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OPTICAL AND STRUCTURAL STUDY OF SOME B^{II} A^{VI} BINARY COMPOUNDS

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ABSTARCT

The compounds B^{II} A^{VI} (ZnO, CdO, ZnS, CdS, ZnSe, CdSe, ZnTe, CdTe, HgS, HgSe and HgTe) and their alloys have been the material of considerable technological interest. Polycrystalline films of CdS, CdSe and CdTe have been deposited onto ultra clean glass substrate by sintering process. 10 min sintering time and 227^{o} K sintering temperature were found to be optimum. The optical band gap of these films were determined by reflection measurements in wave length range 400-900nm. The crystal structure of these films was studied from X-ray diffraction patterns. The films were polycrystalline in nature having hexagonal wurtzite. Sintering is less time consuming, less pollutant, of maximum material utility and offers a suitable method for preparing films.

Key Words:- (Sintering, bandgap, reflection spectra, Crystal structure, Cadmium Chalcogenides).

Introduction

Major part of the world is facing a crisis regarding the cost, availability and pollution effects of fossil fuels. We must develop and use alternative energy sources, especially long term natural resources, the sun, to make ourselves self reliant. Solar energy is an infinite source of energy. If only $1/10^6$ part of solar energy received on earth surface is utilizd, we will get rid off this problem, solar cells are used to convert solar energy into electrical energy directly by using the pbotovoltaic effect. High efficiency solar cells have been produced by using single crystal such as Si and GaAS, but because of their high cost they can not be used on large scale. Thin film solar cells give hope to meet the cost goals which are necessary to provide the needs for energy production by photovoltaics.

Materials of B^{II} A^{VI} class of periodic table and their related compounds are among the leading candidates of the next generation of photovoltaic solar cells[1-3]. In the last twenty years, there has been a rapid development of investigation in the domain of semiconducting films of B^{II} A^{VI} compounds. From the group of B^{II} A^{VI} compounds the most widely used elements are photovoltaic devices with heterojunction between CdSe and CdTe films. These compounds have an important role in the fabrication of active thin film devices[4-6]. They find application in photovoltaic devices, photoelectrochemical solar cells, solar control coatings, lasers, light emitting, diodes, thermo-photovoltaic energy converters, photo luminescent devices[7-9]. Cadmium chalcogenides form a technically important class of materials owing to their wide spread utility in a variety of electronic and opto-electronic devices. The root causes of their popularity are their high absorption coefficient with an allowed direct type of transitions. CdS has been the subject of intensive research because of its intermediate band gap, reasonable conversion efficiency, high absorption coefficient, stability and low cost[10-11]. CdS with a band gap of 2.35eV is an ideal material for use as the window layer of heterojunction solar cells.

CdSe is used in transistors and photo detectors.

CdTe in film form is very promising photovoltaic material due to its near optimum energy gap 1.46eV. CdTe based solar cells have achieved efficiencies greater than 16%, in which CdTe absorber layer is prepared by close space sublimation process. Sintering process has carried out for the synthesis of Cadmium chalcogenides (CdS, CdSe, CdTe) and studies on theis structural and optical properties are presented in this paper.

Experimental Methods :

A variety of thin film deposition techniques are e.g. vacuum evaporation (Thermal Evaporation, Flash Evaporation, Laser Evaporation), sputtering method (glow discharge sputtering, Magnetron sputtering etc.) Epitaxial deposition (Hot wall epitaxy, vapour phase epitaxy etc.) Chemical Deposition (screen printing, sintering, spray pyrolysis etc.) are available offering great flexibility for thin film preparation.

In the present work we have used the technique of screen printing followed by sintering process for the deposition of films.

CdS, CdSe and CdTe of 99.999% purity were used for preparing sintered films. As the weights of these are large, we reduced them in the same proportion. Appropriate amount of CdS, CdSe and CdTe are taken and then to the appropriate amount of CdS & CdTe 10% weight of $CdCl_2.2\left(\frac{1}{2}H_2O\right)$ used as adhesive while for CdSe, $ZnCl_2$ is used as adhesive, and ethylene glycol ($CH_2OH.CH_2OH$) is added as binder and mixed thoroughly. The paste thus formed was screen printed on ultra clean glass substrate, which has been cleaned by soap solution, embry powder, isopropyl alcohol and finally washed with distilled water. The samples thus prepared were dried at 120°C for 3 hours in open air and then heated at 400°C for 15 minutes to remove the organic materials. To avoid the cracks in the samples the drying process in carried out at lower temperature. After this the films were sintered at 550°C for 10 minutes to get a stable sintered film.

