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ESTIMATION OF 'x' IN $Cd_{1-x}Zn_xTe$ THIN FILMS USING X-RAY DIFFRACTION ANALYSIS

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ABSTRACT

In this work, thin films of $Cd_{1-x}Zn_xTe$ of 1µm and 100nm thickness are fabricated on plain glass substrates with 'x' varying from 0.0567 to 0.2210. These fabricated films are subjected to X-Ray Diffracton (XRD) studies. A methodology has been developed in this paper for determining the stoichiometric value 'x' in $Cd_{1-x}Zn_xTe$ 1µm and 100nm thin films from XRD analysis. Evaluated values of 'x' obtained from XRD analysis are compared with experimentally designed values of 'x' for these fabricated films. The values of 'x' obtained from the developed method are well matched with the experimentally designed values of 'x' for $Cd_{1-x}Zn_xTe$ 1µm thin films as compared to $Cd_{1-x}Zn_xTe$ 100 nm thin films.

Keywords - **$Cd_{1-x}Zn_xTe$, Stoichiometric value, Thin films, X-Ray Diffraction (XRD) analysis.**

I. INTRODUCTION

High resistivity II-VI semiconductor compounds e.g. ZnTe, CdTe and their alloys $Cd_{1-x}Zn_xTe$ with stoichiometric value 'x' are the potential materials used for optoelectronic devices [1-5]. Introduction of Zn into CdTe makes the lattice of $Cd_{1-x}Zn_xTe$ tunable, by adjusting the Cd/Zn ratio [6]. The value of 'x' in $Cd_{1-x}Zn_xTe$ lies between 0 and 1. In case of 'x' = 1, the material is ZnTe and in case of 'x' = 0, the material is CdTe. So, the properties of $Cd_{1-x}Zn_xTe$ film vary with the concentration of 'x'. So, determination of 'x' in the CZT matrix is an important aspect. Determination of 'x' from the empirical relation between 'x' and band gap of the material is a well known method [7]. In this paper, a methodology has been developed for determining the value of 'x', embedded in $Cd_{1-x}Zn_xTe$ 1µm and 100nm thin films from X-ray Diffraction (XRD) analysis.

Designable semiconductor band gap is helpful for controlling the resistivity as well as the valence and conduction band alignment at the semiconductor interface. In the recent years, major attention has been given to the investigation of electrical, optical and structural properties of $Cd_{1-x}Zn_xTe$ thin films in order to improve the performance of the device and also for finding new applications. Owing to extensive research and industrial work conducted by teams of solid-state physicists, engineers and medical physicists, CdTe/CZT detectors are now widely used. CdTe/CZT-based surgery probes have large impact on patient management in surgical oncology. Excellent large-field of view modules have already been realized as reported in [8]. The performance of a CZT dual Positron Emission Tomography (PET), dedicated for breast cancer, is studied by a group of researchers and these are reported in [9].

Studies in [10] report on dedicated emission mammotomography with CZT imaging detector. A comprehensive review of the material properties of $Cd_{1-x}Zn_xTe$ with varying zinc content is reported in [11]. Some studies on the structural and optical properties of II-VI compound semiconductors are proposed previously and these are reported in [12-22]. The range of 'x' in $Cd_{1-x}Zn_xTe$ lies preferably within $0.05 \leq$ 'x' ≤ 0.95 [19, 23].

In this work, proper methods are adopted to fabricate $Cd_{1-x}Zn_xTe$ thin films of 1µm and 100nm thickness and these are discussed in section II of this paper. The mathematical calculation for obtaining experimentally designed value of 'x' is discussed in section III of this paper. A new methodology has been developed in this work for determining 'x', in $Cd_{1-x}Zn_xTe$ 1µm and 100nm thin films from XRD results and this is discussed in section IV of this paper. The significance of the results of this work is discussed in section V of this paper. The work is concluded in section VI of this paper.

II. MATERIALS AND METHODS

In this work, physical deposition method is adopted to fabricate large area $Cd_{1-x}Zn_xTe$ thin films of 1µm and 100nm thickness. Surface cleaning of the substrate has predominant effect on the growth of the film on it. Thus prior to deposition, glass substrates are carefully cleaned. Commercially available glass slides of dimensions 23 mm x 37 mm x 1 mm are dipped in chromic acid for two hours. These are washed with detergent and finally ultrasonically cleaned with acetone before use.

