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The Optical Parameters of $Zn_xCd_{(1-x)}Te$ Chalcogenide Thin Films

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ABSTRACT

A procedure to make optical quality thin films of $Zn_xCd_{(1-x)}$ Te by use of thermal evaporation of the ternary compound has been investigated. Structural and optical properties of $Zn_xCd_{(1-x)}$ Te solid solution with x = 0.1 to 0.5 were synthesized, from the resulting ZnTe and CdTe composition used in preparation of thin films. Structural investigation indicates they have polycrystalline structure. Composition was confirmed from EDAX while SEM picture shows homogeneity in films. Plots of $(\alpha h\nu)^2$ versus $(h\nu)$ yield straight line indicating direct transition occurs with optical band gap energies in the range 1.7 - 2.3 eV. It is also found with increase Zn content the band gap of the films increases. Refractive indices and extinction coefficients have been evaluated in the spectral range (200 - 2500 nm).

Keywords*: *Thermal Evaporation, EDAX, XRD, Optical Band Gap

1. Introduction

Solid solution formation in semiconductors has been of interest for a number of years. An important question regarding ternary zinc-blende compound semiconductors is concerned with the structural and dynamic changes that can occur upon replacement of either cations or anions in the binary base material The II-VI compounds semiconductors and solid solutions based on them are promising source for various types of thin film devices such as thin film transistors [1], Solar cells [2] and photoconductors [3].

Thin films of $Zn_xCd_{(1-x)}Te$ were prepared by variety of techniques, such as, two source vacuum evaporation [6], molecular beam epitaxy [7], chemical vapour deposition and closed space vapour transport [8,9], physical vapour transport (PVT) [10], vertical Bridgman growth [11]. In the recent study $Zn_xCd_{(1-x)}Te$ thin films are deposited by thermal evaporation at substrate temperature (373 K) and the films are annealed and then characterized by energy dispersive X-ray analysis (EDAX) and scanning electron microscopy (SEM) technique for composition and surface morphology of the films. Optical properties of the films were studied by optical transmittance and reflectance measurement.

2. Experimental Details

For the preparation of ternary semiconductors, $Zn_xCd_{(1-x)}$ Te the constituent compounds ZnTe (Purity - 99.999%, Aldrich Co. Make, USA) and CdTe (Purity - 99.99+%, Aldrich Make, USA) have been taken in molecular stiochoimetry proportional weights and crushed and mixed homogenously. The different sets of samples of varying compositions (x = 0.1 to 0.5) were deposited via sublimation of the compound in vacuum higher than 10^{-5} mbar under controlled growth conditions of various compositions onto the amorphous precleaned glass substrates at the temperature of 373 K. The thicknesses of films were controlled by using quartz crystal thickness monitor model No.DTM-101 provided by Hind-High Vac. The deposition rate was maintained 10-15 Å/sec constant throughout sample preparations. The source to substrate distance was kept constant (15 cm) and substrate was kept at constant temperature (373 K). Deposited samples were kept under vacuum overnight. All the samples are deposited under the similar optimized condition. These samples were annealed at reduced pressure of 10^{-5} mbar for the duration of 3 hours at the temperature of 573 K and maintain carefully. These samples were then used for various characterizations. X-ray diffraction (XRD) studies were carried out using a Rigaku, Miniflex, Japan X-ray diffractometer. The XRD patterns were recorded in the 2θ range of 20˚ - 80˚ glancing angle 30˚ using CuKα radiation (λ = 1.5418 Å). The morphology of the $Zn_xCd_{(1-x)}Te$ thin films was examined using Scanning Electron Microscope (SEM) (model 501, Philips, Holland with EDAX attachment) using acceleration voltage variable from 1.6 KV to 30 KV. For this purpose thin layer of gold (50Å) was deposited on the film using physical vapour deposition. UV-Vis spectra of the samples were recorded on a HITACHI-MODEL-330 UV-Vis spectrophotometer in the wavelength range 200 - 2500 nm.

3. Results and Discussion

All the $Zn_xCd_{(1-x)}Te$ films prepared by the above technique were polycrystalline of multi phase structure indicating preferential of the film crystallites corresponding to textured (100)H and (220)C growth [14].