RESULTS AND DISCUSSION

Spectroscopic properties

In these sintered films very low transmission and very high absorption were observed. Therefore, we have confined our studies to the reflection studies of these sintered films. The optical reflectance of these films was measured in the appropriate wave length range. In the present investigation, we have used spectrophotometer (Hitachi model U-3400) for reflection studies.

Fig 1 (a), 2 (a), 3 (a), represent the reflection spectra of CdS, CdSe & CdTe respectively. The reflection spectra of these films showed sharp down fall which corresponds to the energy band gap is shifted towards lower wave length. The spectra also showed that, as the sintering temperature increases the energy band gap increases. Fig 2(c) & Fig 3(c).

For the determination of band gap the graph between.

$\left[h\nu \ln\left(\frac{R_{max}-R_{\min}}{R-R_{\min}}\right)\right]^2$ versus photon energy h□

as shown in figure 1(b), 2(b) and 3 (b) have been plotted, a staright line is obtained. The extrapolation of the straight line to $(\alpha h\nu)^2 = 0$ (i.e. energy axis), give the value of band gapes of the film material. The value of the band gap are 2.35 eV for CdS, 1.68 eV for CdSe and 1.46 eV for CdTe. These values are very close to the values reported in other studies.[12-13] The mode of optical transitions in these films is of band to band direct type. In case of Cadmium chalcogenides the plot of electron energy E as a function of electron wave vector K (E–K band diagram) indicates that the top of valence band has the same K value as the bottom of conduction band and hence the

transitions are of direct type. The absorption coefficient was estimated using Tauc relation $\alpha h\nu = A\left(h\nu - E_g\right)_{½}$ where h□ and E_g represent photon energy and band gap, A is constant. The absorption coefficient was found of the order of $10^4 cm^{-1}$ in case of CdS.

Structural Properties

The structural characterization of these films was carried out by taking XRD pattern of the films. A Philips PW1140/09 X-ray diffractometer was employed for studying the structure of films. The copper target was used as a source of X-rays with □=1.5405A° (CuK□ □). X-ray diffraction pattern of CdS, CdSe and CdTe films are shown in the figure (4) (5) (6). The X RD patterns do not show the peaks of oxides of Cadmium. The presence of sharp structural peaks in X RD patterns confirm the polycrystalline nature of these films. The X-ray diffraction data of each film are shown in tables 1-3.

Table - 1

X-ray diffraction data of CdS sintered film.

S. No.	2 θ	d (Exp) (A°)	d* (ASTM) (A°)	Plane (hkl)
1.	43.08	2.067	2.068	110
2.	48.0	1.896	1.898	103
3.	51.0	1.790	1.791	200
4.	52.0	1.758	1.761	112
5.	53.0	1.727	1.731	201
6.	54.8	1.875	1.674	004
7.	58.4	1.582	1.580	202
8.	61.0	1.518	1.520	104
9.	69.5	1.353	1.354	210
10.	71.0	1.328	1.327	211
11.	72.5	1.304	1.303	114
12.	75.7	1.255	1.257	105
13.	80.4	1.194	1.194	300

Table 2

X-ray diffraction data of CdSe sintered film

S. No.	2θ (degree)	d (Exp) (A°)	d* (ASTM) (A°)	Plane (hkl)
1.	23.9	3.720	3.720	100
2.	25.5	3.490	3.510	002
3.	27.1	3.288	3.290	101
4.	35.2	2.548	2.544	102
5.	42.1	2.145	2.151	110
6.	45.9	1.976	1.980	103
7.	49.8	1.830	1.834	112
8.	50.60	1.8023	1.800	201
9.	55.20	1.6488	1.6450	202
10.	66.30	1.4086	1.4070	210

Table 3

X-ray diffraction data of CdTe sintered film

S. No.	2θ (degree)	d (Exp) (A°)	d* (ASTM) (A°)	Plane (hkl)
1.	23.6	3.66	3.75	002
2.	39.2	2.962	2.955	110
3.	46.43	1.965	1.919	201
4.	62.3	1.490	1.495	210
5.	71.5	1.318	1.323	300
6.	76.10	1.245	1.249	302
7.	84.40	1.146	1.145	220
8.	89.30	1.096	1.096	116

The experimental d_value are calculated from the Bragg's equation 2d sin □ □ □ n□ (here $n=1$, □=1.1.5405Å), by taking the values of □ corresponding to the peaks of XRD pattern. The observed d-values of these sintered films are in good agreement with ASTM data (d*) of these films and show the hexagonal wurtzite structure of the films as also reported by Y. S. Seol et al[14] V. Snejdar[15], E.U. Masumdar et al[16] and P. J. Sebastian[17-19], Thus it is concluded that these films are of polycrystalline nature and have hexagonal wurtzite structure.

