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Structural and Optical Properties of CdS_xTe_{1-x} Thin Films Fabricated by Thermal Evaporation.

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ABSTRACT

CdS_xTe_{1-x} films in the range of (x=0.9, 0.8, 0.7) about 300 nm thickness have been formed on glass substrates by thermal evaporation . X-ray results showed that the CdTe film was polycrystalline with cubic zinc blend structure and had preferred growth of grains along the (111) crystallographic direction. Also, CdS was polycrystalline with hexagonal wurtzite structure and had preferred growth of grains along (002) crystallographic direction while CdS_xTe_{1-x} films studied the phase change with an inversion point related to the x-value . Transmittance and absorbance spectra of the films were measured as a function of wavelength (300-1100) nm . Then the band gap of the films calculated by using absorption spectrum, where the direct optical energy gap for CdTe is 1.48 eV and for CdS is 2.5 eV while the direct optical gap of CdS_xTe_{1-x} films be limited to between CdS and CdTe, and varied non-linearly, showing downward with decrease x-value .Also the refractive index (n) of these films are discussed.

1. Introduction

The II-VI Semiconductors with a wide range of band gap energies find potential applications in a variety of optoelectronic devices .The development of thin film solar cells makes use of at least two kinds of semiconducting layers; a wide bandgap window material and a narrow bandgap absorber material . The one most researched absorber materials is CdTe and the majority of researchers used a n-CdS layer as a window material[1-3] . CdTe is very well studied for use as active material in thin film solar cells due to its special properties [4] : CdTe has an energy gap of 1.45 eV, and therefore is well adapted to the spectrum of solar radiation . The energy gap of CdTe is direct, leading to very strong light absorption, CdTe has a strong tendency to grow as an essentially highly stoichiometeric, but p-type semiconductors film can form an p-n heterojunction with CdS. CdS/CdTe heterojunction solar cell is a strong candidate of the low cost –effective thin film solar cells with the cell efficiency of over 16.5%[5-7]. In fabricating CdS/CdTe heterojunction, 400 C° CdCl2 heat treatment was used. It is known that the CdCl2 treatment recrystallizes both CdS, CdTe to enhance grain size, and interdiffusion the CdS/CdTe layers to introduce a CdSxTe1-x graded layer capable of reducing defects due to a lattice- mismatch at the CdS/CdTe interface [8]. The solar cell of the thicker CdTe layer showed more interdiffusion at the CdS/CdTe interface and better photovoltaic characteristics [7] . The formation and characterization of CdSxTe1-x was recorded by different authors [9-12] . In this paper, we explain the preparation CdSxTe1-x alloy films with x-value (0.9, 0.8, 0.7) by thermal co-evaporation on glass substrates. The characteristics of the films have been investigated by X-Ray Diffraction (XRD), the transmittance and optical absorption measurements by (UV-VS-Spectrophotometer) we have studied these alloy films in order to improve the photovoltaic(PV) performance.

2. The Experimental part

A thermal evaporation apparatus (Edward coating unit 306) was used at high vacuum of about 10-6 Torr to prepare the polycrystalline CdTe, CdS and CdSxTe1-x where x=0.9,0.8.0.7 at R.T . The deposition rate was 0.8 nm/sec .which depends on the

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molecular weight of high purity compounds CdS and CdTe powder with 99.99% purity was purchased from Sigma-Aldrich Company . All samples were deposited on glass substrates were cleaned with alcohol . The films prepared were evaporated using molybdenum boat, with a thickness 300 nm. In the case of preparation the ternary alloy CdSxTe1-x, the technique of two independent sources are used to evaporate the different compositions of CdTe and CdS with appropriate evaporation rates for these

Table. 1.The Grain size, Phases and Planes of CdS_xTe_{1-x} thin films with x-value