From the **Figure 1** X-ray diffractograms of various compositions it is observed that for x = 0.1 and x = 0.2 there are only two prime peaks which corresponds to (100) plane of hexagonal CdTe and (220) plane of cubic ZnTe [14]. Diffraction analysis suggests that all the samples of various compositions are polycrystalline nature. However the charactertics peak of hexagonal CdTe and cubic ZnTe changes their angular position and relative intensities for different compositions suggesting multi phases and inhomogeneity in the growth of films. The samples of compositions (x = 0.1, 0.2 and 0.4) exhibit predominant diffraction lines corresponding to (100) plane of CdTe (H) may be attributed to the characteristics growth with (100) reflecting plane as a preferred orientation. While the sample (x =0.3 and 0.5) exhibits pre- dominant diffraction lines corresponding to (111) plane of ZnTe (C) is again attributed to the charactertics growth with the (111) reflecting plane as preferred ori- entation. The shifting of peak positions of these promi- nent diffraction lines suggests the formation of solid so- lution corresponding to $Zn_xCd_{(1-x)}Te$ material from the basic starting compounds CdTe and ZnTe.

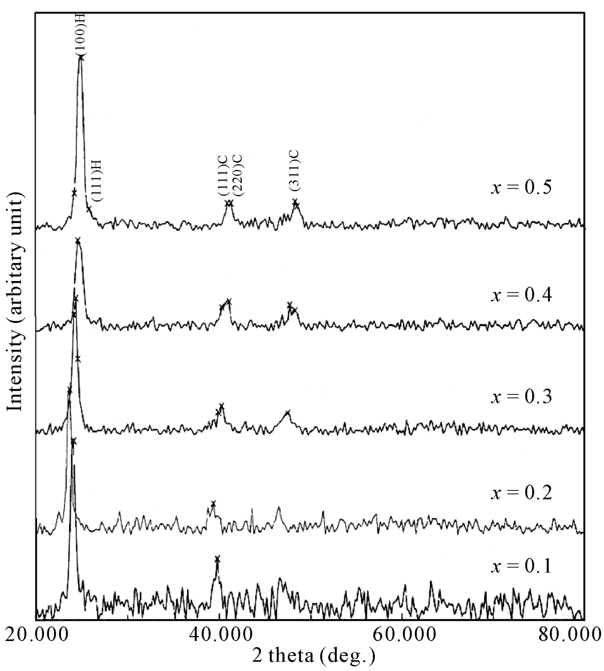

Figure 1. X-ray diffractograms of various $Zn_xCd_{(1-x)}Te$ structures.

From the scanning electron micrographs, it is found that the thicknesses of the films samples are too small to observed structure patterns. However films surfaces are very smooth. In all the compositions it has been observed that the reflectivity of the film gradually increases, which is quite natural that the reflectivity of the film is expected to increases with the increase of ‘x’ composition. The same observation as above shows the straitions, which are exactly parallel equidistance and extend from one end to another end. These straitions indicate the oscillatory growth [15], which indicate at the one end and terminate at the other end. It may be said that the oscillatory growth in the film which is manifested by straitions has been initiated by the presence of small composition of Zn (x = 0.1) in **Figure 2** and these oscillatory growth has been found to reduce successively with the composition x = 0.3 and x = 0.4. It is about reduce with composition of x = 0.5. The composition of starting basic ingredients and film composition comparison is presented in the **Table 1** and expressed in atomic percentages. The atomic percentage of basic ingredient seems to be in agreements with that obtain from EDAX analysis. From this table it is remarkable point to note that for composition (x = 0.3) the atomic percentage of basic ingredient taken is very close to atomic percentage obtain from EDAX spectra.

The reflectance and transmittance spectra of these sam-

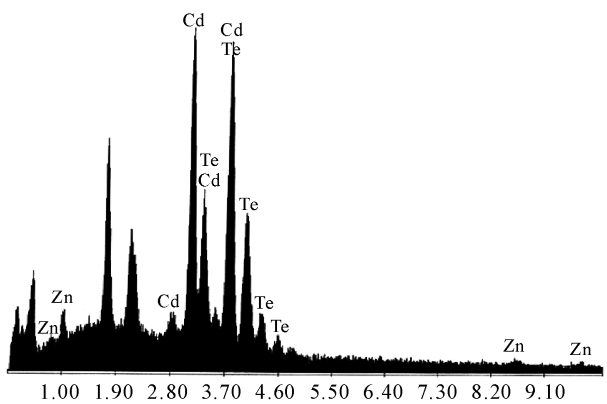

Figure 2. EDAX of ternary compound $Zn_xCd_{(1-x)}Te$ Thin Film. (x = 0.1).