Table 4

Lattice Parameters of CdS, CdSe and CdTe films

S. No.	Sample (Film)	d (A)	a (A)	c (A)
1.	CdS	1.896	4.135	6.704
2.	CdSe	3.720	4.296	6.983
3.	CdTe	3.660	5.922	7.320

The lattice constants a and c of each film corresponding to the strongest diffraction peak have been determined using the following equations:-

$$\frac{1}{d^2}=\frac{1}{a^2}\left[\frac{4}{3}\left(h^2+hk+k^2\right)+\frac{l^2}{\left(c/a\right)^2}\right] \qquad \text{_____(1)}$$

The equation (i) for two different planes ($h_1k_1l_1$) & ($h_2k_2l_2$) can be written as

$$\left(\frac{d_2}{d_1}\right)^2=\frac{\left[\frac{4}{3}\left(h_1^2+h_1k_1+k_1^2\right)+\frac{l_1^2}{\left(c/a\right)^2}\right]}{\left[\frac{4}{3}\frac{\left(h_2^2+h_2k_2+k_2^2\right)}{}+\frac{l_2^2}{\left(\frac{c}{a}\right)^2}\right]} \qquad \text{.... (ii)}$$

On substituting the value of h_1,k_1,l_1 and h_2,k_2,l_2 in above equation (ii) we determine the value of $\frac{c}{a}$ and on subsisting the value of $\frac{c}{a}$ in equation (1), we calculated a and then calculate c as c/a is already known.

The constants a and c are in agreement with the standard lattice constants.

The optical band gap and lattice parameter and high value of absorption coefficient make these materials suitable and smart for various types of solid state devices.

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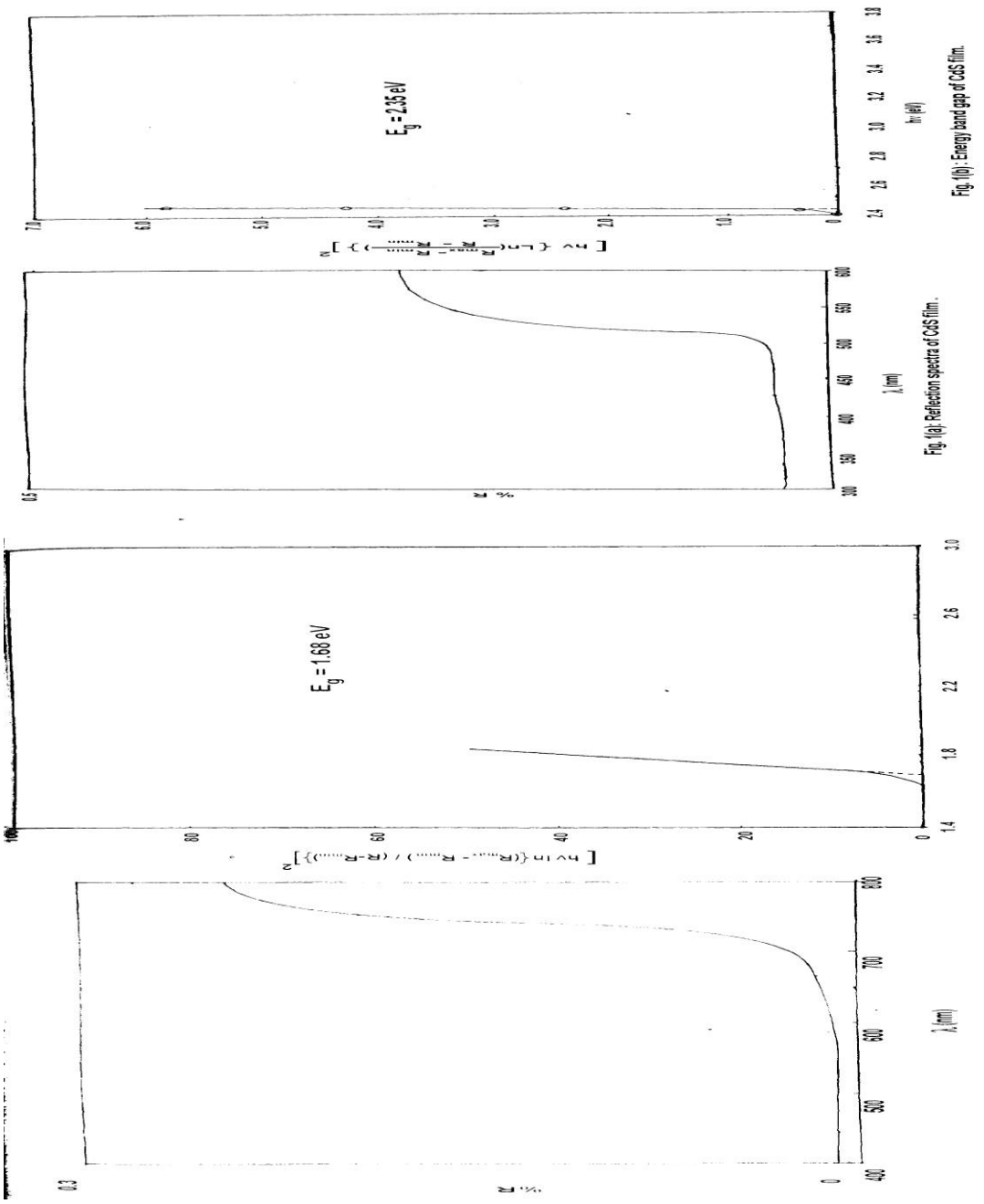