X	Grain size	2θ	hkl	d(Å)	Crystal System
1	29 nm	26.61	002	3.3471	Hexagonal
		28.30	101	3.1509	Hexagonal
		48.05	103	1.8919	Hexagonal
0.9	27 nm	24.16	111	3.5939	Cubic
		25.73	100	3.4585	Hexagonal
		26.42	002	3.3706	Hexagonal
0.8	20 nm	24.45	111	3.6367	Cubic
		25.25	002	3.5238	Hexagonal
		26.64	101	3.3427	Hexagonal
0.7	22 nm	24.85	111	3.6213	Cubic
		25.95	100	3.4644	Hexagonal
		26.50	101	3.3562	Hexagonal
		27.10	002	3.0775	Hexagonal
		45.15	003	2.1984	Hexagonal
0	44 nm	23.92	111	3.7162	Cubic
		39.56	220	2.2758	Cubic
		46.67	311	1.9443	Cubic

sources because of the different melting points of CdS 1750 C̊ and CdTe 1041 C̊ . The crystal structure of the films was determined by X-ray diffraction (XRD) using SHIMADZU, XRD-7000, X-RAY DIFFRACTOMETER with Cukα radiation (λ=1.5406 A°) . The optical absorption and transmission spectra of the prepared thin films were obtained by (UV-VIS-Spectrophotometer) Model JENWAY (6800 UV/VIS) in the spectra range of 300 to 1100nm.

3. Results and Discussion

3.1 Structural properties

The crystalline of the prepared thin films were analyzed by X-ray diffractometer, and it showed that all films are polycrystalline . By comparing the experimental XRD data with ASTM cards, found that the CdTe film (x=0) had exhibited a pure cubic phase with different orientations while the CdS film (x=1) had a hexagonal phase with many planes . The same results were found by J.Touskova et al [13,] . The phases and planes of CdSxTe1-x are illustrated in table(1), which shows that existence of the cubic phase together with the hexagonal one of 0<x<1 . This is due to the polycrystalline behavior of thin films tending to present a multiphase structure . Similar results found by E.K.AL-Shakarchi [14] and R.Dhere et al [9] . K.R Murali et al [10] found that the peaks shifted twords low 2θ side as the concentration of CdTe increased in the ternary .The grain size of films are in the range of 20 to 44 nm calculated by using Scherrer formula [15] depending on the x-value as shown inTable.1, and the grain size of CdS_xTe_{1-x} at 0<x<1 are smaller than that for CdS and CdTe.

$$D_{hkl} = K\lambda / \beta Cos\theta$$

Where K is a shape factor, β is the width half maxima (FWHM) of the XRD peak at 2θ, recorded with an incident wavelength (λ=1.54 A˚).

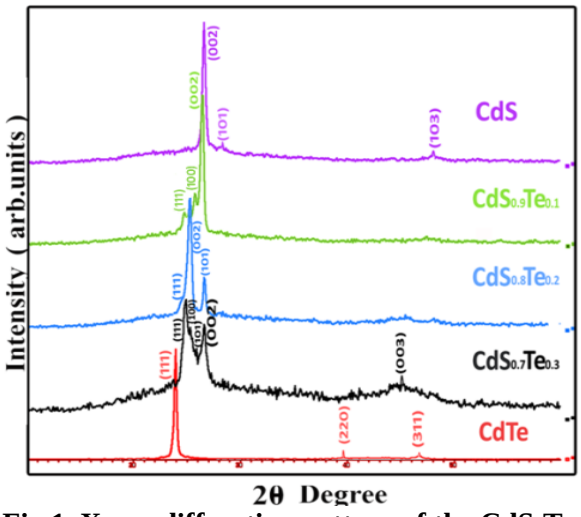

Fig.1. X-ray diffraction pattern of the CdS_xTe_{1-x} films deposited at different x-value 0<x<1

3.2 Optical properties

The Absorbance (A) and transmittance (T) spectra of the CdS_xTe_{1-x} thin films were recorded in the range (300 -1100) nm . Fig.2 shows the plot of α versus the wavelength λ of the films that had a high α at the visible range and decreased with λ at nearly sharp behaviour to become nearly constant at NIR range . The Absorption edge shifted to the NIR region with increasing x, which related to the CdS and CdTe energy gap (Eg), (2.5-1.48 eV) respectively . Fig.3 shows the plot of transmission (T) versus λ for the CdS_xTe_{1-x} films that have high T>80%, the position of

the band gap in the wavelength scale is shown with dotted lines . Optical band gaps of the samples were determined from the intercept of $(\alpha h\upsilon)^2$ versus hυ plots as shown in Fig.4 . The plots were linear suggesting direct band nature of the films [10] . The energy gaps (Eg) are (2.5, 2.45, 2.4, 2.1, 1.48 eV), for films of different compositions where x=(1, 0.9, 0.8, 0.7, 0) respectively . It is observed that the band gap shifted towards CdTe side as x increased . The relation of Eg with x given by the following equation.

