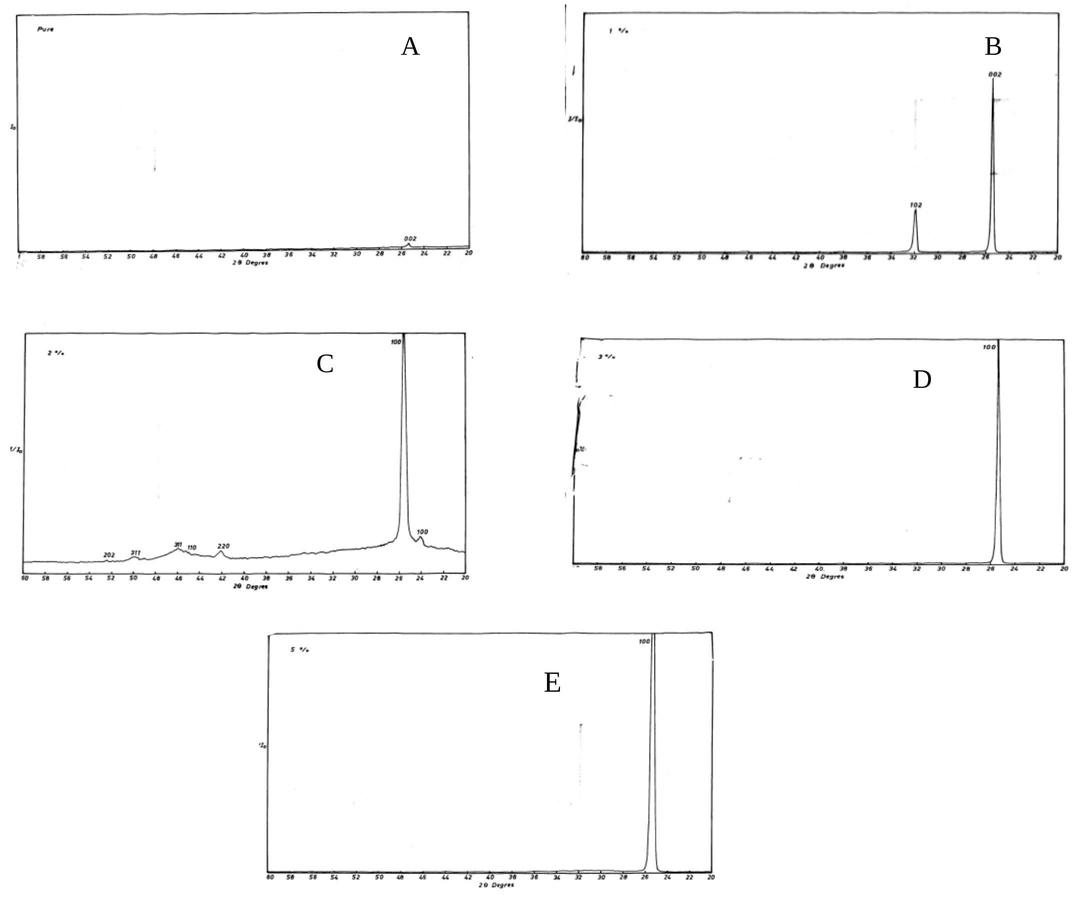

Fig.(1) X-ray diffraction pattern for CdSe:Cu film at A-pure CdSe, B-doped with 1wt% Cu, C- doped with 2wt% Cu, D- doped with 3 wt% Cu, E- doped with 5 wt% Cu.

have obtained that the structure is hexagonal and cubic, and they found that there is a strong peaks at the plane (002) which agree with our results.

We can see from Fig.(1) that the doping samples will shift the peaks towards higher 2θ from 25.4 before doping to 25.5 after doping for the plane (002), and the value of d-spacing from 3.51A to 3.49A and this may be due to substitute the Cu ions instead of Cd^{+2} because the radius of Cu(1.28A) is smaller than the radius of Cd(1.43A) which lead to shift the peaks and decrease the interplaner distance(d), and this results agree with Shreekanthan et al[13] and sathyalatha[14].