In order to design the six different compositions of $Cd_{1-x}Zn_xTe$ thin films of 1µm and 100nm thickness, six different % ratio of the stack layer of ZnTe/CdTe is chosen and these are 20:80, 30:70, 40:60, 50:50, 60:40 and 70:30. For these six ratios of the stack layer of ZnTe/CdTe, six different values of 'x' are obtained. The mathematical detail is discussed with a sample calculation in section III of this paper.

For the film fabrication, 500W RF Sputtering unit has been used. ZnTe and CdTe targets are placed in the target holders of the RF sputtering unit. Plain glass substrates are kept at the bottom of the target holder and temperature to the order of 100°C is maintained on the substrates. Argon gas is injected from outside and pressure of the order of 10^{-2} Torr has been maintained. At this pressure, the RF unit is energized and a power of 500W with

a frequency of 13.56 MHz is applied between the target and the substrate. On application of this RF power the target gets energized and vapour of the target material produced deposits on the substrate. At the substrate temperature the film gets crystallized and the thickness is dependent on the sputtering time. Both CdTe and ZnTe targets are sputtered sequentially and a stack layer of ZnTe/CdTe is thus obtained. The stack layer is then annealed in vacuum (10^{-5} Torr) for an hour at 300°C. Both Cadmium and Zinc tried to inter-diffuse among each other to get into a stabilized state. Applications of thermal energy initiate both cadmium and zinc inter-diffusion. However, the stoichiometric ratio of cadmium and zinc is not equal and as a result the film is formed in the form of $Cd_{1-x}Zn_xTe$. The value of 'x' decides whether the film is CdTe or ZnTe. Thickness and deposition time for CdTe and ZnTe layers for each composition of $Cd_{1-x}Zn_xTe$ films of 1µm thickness are tabulated in Table 1(a). Similarly, thickness and deposition time for CdTe and ZnTe layers for each composition of $Cd_{1-x}Zn_xTe$ 100nm thin films are tabulated in Table 1(b).

III. SAMPLE CALCULATION OF 'X'

In this section, the mathematics to determine 'x' in $Cd_{1-x}Zn_xTe$ film is discussed with a sample calculation. For this purpose, one out of the six samples is considered and this is a 1µm stack of CZT comprised of ZnTe film deposited on CdTe film. Percentage thickness ratio of ZnTe : CdTe layer is 60:40 and this can be expressed as given in Eq. (1.1).

$$\frac{\%ZnTe}{\%CdTe}=\frac{60}{40}=\frac{n_{ZnTe}}{n_{CdTe}}=\frac{\frac{m_{ZnTe}}{M_{ZnTe}}}{\frac{m_{CdTe}}{M_{CdTe}}} \quad (1.1)$$

where,
m_{ZnTe} and m_{CdTe} are the masses of ZnTe and CdTe layers respectively to attain the % ratio ZnTe : CdTe as 60:40.
M_{ZnTe} and M_{CdTe} are the molar masses of ZnTe and CdTe respectively and these values are M_{ZnTe} =193 gms/mol and M_{CdTe}=240 gms/mol. On putting these values, Eq. (1.1) becomes,

$$1.5=\frac{\rho_{ZnTe}.T_{ZnTe}.A.240}{\rho_{CdTe}.T_{CdTe}.A.193} \quad (1.2)$$

where,
'A' is the cross-sectional area of the substrate. ρ_{ZnTe} and ρ_{CdTe} are the density of ZnTe and CdTe layers respectively and these values are ρ_{ZnTe} = 6.34 gms/cc and ρ_{CdTe}=5.85 gms/cc. T_{ZnTe} and T_{CdTe} are the values of thickness of ZnTe and CdTe layers respectively. On putting these values, Eq. (1.2) becomes,

$$\frac{T_{ZnTe}}{T_{CdTe}}=1.113022477 \quad (1.3)$$

$$T_{ZnTe}+T_{CdTe}=1\mu m \quad (1.4)$$

Solution of Eq. (1.3) and Eq. (1.4) gives the values of the thickness of CdTe and ZnTe layers and these are,
T_{CdTe} = 473.26 nm and T_{ZnTe} = 526.74 nm. (1.5 a)
Deposition rates for CdTe and ZnTe targets are 78 nm/min and 45 nm/min respectively. (1.5 b)
From Eq. (1.5 a) and Eq. (1.5 b) the deposition times for CdTe and ZnTe layers for this sample are obtained and these values are t_{CdTe} = 6 mins 4 sec and t_{ZnTe} = 11 mins 42 sec respectively. (1.5 c)
So, mass of ZnTe layer, $m_{ZnTe} = 3339.53.A.10^{-7}$ gms
and mass of CdTe layer, $m_{CdTe} = 2768.57.A.10^{-7}$ gms.
Molar mass of Zinc, M_{Zn} = 65.38 gms/mol.
So, $1139.29.A.10^{-7}$ gms of zinc is present in $3339.53.A.10^{-7}$ gms of ZnTe.
∴ Fraction of zinc in this CZT matrix

$$=\frac{1139.29.A.10^{-7}}{(2768.57+3339.53).A.10^{-7}}=0.1865 \quad (1.6)$$

Similarly, for other % ratios of ZnTe : CdTe layers for both the thickness domains considered in this study, the values of 'x' are calculated and these results are tabulated in Table 1(a) and Table 1(b).

