INVESTIGATION ON COMPOSITIONAL, OPTICAL AND STRUCTURAL PROPERTIES OF $Cd_{1-x}Zn_xTe$ THIN FILMS FOR PHOTOVOLTAICS

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ABSTRACT- *Polycrystalline semiconductors belonging to group II-VI have come under improved inspection due to the fact of their cost reduction for the applications in photovoltaic devices. These are auspicious materials for efficacious devices such as photovoltaics (Solar cells) and optoelectronics (X-ray and Gamma-ray detectors). Among the group II-VI semiconducting materials, $Cd_{1-X}Zn_XTe$(CZT) have achieved great attention in bandgap tailoring as we have tailored its bandgap to the value between 1.48-2.26eV by varying the 'Zn' content i.e, varying the value of 'X' from 0 to 1. Thin films of CZT having variable compositions ($0 \leq X \leq 1$) has been deposited on ultrasonically cleaned substrates (glass) using thermal evaporation technique in the high vacuum conditions i.e, 10^{-6} torr. The optical (UV-Vis spectrscopy), compositional (Energy dispersive analysis of X-rays) and structural properties (X-ray diffractometry) of CZT's thin films have been inspected. The bandgaps of these films were calculated by drawing graphs between the values of energy E(eV) and $(\alpha h\nu)^2$ by using UV-Vis spectrophotometer's data. X-ray diffraction patterns determined the structural analysis of these thin films after deposition. The entire range of as deposited films were studied, the nature of thin films were polycrystalline in bearing zinc blend (111). The results obtained by our current investigation will be exploited in utilizing the material (CZT) for its applications in photovoltaics.*

Keywords: Photovoltaics, CZT, Thermal Evaporation Technique, UV-Visible Spectroscopy, EDX, XRD.

INTRODUCTION:

In the wide spectrum of optoelectronics devices, the potential knacks of compound semiconductors are collecting a great deal of attention in recent era [1]. We can tailor the properties of these ternary compounds by tailoring the bandgaps and hence bulging these compounds as significant materials for future progressions within the field of device fabrication like solar cells, X-Ray and gamma-ray detectors, electro-Optical modulators, LED's, nuclear radiation detectors etc [1-3]. The $Cd_{1-x}Zn_xTe$ ($0 \leq X \leq 1$) is a ternary semiconductor alloy formed when 'Cd' is replaced by 'Zn' and having Zinc blende-type structure (111). Various desirable properties such as bandgap tuneability, lattice parameter with alloy composition and high values of transmittance can be achieved. These characteristics have gained the attraction of many scientists and researchers to perform experiments with this material [3-5].

$Cd_{1-x}Zn_xTe$'s bandgap lies within the range of 1.48-2.26eV depending on the percentage of 'Zn' content. $Cd_{1-x}Zn_xTe$ is the best material for top cell structure in solar cells owing to the low leakage of currents and high quantum efficiencies which empowers the operation of photovoltaics (Solar cells) and other detectors (gamma-ray & X-ray) most probably at room temperature [5]. $Cd_{1-x}Zn_xTe$ thin films having bandgap in the range of 1.65-1.75eV are best suitable for its use in tandem solar cells' structure[2] particularly for absorber layer which must have longer carrier life time, large absorption co-efficient[7] and lower carrier mobility as compared to the window layer[6-8].

Thermal evaporation is used for deposition of $Cd_{1-x}Zn_xTe$ thin films onto glass substrates. Thermal evaporation has several advantages like high growth rates and high efficiency of material utilization [6].

EXPERIMENTAL DETAILS:

In the current investigation, the thin films of $Cd_{1-x}Zn_xTe$ with different compositions of 'Zn' were deposited by using the thermal evaporation under high vacuum [9]. The $Cd_{1-x}Zn_xTe$ alloy was prepared by mixing the powders mechanically with the help of mortar and pestle for 90min for each composition to get uniformly mixed powders while taking into account the stoichiometric ratios of compounds (CdTe and ZnTe).

The two compounds in finally mixed powder form have been taken as follows;

Weight of CdTe = $240(1 - X)$ g,

Weight of ZnTe = 192.97 (X) g,

We reduced the weights by to a same factor (proportion) as these weights were large in quantity. Erstwhile to the development of thin films, the glass substrates (1×3 inch) were cleaned by detergent cleaning treatment for 10mins, ultrasonically cleaned in acetone bath for 30 min and then by Isopropyl-Alcohol for 15mins, finally dried them with an air gun. Thermal evaporation technique utilized the resistive heating by the passage of high electric current and a temperature of 530ºC-600ºC has been achieved using this technique under vacuum ~ 10^{-6} torr. Tantalum boat is used as container for source material i.e, finely mixed powder of $Cd_{1-x}Zn_xTe$ for the reason that it can withstand high temperature upto 1600ºC. 'He' gas was used as a filler as to sweep out the residual dust particles and other contaminations, inside the working chamber. Z-ratio was 0.875 and the growth rate was set at 5 Aº/s. All the films of $Cd_{1-x}Zn_xTe$ were deposited using the same conditions of the experiment.