The relative intensity of the peaks increases with increasing the doping concentration and these results are agreement with other researchers[3,15,16]. The value of lattice constant was calculated by computer programs, and we are found that the value of these constant equal to (a=3.741,c=7.096)A°. The crystallite size for these samples are various from (20 to 81.4)nm for doping from pure to the 5wt%Cu as shown in Table(1) and Fig.(2), and this is attributed to the improvement in the crystal structure by doping and crystallite it in the plane(002) with high intensity and hexagonal structure, this is agree with Shreekanthan et al[13] , whereas the researchers Sathyalatha[14] have obtained grain size 430A for CdSe:Ag from X-ray diffraction studies.

Table(1) X-ray diffraction data for CdSe:Cu films with variation of Cu content.

Cu wt %	hkl	$(I/I_o)_{stand}$	d_{stand}(A°)	2θ	dnm	D(A°)	(I/I_o)
pure	2	75	3.509	25.4	3.51	20.3	2
1	2	75	3.509	25.4	3.51	27.2	75
	102	35	2.55	34.5	2.59	-	35
2	2	100	3.509	25.5	3.49	40.7	100
	100	75	3.71	24.1	3.69	-	15
	110	85	2.15	42.1	2.15	-	10
	103	70	1.979	45	2.01	-	8
	200	12	1.86	46.8	1.97	-	10
	112	50	1.83	50	1.82	-	5
	201	12	1.8	52.4	1.75	-	4
3	2	70	3.509	25.5	3.49	81.4	100
5	2	70	3.509	25.5	3.49	81.4	100

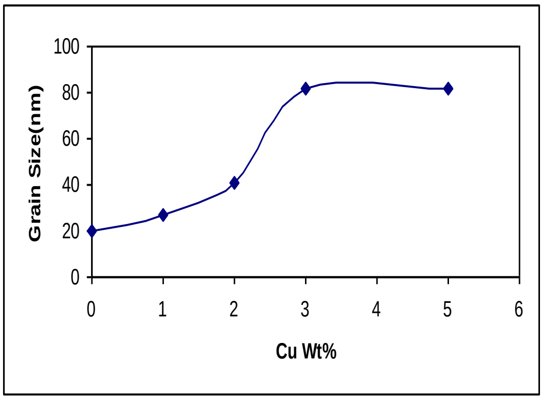

Fig.(2) Variation of a grain size as a function of Cu content for CdSe films for (002) plane

4-Conclusions:

1- The pure CdSe films have been found to consist amorphous structure with very small peak at (002)plane and the films were polycrystalline for doped CdSe with (1&2wt%) Cu content and it has better crystallinty as the Cu contents increased to (3 &5wt%).

2- The crystal structure of all CdSe:Cu films are hexagonal.

3- The relative intensity of the peaks increases with increasing the doping concentration.

4- The crystalline size were found to increase with increasing Cu content.

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تأثير نسب التطعيم بالنحاس على الخصائص التركيبية لأغشية CdSe

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الخلاصة:

حضرت أغشية CdSe بطريقة التبخير الحراري في الفراغ بالسمك 1µm. . تمت عملية التطعيم بالنحاس باستخدام التلدين بوجود غاز الأركون . درست الخصائص التركيبية باستخدام تحليلات الأشعة السينية ودرس تأثير نسب النحاس المضافة على الاتجاهية , الشدة النسبية, حجم الحبيبات وثابت الشبيكة. تمتلك أغشية CdSe النقية تركيب عشوائي مع قمة صغيرة بالاتجاه(002). ولوحظ إن الأغشية المطعمة بالنحاس ذات النسب (1&2wt%) هي ذات تركيب متعدد البلورات وبثابت شبيكة (a=3.741,c=7.096)A° وتتبلور الأغشية بصورة اكبر بإضافة نسب أكثر من النحاس Cu (3&5wt%) . تشير الانعكاسية من المستويات(201) and (112), (110), (102). (002)] الى ان التركيب الشائع هو السداسي , لذلك يكون تركيب اغشية CdSe:Cu سداسي عند نسب النحاس(pure, 1&2wt%) وسداسي أيضا عند النسب(3&5wt%) . وجد بأن الحجم الحبيبي يعتمد على تركيز الشوائب المضافة ويتغير بين(20.3-81.4)nm ويزداد بزيادة تركيز النحاس.