Optical characterization of the $CdZnSe_{2x}Te2_{(1-x)}$ thin films deposited by spray pyrolysis method

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Abstract- $CdZnSe_{2x}Te_{2(1-x)}$ thin films for different composition parameters 'x' have been deposited on large substrate area by the spray pyrolysis method which is simple, inexpensive and economical at 300^o substrate temperature. From the optical transmission and reflection spectra, absorption coefficients were calculated . Band gap energy were determined from absorbance measurements in visible range using Tauc theory. Band gap energy values are found to lie in the range 2.04-2.52 eV for the films with composition parameter, x= 0 to 1. It shows that the main transition at the fundamental absorption edge is a direct allowed transition. The optical constants such as optical band gap, extinction coefficient, refractive index and dielectric constant have been calculated for these films The values obtained by this method are suitable for many scientific studies and technical applications such as solar cells, heat mirrors , transparent electrodes, piezoelectric devices, sensors etc.

Index Terms- thin films,spray pyrolysis,optical constants, band gap energy.

I. Introduction

The II-VI compounds such as CdTe, CdSe,ZnSe,ZnTe,CdZnSe,CdZnTe etc.are becoming more interesting and important because of their major contribution in solar cells[1] and various optoelectronic devices [2-5],field effect transistors[6],light emitting diodes [7-8] photocatalysts[9]. Cadmium zink selenide,one of the II-VI group semiconductor material,plays a prominent role in the modern material science and technology.CdZnSe and CdZnTe are n-type semiconductor materials having wide band gap covering maximum electromagnetic spectrum[10].

There are many methods of depositing II-VI alloy compounds such as thermal evaporation [11], vapour phase deposition of high quality II-VI alloy crystals[12],spray pyrolysis [13-20], electrodeposition[21],chemical bath deposition[22].

Spray pyrolysis technique is most simple and economical method. The advantage of the technique is that just by varying the concentration of precursors and substrate temperature, it is possible to control stoichiometry of the deposits. Hence the thin films of $CdZnSe_{2x}Te_{2(1-x)}$ have been prepared by spray pyrolysis technique.

We can determine direct or indirect band gap from optical absorption spectra. Absorption coefficient 'α'

Can be determine from relation $\alpha = (1/t)\ \ln(1/T)$, (1)

Where t- thickness of thin film and T- transmittance.

The evaluation of refractive index of optical material is of importance for applications in integrated optical devices such as modulators, filters where refractive index of material plays vital role in fabrication of these devices.

Aim of the study is to investigate optical properties of $CdZnSe_{2x}Te_{2(1-x)}$ thin films to calculate optical constants such as optical band gap, extinction coefficient ,refractive index and real and imaginary parts of dielectric constant.

II. Experimental

2.1 Materials:-

The deposition was carried out onto commercial available glass substrate. The chemicals used were of analytical reagent grade. Aqueous solutions (0.02M) of $ZnCl_2$, $CdCl_2$, $TeCl_4$ and SeO_2 were used for spraying the films. Composition parameter 'x' in $CdZnSe_{2x}Te_{2(1-x)}$ was varied as x= 0, .25 ,.50, .75, 1 in steps and films were deposited on glass substrate. Temperature of substrate was maintain at 300^0C and was measured by precaliberated opper constantan thermocouple. Spray rate was maintained at 3.5 ml/min. and spraying was done in air at 12 Kg/Cm^2 pressure. The sprayer was mechanically moved to and fro to avoid formation of droplets on the substrate and to ensure the instant evaporation from the substrate. The films were allowed to cool at room temperature. The thickness of the films were calculated by weighing the glass substrate before and after deposition on unipan- microbalance. The density of mixed crystal film material formed on the glass substrate was calculated by adding the standard densities of CdZnSe and CdZnTe in proportion to x and 1-x. The thickness of film so obtained was of the order of 0.1730 μm. The colour of the film changes from whitish to grey as composition parameter changes from 0 to 1.

2.2 Optical measurements:-

The optical absorption spectra of $CdZnSe_{2x}Te_{2(1-x)}$ thin films at room temperature were obtained on shimadzu uv-1800 series spectrophotometer in the wavelength range 350 – 1100 nm. For the calculation of absorption coefficient (α) at various wavelengths the method used by Rubin et.al.[23] was adopted. For the sample of thickness ' t' , α is given by the relation,

$$\alpha = (1/t)\ \ln(I_0/I), \quad (2).$$

where I_0 and I are the intensities of incident and transmitted radiations respectively.

Absorption coefficient is also related to % transmittance by
$\alpha = (1/t) \ln(1/T)$ (3).

To find absorption coefficient the graph was plotted between % transmittance and wavelength as shown in fig.1.F graph value of absorption coefficient (α) at each wavelength was calculated using above relation.

Optical band gap can be determine from the graph between $(\alpha hv)^2$ and (hv)and extrapolating the graph on (hv) axis.
The extinction coefficient ' k' is related to absorption coefficient ' α ' by the relation,

$$K = \alpha \lambda / 4 \pi. \quad (4)$$

Refractive index 'n' for the film is calculated using the relation,

$$n = (1 + R)/(1-R) + [4R/(1+R)^2 - k^2]^{½}. \quad (5)$$

Where R is the reflection.