Fig. 1(b): Energy band gap of CdS film.

Fig. 1(a): Reflection spectra of CdS film.

Fig. 2(b) : Energy band gap of CdSe sintered film

Fig. 2(a) : Reflection spectra of CdSe sintered film

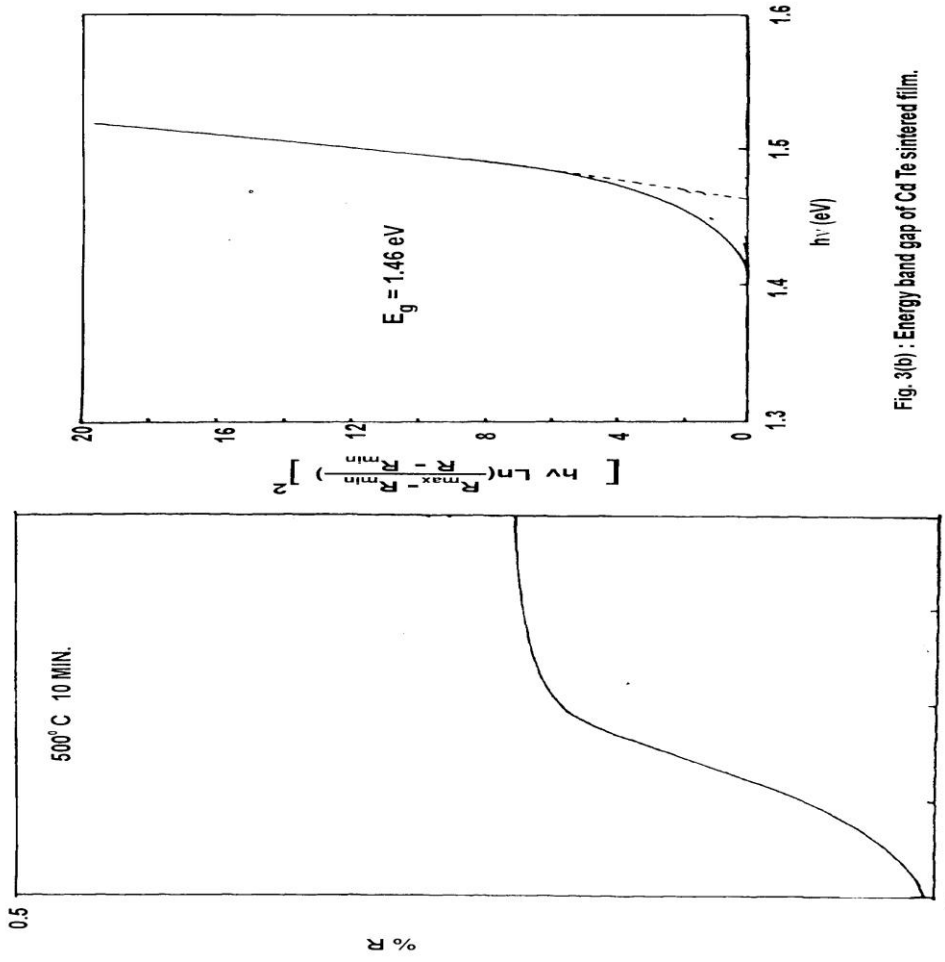

Fig. 3(a) : Reflection spectra of Cd Te sintered film.