Table 1(a) Thickness and Deposition Times of ZnTe and CdTe layers in 1µm CZT Films

S..No.	(%ZnTe):(%CdTe)	Thickness of ZnTe layer T_{ZnTe} (nm)	Thickness of CdTe layer T_{CdTe} (nm)	Deposition time of CdTe layer t_{CdTe}	Deposition time of ZnTe layer t_{ZnTe}	Fraction of Zinc in CZT matrix, 'x'
1	20:80	156.48	843.52	10 mins 49 sec	3 mins 29 sec	0.0567
2	30:70	241.29	758.71	9 mins 44 sec	5 mins 22 sec	0.0870
3	40:60	330.97	669.03	8 mins 35 sec	7 mins 21 sec	0.1182
4	50:50	425.95	574.05	7 mins 22 sec	9 mins 28 sec	0.1510
5	60:40	526.74	473.26	6 mins 4 sec	11 mins 42 sec	0.1865
6	70:30	633.88	366.12	4 mins 42 sec	14 mins 5 sec	0.2210

Table 1(b) Thickness and Deposition Times of ZnTe and CdTe layers in 100 nm CZT Films

S.No.	(%ZnTe):(%CdTe)	Thickness of ZnTe layer T_{ZnTe} (nm)	Thickness of CdTe layer T_{CdTe} (nm)	Deposition time for CdTe layer t_{CdTe}	Deposition time for ZnTe layer t_{ZnTe}	Fraction of Zinc in CZT matrix, 'x'
1	20:80	15.65	84.35	1 min 5 sec	21 sec	0.0567
2	30:70	24.13	75.87	58 sec	32 sec	0.0870
3	40:60	33.10	66.90	51 sec	44 sec	0.1182
4	50:50	42.60	57.40	44 sec	57 sec	0.1510
5	60:40	52.67	47.33	36 sec	1 min 10 sec	0.1865
6	70:30	63.39	36.61	28 sec	1 min 25 sec	0.2210

IV. DETERMINATION OF 'X' FROM XRD ANALYSIS

X-ray diffraction (XRD) spectra of the fabricated films are recorded on Rigaku Miniflex (Japan) powder diffractometer using Cu Kα radiation (1.5406 Å). The scanning angle range, 2θ of the diffractometer, is from 20º to 70º. XRD spectra of $Cd_{1-x}Zn_xTe$ 1µm and 100 nm thin films for the composition at 'x' = 0.1865 are shown in Fig. 1(a) and Fig. 1(b) respectively as sample results.

At constant temperature, crystal lattice constant of an alloy bears a linear relationship with the concentrations of the constituent elements [24]. For a simple cubic lattice, the lattice constant bears a relation with d-value where'd' is the spacing between adjacent parallel planes [25]. So, this implies that the 2θ values of the peaks of $Cd_{1-x}Zn_xTe$ 1µm and 100 nm thin films at 'x' = 0.1865, as shown in Fig. 1 (a) and Fig. 1(b) respectively will lie in between the 2θ values of the peaks of the corresponding planes of CdTe and ZnTe cubic crystals. On the basis of this idea and standard JCPDS files, CZT peaks in the XRD spectra of $Cd_{1-x}Zn_xTe$ 1µm and 100 nm thin films at 'x' = 0.1865 are identified and the details of these results are tabulated in Table 2(a) and Table 3(a) respectively. Peaks other than CZT are also identified in the XRD spectra of $Cd_{1-x}Zn_xTe$ 1µm and 100 nm thin films at 'x' = 0.1865 and the details of these results are tabulated in Table 2(b) and Table 3(b) respectively. Similarly, for other values of 'x', XRD spectra are obtained for both $Cd_{1-x}Zn_xTe$ 1µm and 100 nm thin films and in those XRD spectra, CZT and other peaks are identified.