$E_g(x) = 58.49x^4 - 157.2x^3 + 139.6x^2 - 39.86x + 1.48$

The absorption coefficient (α) was calculated as : $\alpha = 2.303\frac{A}{t}$ where

(*A*) Is the absorbance and *t* is the film thickness [16] . Fig.5 showed the change of refraction index (n) versus the wavelength of the films that have a high (n) at the range of (480-1100nm) equal to about 2.6, the maximum value depend on the x value and shifted towards NIR with increasing Te, similar results found by D.A. Wood et al [17], the refractive index of the films were obtained by using the equation [18]:

$$n = \left[\left(\frac{1+R}{1-R}\right) - (1+k^2)\right]^{1/2} + \frac{1+R}{1-R}$$

were *R* is the ratio of the reflectance which calculated by using the equation:

R= 1-T-A

k is the extinction coefficient which related to absorption coefficient by :

$k = \alpha\lambda/4\pi$

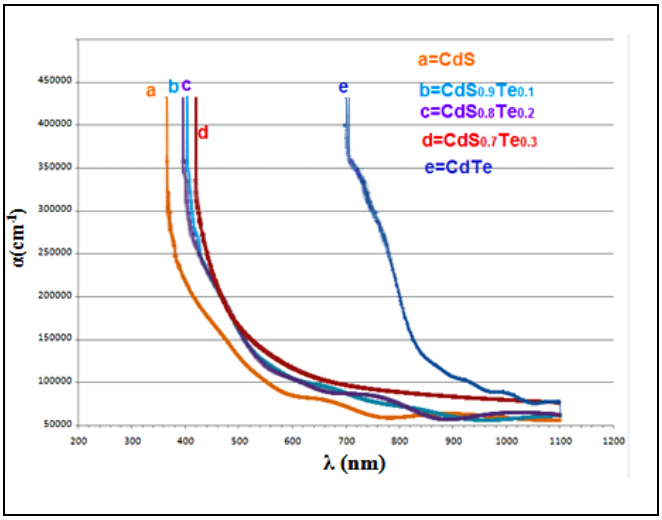

Fig.2. Absorption coefficient with wavelength of the CdSxTe1-x thin films .

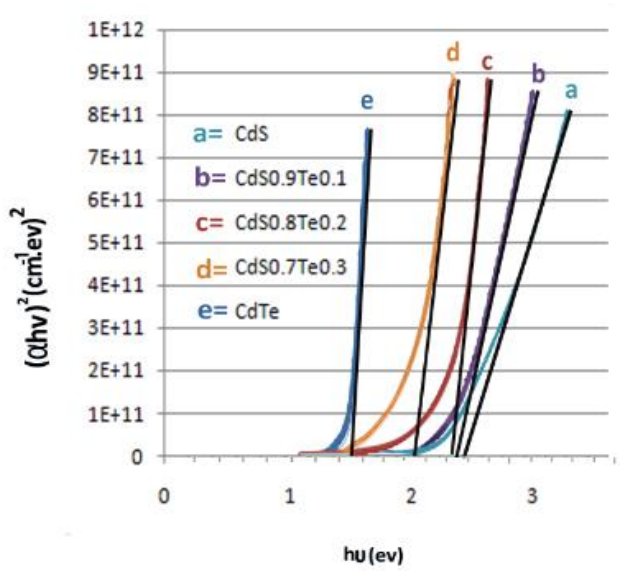

Fig.3. Transmittance spectra of the CdS_xTe_{1-x} thin films .

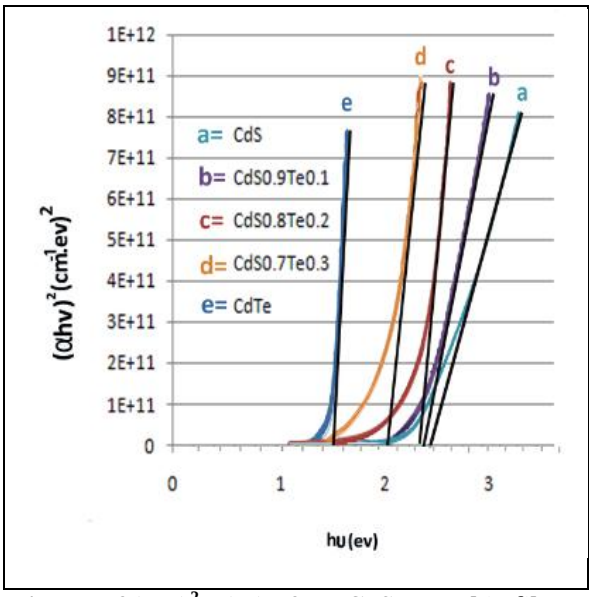

Fig.4. Plot of $(\alpha h\upsilon)^2$vs(hυ) of the CdS_xTe_{1-x} thin films .