Table 1. EDAX data for $Zn_xCd_{(1-x)}Te$ composite thin films.

Basic Ingredient Taken				EDAX Composition		
'x'	At% Zn	At% Cd	At% Te	At% Zn	At% Cd	At% Te
0.1	5	45	50	7.07	40.52	52.41
0.2	10	40	50	13.42	37.78	48.81
0.3	15	35	50	15.59	34.46	49.96
0.4	20	30	50	28.20	25.90	45.90
0.5	25	25	50	31.49	20.95	47.56

ples were recorded using Hitachi Spectrophotometer model-330 in spectral region 200 - 2500 nm. Using these data, the absorption coefficient α has been calculated by applying the relation [12]. Absorption coefficients have been evaluated using percentage transmittance data as a function of wavelength presented in **Figure 3** for the samples of different compositions. The plot of $(\alpha h\nu)^2$ versus $h\nu$ are plotted and shows clearly linear dependence for the value of $p = ½$. This is attributed to an allowed and direct transition with direct band gap energies. The evaluated band gap energies are 1.7 eV, 2.05 eV, 2.2 eV, 2.3 eV and 1.5 eV for the samples of compositions $x = 0.1$ to 0.5 respectively clearly indicating dependence on compositions of films. Band gap energies are to be composition dependent. Band gap energy increases with the increasing 'x', this is as expected as band gap energy for ZnTe is 2.26 eV and band gap energy for CdTe is 1.5 eV [16].

CdZnTe thin films of thickness 450 - 1400 nm have been evaporated under vacuum onto unheated glass substrates, using a multilayer method [17]. He reported variation of optical band gap between 1.16 and 1.63 eV. Band-to-band transitions which give rise to the optical absorption in the visible region of the spectrum may be interpreted in terms of direct allowed transition with the band gap in the range of 2.05 - 1.92 eV. [18]. The band gap energy of the films measured by optical transmittance measurement is 1.523 eV [14]. Polycrystalline thin films of CdZnTe and CdMnTe have been grown by molecular beam epitaxy and metal-organic chemical vapor deposition [19]. He reported with band gaps of 1.65 - 1.75 eV for the top of a two-cell tandem design. P-i-n cells were fabricated and tested using Ni/p^+-ZnTe as a back contact to the ternary films. CdTe cells were also fabricated using both growth techniques.

Near normal incidence reflectance and transmittance data have been used to determine optical constant 'n' and 'k' [13]. The variation of refractive indices and extinction coefficients as a function of wavelength as represented in **Figure 4** for the samples of compositions

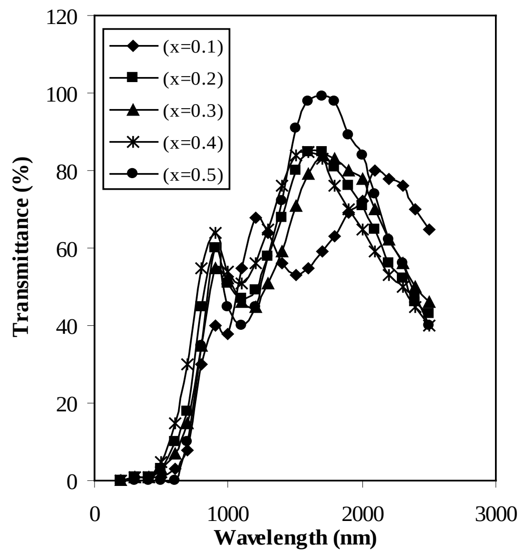

Figure 3. Spectral behaviour of transmittance with wavength.