The recorded spectra were in the wavelength range of 400–1100 nm, using a UV–Vis spectrometer (Model U-4300). X-ray diffractometer was used to determine the aspects about the structural properties. Compositions of these as deposited thin films were approved by energy dispersive X-rays' analysis (EDX) [9-10].

RESULTS AND DISCUSSIONS:

Samples were characterized as UV-Visible spectroscopy, X-ray diffractometry and Energy dispersive analysis of X-rays and results have been discussed to achieve the desired properties and described below.

UV-VIS Spectroscopy:

The determination of the bandgap was brought about while taking into consideration the graphs drawn between energy 'E'(eV) taken on x-axis and $(\alpha h\nu)^2$ which is of the order of 10^{-24} on y-axis. The conversion of transmittance values to the absorption coefficients was done while using the following mathematical relation (1),

$$\alpha = (1/d)\ln(100/T) \quad (1)$$

Where'd' is the film thickness that is of the order of 500nm and 'T' is representing transmittance values [11]. Almost all the compounds belonging to group II-VI are semiconductors with direct bandgaps. We can also calculate the absorption coefficient with the help of Tauc's relation [12], specified by (2),

$$\alpha h\nu = A(h\nu - E_g)^n \quad (2)$$

Where 'hν' be the energy of photons, for different transitions, the constant 'A' should have different values, E_g be the value of bandgap. Finally, the bandgap calculation was done using the graphs drawn in Fig:1, for different values of absorption and for different compositions as in the following graphs.

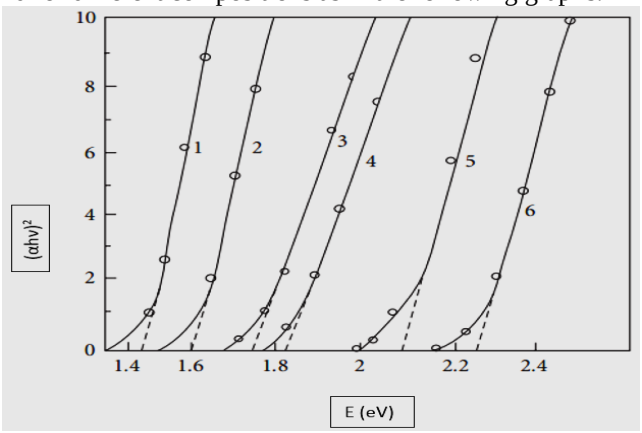

Fig1: Graphs drawn between Energy(E) and $(\alpha h\nu)^2$ for bandgap calculations as compositions of 1(x=0), 2(x=0.2), 3(x=0.4), 4(x=0.6), 5(x=0.8) & 6(x=1).

We have noted an incremental enhancement in the bandgap of CZT's thin films by increasing the value of 'x' i.e, Zn-content (shown in Fig:2) within the compound $Cd_{1-X}Zn_XTe$ which is the main goal of our project as to cover a broad range of E-M spectrum for the better efficiency of solar cell as its major application. The variation in the bandgap was in the range of 1.48-2.26 eV which is in agreement with the literature [13].

This analysis revealed the fact that despite of its least sticking coefficient of about 5%, 'Zn' content having numerous quantity is present within the mixture. By the disparity of composition in this way we can control the stochiometry of these types of compound semiconductors while tailoring their bandgaps with the replacement of 'Cd' by 'Zn' which later on will be proved to be the one of cheaper and easier techniques.

This image of EDX analysis was taken for the composition($Cd_{1-X}Zn_XTe$) x =0.2 as shown in Fig(3), and it was noted that for greater concentrations of 'x' i.e, 0.4, 0.6, 0.8 and 1 there noted a sharpness in the peaks given by the same elemental analysis.

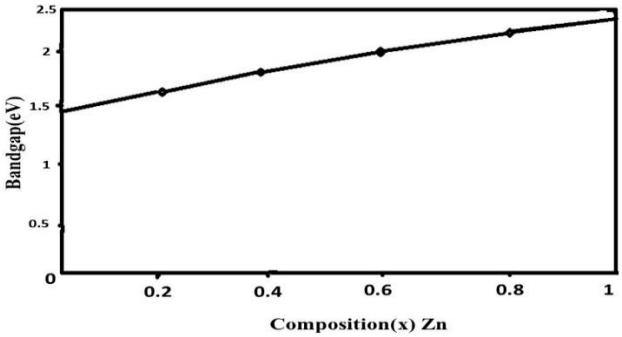

Fig 2: Variation of bandgap by increasing 'Zn' content in $Cd_{1-X}Zn_XTe$ alloy

Energy dispersive analysis of X-rays (EDX):