Also, on the basis of this idea, a method has been developed in this work to determine the value of 'x' in $Cd_{1-x}Zn_xTe$ 1µm and 100 nm thin films. The calculations of 'x' from XRD analysis of $Cd_{1-x}Zn_xTe$ 1µm and 100 nm thin films for experimentally designed value of 'x' = 0.1865, are explained in Table 4(a) and Table 4(b) respectively as sample results.

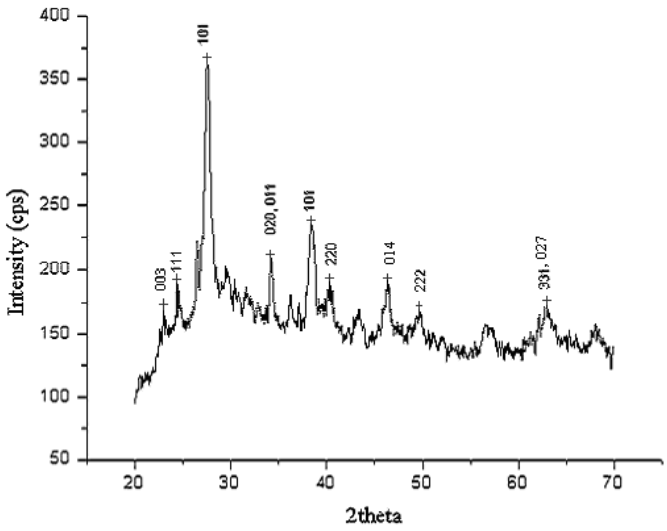

Fig. 1(a) XRD spectra of 1µm $Cd_{1-x}Zn_xTe$ thin film at 'x' = 0.1865

Table 2(a) Details of CZT peaks in $Cd_{1-x}Zn_xTe$ 1µm thin film at 'x' = 0.1865

S. No.	Peak No.	2theta (deg)	I/Io	Planes	JCPDS Card No.
1	5	24.02	14	003	CZT-471296
2	6	24.47	18	111	CdTe-752083-ZnTe 800022
3	15	40.37	26	220	CdTe-752083-ZnTe 800022
4	15	40.37	26	220	CZT-471296
5	21	49.64	18	222	CdTe-752083-ZnTe 752085
6	28	63.62	8	027	CZT-471296
7	28	63.62	8	331	CdTe-752083-ZnTe 800022

Table 2(b) Details of other peaks in $Cd_{1-x}Zn_xTe$ 1µm thin film at 'x' = 0.1865

S. No.	Peak No.	2theta (deg)	I/Io	Planes	JCPDS Card No.
1	8	27.56	100	101	Te-850555
2	13	38.33	33	101	Cd-851328
3	10	35.19	10	020, 011	CdTe-410941
4	19	46.49	15	014	ZnTe-830966

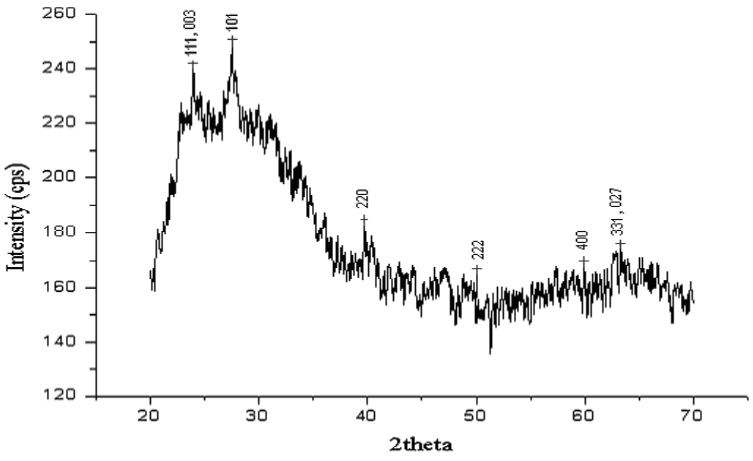

Fig. 1(b) XRD spectra of $Cd_{1-x}Zn_xTe$ 100 nm thin film at 'x' = 0.1865

Table 3(a) Details of CZT peaks in $Cd_{1-x}Zn_xTe$ 100 nm thin film at 'x' = 0.1865

S. No.	Peak No.	2theta (deg)	I/Io	Planes	JCPDS Card No.
1	3	23.93	89	111	CdTe-150770-ZnTe-800022
2	3	23.93	89	003	CZT- 471296
3	10	39.68	62	220	CdTe-150770-ZnTe-800022
4	10	39.68	62	220	CZT- 471296
5	13	49.82	48	222	CdTe-752083-ZnTe-800002
6	16	59.93	58	400	CdTe-752083-ZnTe-800022
7	21	62.93	47	331	CdTe-150770-ZnTe-752085
8	21	62.93	47	027	CZT- 471296