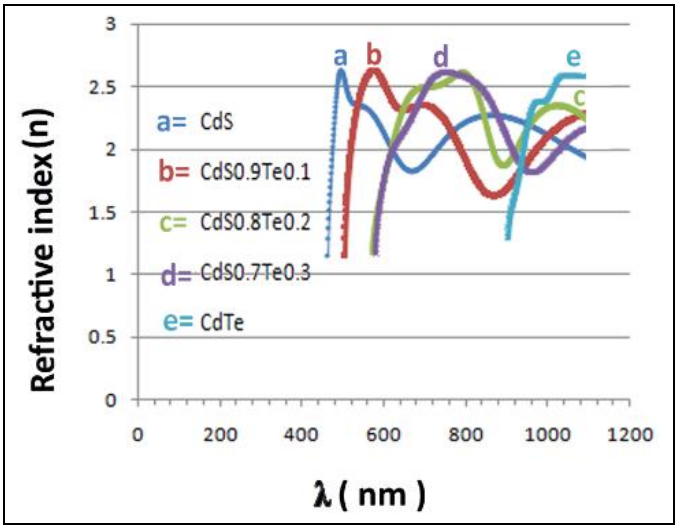

Fig.5. Refractive index versus wavelength for CdS_xTe_{1-x} thin films .

4. Conclusion

A polycrystalline CdS_xTe_{1-x} thin films of nano grain size were prepared by thermal evaporation technique, with different phases . A graded direct optical energy gap were found ranged from (1.48-2.5) eV depending on the x-value .The films give a transmission of greater than 80% in the visible and NIR range this refers to the possibility of using this films as a window layer in solar cells. The refractive index give an interference shape of higher value equal to about 2.6 for all films in the visible and NIR wavelength range .

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الخصائص التركيبية والبصرية لاغشية CdS_xTe_{1-x} الرقيقة المحضرة بطريقة التبخير الحراري تحت الفراغ .

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الخلاصة

تم تحضير اغشية CdSxTe1−x الرقيقــة عند قيم (x) تساوي (٠,٩ ، ٠,٨ ، ٠،٧) وبسمك (٣٠٠) نانومتر تقريباً على قواعد زجاجية بطريقة التبخير الحراري تحت الفراغ . اظهرت نتائج حيود الاشعة السينية (XRD) ان غشاء تلوريد الكادميوم (CdTe) متعدد التبلور بتركيب مكعبي (ركائز الخارصين) عند اتجاه النمو الحبيبي المفضل (١١١)، كما اظهرت نتائج حيود الاشعة السينية ان غشاء كبريتيد الكادميوم (CdS) متعدد التبلور ذو تركيب سداسي عند اتجاه النمو الحبيبي المفضل (٠٠٢) بينما اظهرت نتائج حيود الاشعـــة السينية لاغشية CdSxTe1−x تغيراً في الطور بالاعتمــاد على تغير قيمة (x) في المزيج . تم قياس اطياف الامتصاص والنفاذ لجميع الاغشية المحضرة كدالــة للطول الموجي (λ) ضمن المدى (٣٠٠−١١٠٠) نانومتر . وقد حسبت فجوة الطاقــة البصرية (Eg) عن طريق طيف الامتصاص وكانت قيمة فجوة الطاقة البصرية المباشرة لغشاء تلوريد الكادميوم (١,٤٨) الكترون−فولت ولغشاء كبريتيد الكادميوم (٢,٥) الكترون−فولت . بينما كانت قيمة فجوة الطاقة البصرية لاغشية CdSxTe1−x محصورة بين قيم فجوة الطاقة لكبريتيد الكادميوم وتلوريد الكادميوم، وتغير قيمها لم يكن خطياً حيث تقل قيمة فجوة الطاقة للمزيج كلما قلت قيمـــة (x) . وتم كذلك دراسة معامل الانكسار (n) للاغشية المحضرة.