Structural and Optical Properties of CdS\textsubscript{x}Te\textsubscript{1-x} Thin Films Fabricated by Thermal Evaporation.

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Abstract: CdS\textsubscript{x}Te\textsubscript{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 wurzite structure and had preferred growth of grains along (002) crystallographic direction while CdS\textsubscript{x}Te\textsubscript{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\textsubscript{x}Te\textsubscript{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.

Keywords: Thin films, Structural and Optical Properties, CdS\textsubscript{x}Te\textsubscript{1-x}.

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 stoichiometric, 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° CdCl\textsubscript{2} heat treatment was used. It is known that the CdCl\textsubscript{2} treatment recrystallizes both CdS,CdTe to enhance grain size, and interdiffusion the CdS/CdTe layers to introduce a CdS\textsubscript{x}Te\textsubscript{1-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 CdS\textsubscript{x}Te\textsubscript{1-x} was recorded by different authors [9-12]. In this paper, we explain the preparation CdS\textsubscript{x}Te\textsubscript{1-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 CdS\textsubscript{x}Te\textsubscript{1-x} where x=0.9,0.8,0.7 at R.T. The deposition rate was 0.8 nm/sec which depends on the 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 CdS\textsubscript{x}Te\textsubscript{1-x}, the technique of two independent sources are used to evaporate the different compositions of CdTe and CdS with appropriate evaporation rates for these.
The grain size of films are in the range of 20 to 44 nm with an incident wavelength $\lambda= 546$ Å. The optical absorption and transmission spectra of the CdS thin films were recorded in the range of 300 to 1100 nm.

### 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 CdS$_x$Te$_{1-x}$ 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 towards low 20 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 in Table 1, and the grain size of CdS$_x$Te$_{1-x}$ at 0<x<1 are smaller than that for CdS and CdTe.

$$D_{hkl} = \frac{K\lambda}{\beta \cos \theta}$$

Where $K$ is a shape factor, $\beta$ is the width half maxima (FWHM) of the XRD peak at 20, recorded with an incident wavelength ($\lambda=1.54$ Å).

#### Table 1

<table>
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<tr>
<th>X</th>
<th>Grain size</th>
<th>2θ</th>
<th>hkl</th>
<th>d(Å)</th>
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The Absorbance (A) and transmittance (T) spectra of the CdS$_x$Te$_{1-x}$ thin films were recorded in the range (300-1100) nm. Fig.2 shows the plot of $\alpha$ versus the wavelength $\lambda$ of the films that had a high $\alpha$ at the visible range and decreased with $\lambda$ 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 ($E_g$) $(2.5-1.48$ eV) respectively. Fig.3 shows the plot of transmission (T) versus $\lambda$ for the CdS$_x$Te$_{1-x}$ 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 $(\alpha h\nu)^2$ versus $h\nu$ plots as shown in Fig.4. The plots were linear suggesting direct band nature of the films [10]. The energy gaps ($E_g$) 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 $E_g$ 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 ($\alpha$) was calculated as: $\alpha = 2.303A/\lambda$

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]:

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

were \( R \) is the ratio of the reflectance which calculated by using the equation:

\[ R = 1 - T \times A \]

\( k \) is the extinction coefficient which related to absorption coefficient by:

\[ k = \alpha \lambda / 4\pi \]

Fig.2. Absorption coefficient with wavelength of the CdS\(_x\)Te\(_{1-x}\) thin films.

Fig.3. Transmittance spectra of the CdS\(_x\)Te\(_{1-x}\) thin films.

Fig.4. Plot of \( (\alpha h\nu)^2 \) vs \( h\nu \) of the CdS\(_x\)Te\(_{1-x}\) thin films.

Fig.5. Refractive index versus wavelength for CdS\(_x\)Te\(_{1-x}\) thin films.

4. Conclusion
A polycrystalline CdS\(_x\)Te\(_{1-x}\) 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.
References


الخصائص التركيبية والبصرية لاغشية CdS̵₉Te̵₁-x تحت الفراغ 

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الخلاصة

تم تحضير أغشية CdS₧Te₁-x على قواعد زجاجية بطريقة التبخير الحراري تحت الفراغ (XRD) عند تدفق غاز تيريد cadmum (CdTe) في ثلوج مكعبة (كلايكس الخاردين) عند انتقال النمو الادربي المفضل (111) كمكربن ذو تركيب سداسي عند انتقال النمو الحبشي المفضل (002) بينما اظهرت نتائج جودية ازهارية السينية لاغشية CdS₧Te₁-x تغيرا في الطرور بالاعياد على نتائج قيمة (x) في المزيج. تم قياس طفيلة الاختصاص ونفاذ لجميع الاغشية المحضرة كندالة للطول الموجي نم (λ) ضمن النمو (300-1100 نانومتر). وقد حسبت فجوة الطاقة البصرية (Eg) عن طريق طفيلة الاختصاص وكانت قيمة فجوة الطاقة البصرية المباشرة لغشاء تيريد cadmum (1.48 الالكترون-فولت) ولغشاء cadmum (2.5 الالكترون-فولت). بينما كانت قيمة فجوة الطاقة البصرية لاغشية CdS₧Te₁-x محضرة بين فجوة cadmum وكان cadmum ونفاذ cadmum تغير قيمة (x) محضرة. ولذلك دراسة معامل الانكسار (n) للاغشية المحضرة.