Table 3(b) Details of other peak in $Cd_{1-x}Zn_xTe$ 100 nm thin film at 'x' = 0.1865

S. No.	Peak No.	2theta (deg)	I/Io	Planes	JCPDS Card no
1	6	27.47	100	101	Te-850555

Table 4(a): Determination of 'x' from XRD analysis of $Cd_{1-x}Zn_xTe$ 1µm thin film with experimentally designed value of 'x' = 0.1865

S. No.	Peak no.	d-value	planes	JCPDS Card no. for CdTe & ZnTe	$'x' = \frac{d_{Cd_{1-x}Zn_xTe} - d_{CdTe}}{d_{ZnTe} - d_{CdTe}}$
1	6	3.6346	111	CdTe-75-2083-ZnTe 80-0022	0.3140
2	15	2.2323	220	CdTe-75-2083-ZnTe 80-0022	0.2628
3	21	1.8350	222	CdTe-75-2083-ZnTe 75-2085	0.1568
4	28	1.4613	331	CdTe-75-2083-ZnTe 80-0022	0.1099

Average value of 'x' obtained from XRD Analysis of $Cd_{1-x}Zn_xTe$ 1µm thin film is 0.2109

Table 4(b): Determination of 'x' from XRD analysis of $Cd_{1-x}Zn_xTe$ 100 nm thin film with experimentally designed value of 'x' = 0.1865

S. No.	peak no.	d-value	planes	JCPDS Card no. for CdTe & ZnTe	'x'= $\frac{d_{Cd_{1-x}Zn_xTe} - d_{CdTe}}{d_{ZnTe} - d_{CdTe}}$
1	3	3.7154	111	CdTe-150770-ZnTe 800022	0.1056
2	10	2.2695	220	CdTe-150770-ZnTe 800022	0.1342
3	13	1.8287	222	CdTe-752083-ZnTe-800002	0.2059
4	16	1.5421	400	CdTe-150770-ZnTe-800022	0.7134
5	21	1.4756	331	CdTe-150770-ZnTe-752085	0.1298

Average value of 'x' obtained from XRD Analysis of $Cd_{1-x}Zn_xTe$ 100 nm thin film is 0.2578.

Similarly, for all other compositions of $Cd_{1-x}Zn_xTe$ 1µm and 100 nm thin films, the average values of 'x' are obtained from XRD analysis. Experimentally designed values of 'x' and the values of 'x' obtained from this developed method based on XRD analysis are tabulated in Table 4(c) for all the samples of $Cd_{1-x}Zn_xTe$ 1µm and 100 nm thin films.

Table 4(c): Comparison of 'x'

S. No.	Experimentally designed value of 'x'	'x' obtained from XRD analysis of $Cd_{1-x}Zn_xTe$ 1µm thin film	'x' obtained from XRD analysis of $Cd_{1-x}Zn_xTe$ 100 nm thin film
1	0.0567	0.0604	0.1763
2	0.0870	0.1064	0.1806
3	0.1182	0.1221	0.2256
4	0.1510	0.1482	0.2538
5	0.1865	0.2109	0.2578
6	0.2210	0.2247	0.2887

V. DISCUSSIONS

In the X-Ray Diffraction (XRD) patterns of $Cd_{1-x}Zn_xTe$ 1µm and 100 nm thin films, for 'x' varying from 0.0567 to 0.2210, the peaks for CZT along with other peaks are identified as discussed in section IV of this paper. Some peaks are found to lie between those for CdTe and ZnTe. The methodology that has been developed in this paper, for determining the value of 'x' in $Cd_{1-x}Zn_xTe$ thin films from XRD analysis, has given results as discussed in section IV of this paper and these are in good agreement with experimentally designed values of 'x' as observed in Table 4 (c). This developed method for evaluation of 'x' from XRD analysis has given better results for $Cd_{1-x}Zn_xTe$ 1µm thin films as compared to $Cd_{1-x}Zn_xTe$ 100 nm thin films. This may be due to the predominance of two-dimensional effect on $Cd_{1-x}Zn_xTe$ 1µm thin films over 100 nm thin films[21].

VI. CONCLUSION

This study infers that evaluation of 'x' from XRD analysis based on the methodology developed in this work has given results which are in good agreement with experimentally designed values of 'x'. The values of 'x' obtained from this developed method are better matched with the experimentally designed values of 'x' for $Cd_{1-x}Zn_xTe$ 1µm thin films as compared to $Cd_{1-x}Zn_xTe$ 100 nm thin films.

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