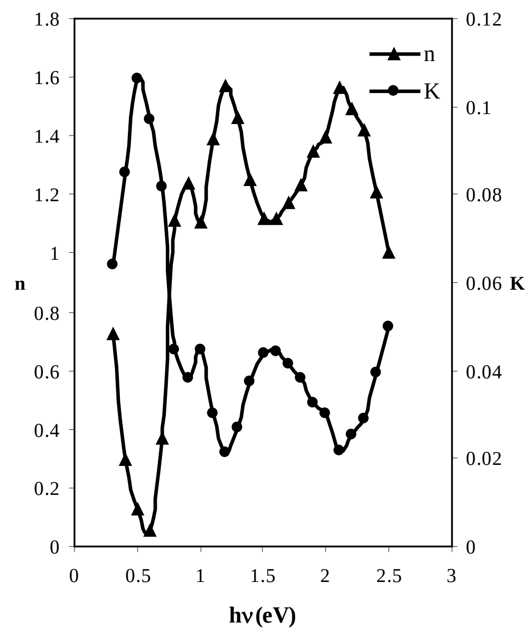

Figure 4. Variation of '*n*' and '*k*' with wavelength for $Zn_xCd_{(1-x)}Te$ ($x = 0.1$).

($x = 0.1$) It is found that variations in refractive indices and extinction coefficients are oscillatory in nature. Secondly variation in n and k seems to be complementary *i.e.* maxima of one and minima of the other at the same wavelength as estimated in **Table 2**.

Polycrystalline $Cd_{0.96}Zn_{0.04}Te$ thin films [20] were desited onto well-cleaned glass substrates kept at room temperature by vacuum evaporation. Optical properties of thin films were studied by optical transmittance meare-

Table 2. Well defined Maxima and Minima in variation of '*n*' and '*k*'.

Composition (x)	λ (μ)	Maxima		Minima	
		'*n*'	'*k*'	'*n*'	'*k*'
0.1	0.6	-	0.10	0.055	-
	0.9	1.23	-	-	0.038
	1	-	0.044	1.10	-
	1.2	1.57	-	-	0.021
	1.5	-	0.044	1.11	-
	2.1	1.56	-	-	0.021
0.2	0.4	-	0.076	1.84	-
	0.9	1.96	-	-	0.019
	1.2	-	0.035	1.92	-
	1.6	1.97	-	-	0.010
0.3	0.4	-	0.065	1.86	-
	0.9	1.96	-	-	0.019
	1.2	-	0.034	1.93	-
	1.7	1.97	-	-	0.010
0.4	0.4	-	0.078	1.84	-
	0.9	1.96	-	-	0.017
	1.1	-	0.031	1.93	-
	1.6	1.97	-	-	0.010
0.5	0.9	1.95	-	-	0.021
	1.1	-	0.046	1.90	-
	1.7	1.99	-	-	0.0007

ment and spectroscopic ellipsometry (SE). The spectra of various optical constants obtained from the SE ε(E) data (ε1, ε2, *R*, *n*, *k* and α) revealed three distinct critical points (E1, E1+Δ1 and E2). The band gap energy of the films determined by transmittance measurement was 1.523 eV at room temperature. He reported refractive indices 'n' varies between 2.4 to 2.6 and extinction coefficient '*k*' varies 0.5 to 1.

Optical properties of $Zn_xCd_{(1-x)}Se$ films [21]. He reported variation in n and k in the wavelength range 600 - 1000 nm is very close matching with present work. They also reported the band gap energy increases with increasing Zn component in $Zn_xCd_{(1-x)}Se$ films. At higher wavelengths the experimental results T and R satisfy the relationship T + R = 1. This indicates that neither absorption nor scattering of light occurs beyond the absorption edge. The appearance of maxima and minima results from interference effect and their number increases with increases film composition. These results are satisfactory and as theoretically expected.

4. Conclusions

- Homogeneous polycrystalline of multi phase structure of the thin films of $Zn_xCd_{(1-x)}Te$ have been successfully deposited by thermal evaporation technique using basic ingredient ZnTe and CdTe elemental starting materials.
- EDAX composition seems to be closely matched with starting basic ingredients.
- The dependence of the optical parameters of the films on the light energy supports the direct character of the interband transition through an optical band gap in the range 1.7 - 2.3 eV.
- The variation in optical constants as a function of wavelength is oscillatory in nature having well defined maxima and minima, which depends on the composition of the thin films.

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