Fig. 3(b) : Energy band gap of Cd Te sintered film.

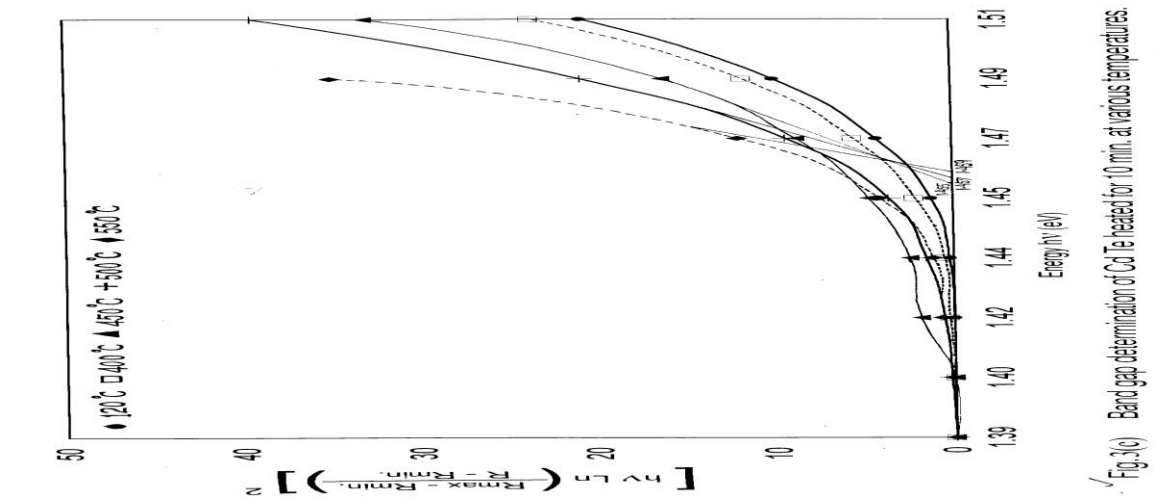

Fig.3(c) Band gap determination of CdTe heated for 10 min. at various temperatures.