Element	Atomic%
Te (L)	53.78
Cd (L)	42.07
Zn (K)	4.13

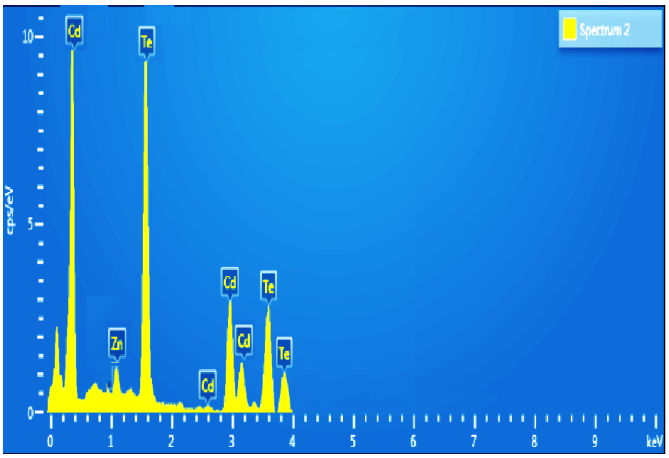

Fig 3: EDAX of thin film of $Cd_{1-X}Zn_XTe$ at X = 0.2

The EDAX provided us the Wt% values for the individual elements and we have converted these values into atomic% using the particular conversion formulae and finally calculated percentages are given above adjacent to the EDAX's image.

Analysis of XRD patterns:

The analysis of X-ray diffraction (XRD), was conceded on these samples and were analysed to collect data about different crystallographic features. At room temperature, traces of XRD for all of the samples were obtained and these traces found to show nearly the same trends. The XRD patterns of composition $Cd_{0.8}Zn_{0.2}Te$ and Cd_0Zn_1Te have shown here in fig4 (a)(b).

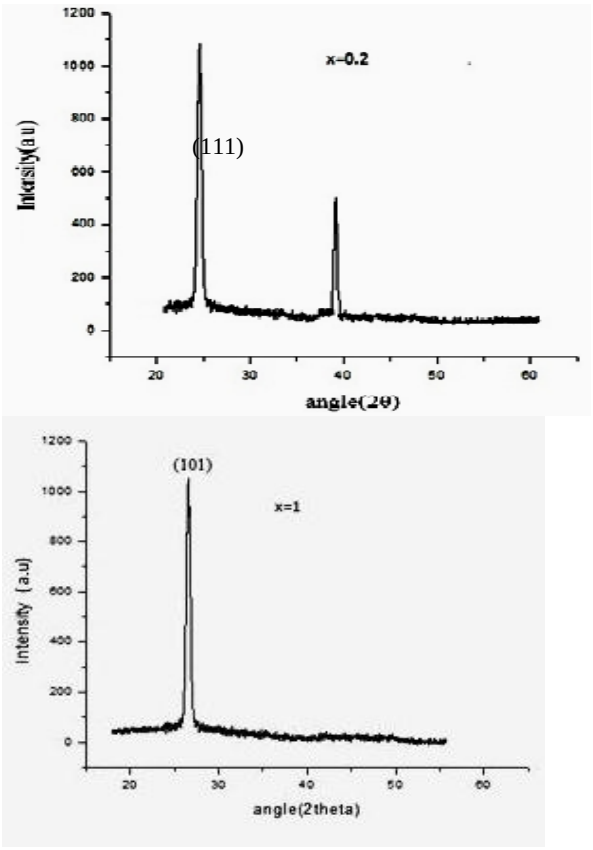

Fig 4 (a)(b): XRD plot of $Cd_{1-X}Zn_XTe$ thin films at X = 0.2 & X = 1 respectively, as angle(2θ) against Intensity(a.u)

The preferential orientation of thin films is cubic (111) plane for the 'Zn' concentration upto x=0.8, also contains the hexagonal (Wurtzite) crystal structure for x=1 i.e,(101) for pure ZnTe shown in fig4(b), also these orientations inveterate the nature of these thin films as polycrystalline. The shifting of the peak is due to the generation of stresses within the lattice caused by the replacement of 'Cd' atom by 'Zn' as the phase changes due the numerous quantities of as deposited Zn-content. The deposition of thin films was done under high vacuum conditions so there is no Oxidation of CdTe or ZnTe peaks within the graph bearing XRD analysis. XRD scans are produced for $Cd_{1-X}Zn_XTe$ (at x = 0.2 & x = 1) and Shown in fig 4(a)(b).

CONCLUSIONS AND FUTURE WORK

The nexus of our investigation is to explore the optical, compositional and structural properties of $Cd_{1-X}Zn_XTe$'s pseudo binary thin films. Thin films of $Cd_{1-X}Zn_XTe$ have high absorption coefficients and their bandgaps can be tailored or altered to any value between 1.48 to 2.26eV by varying 'X' from 0 to 1 i.e, varying the 'Zn' content within the alloy or overall concentration($Cd_{1-X}Zn_XTe$). The property of tailoring the bandgaps is suitable for the proficient absorption within the visible region of the solar spectrum that comprises of about 46% of the entire solar spectrum. Despite of having very least sticking coefficient of about 5%, Zinc was deposited in large amount without the utilization of any adhesive materials during the process of powder mixing. As far as the structural properties are concerned, all the thin films of $Cd_{1-X}Zn_XTe$ are found to have cubic (111) like Zn-blend structure bearing the polycrystalline nature. The thin films of $Cd_{1-X}Zn_XTe$ can be used as the best absorber layers for Solar cells, X-ray and Gamma-ray detectors and Electro-optic modulators etc.

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