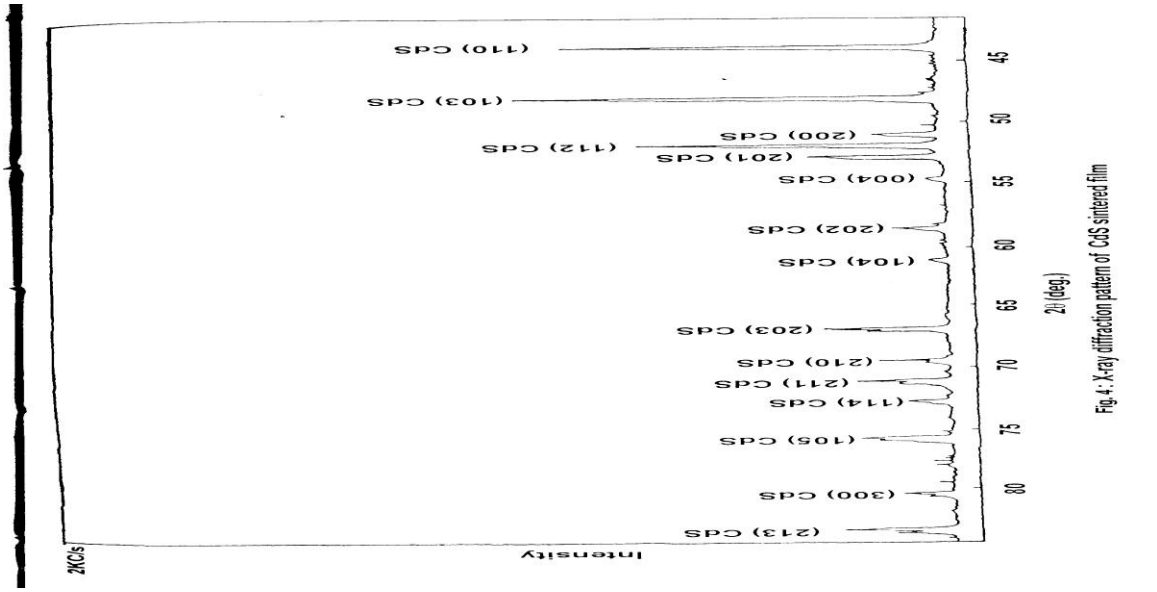

Fig. 4 : X-ray diffraction pattern of CdS sintered film

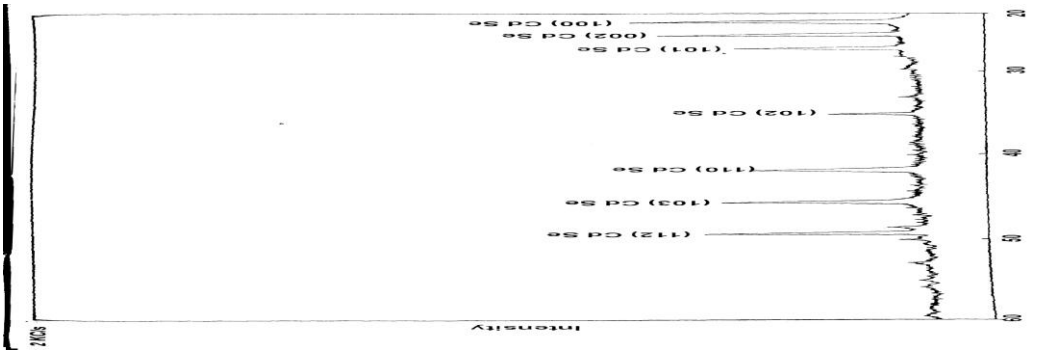

Fig. 5 : X-ray diffraction pattern of Cd Se sintered film.

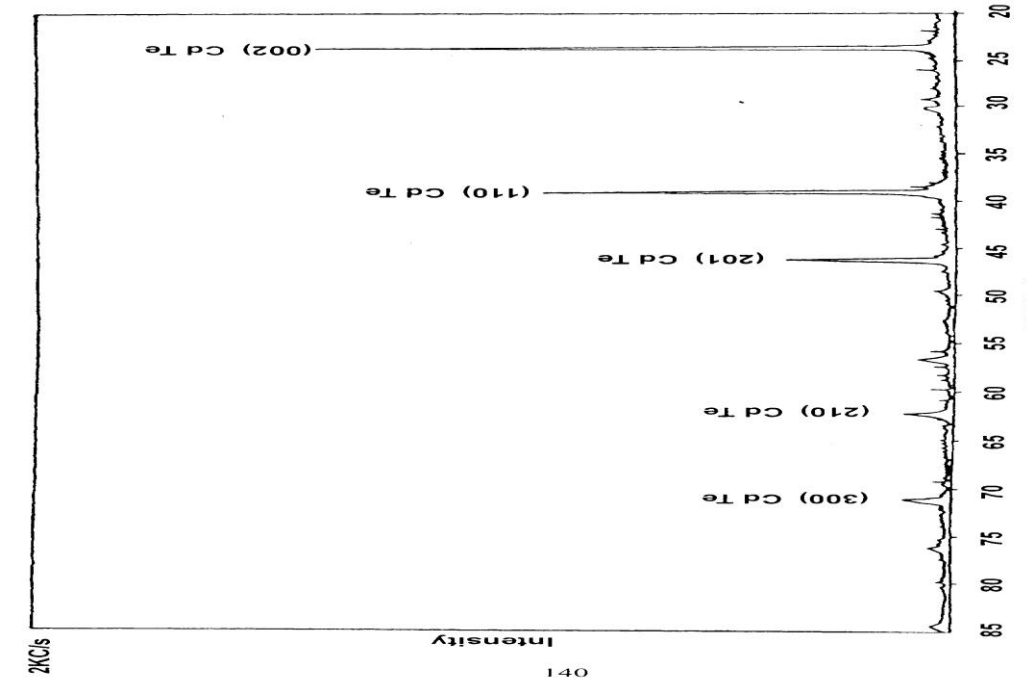

Fig. 6 : X-ray diffraction pattern of Cd Te sintered film.