The real and imaginary parts of dielectric constant are given by the relations [19],

$$\varepsilon_1 = n^2-k^2 \quad (6)$$

$$\varepsilon_2 = 2nk \quad (7)$$

III. Results and Discussion

The transmission spectra of of $CdZnSe_{2x}Te_{2(1-x)}$ for composition parameter x = 0, .25, .50, .75, 1 thin films of thickness 0.1730 µm are shown in **fig.1.**

Average transmission values are 75.5%, 80%, 82%, 92% in the wavelength range 350-1100 nm.It is found that % transmittance depends upon composition parameter ' x'. As x increases, %T also goes on increasing and it is found that $CdZnSe_2$ thin films have higher values of %T.

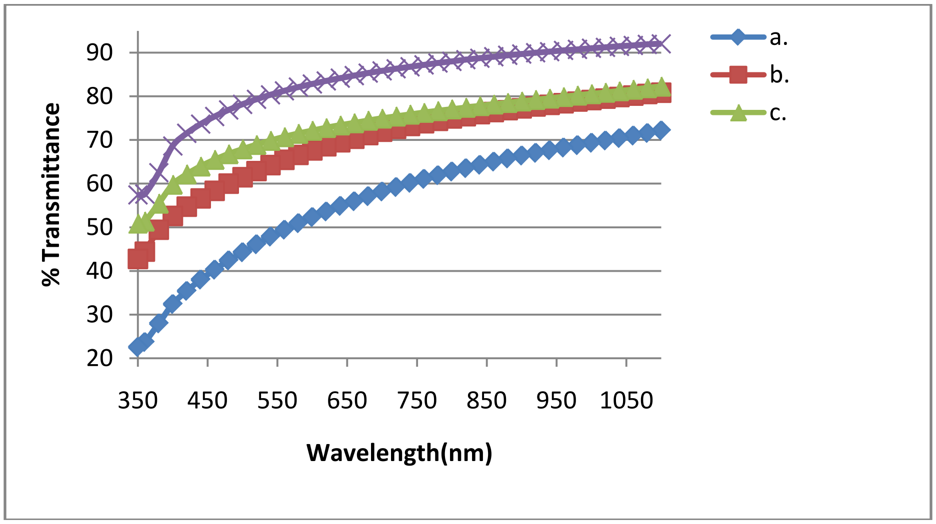

Fig. 1. Optical transmission spectra of the of $CdZnSe_{2x}Te_{2(1-x)}$ thin films for composition parameters a)x=0, b) x=.25, c)x=.5, and d) x=1.

To calculate the optical band gap the graphs are plotted between $(\alpha hv)^2$ vs. photon energy(hv) of the thin films of $CdZnSe_{2x}Te_{2(1-x)}$ of different composition parameters (x=0, .25, .50, .75, 1.) as shown in **fig. 2.**

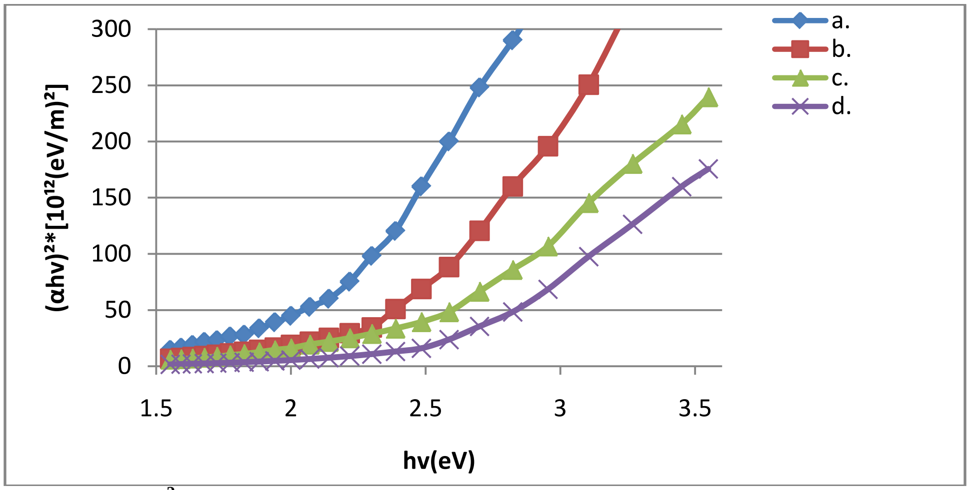

Fig. 2.Plots of $(\alpha hv)^2$ vs. photon energy of $CdZnSe_{2x}Te_{2(1-x)}$ thin films for composition parameter a) x=0, b) x=.25, c) x=.50, d) x=1.

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From the nature of graphs it is seen that each graph is linear above its absorption band edge. This linear relation indicates the direct allowed transition described by relation [24],

$$\alpha = (-A/hv)(hv-E_g)^{1/2} \quad (9)$$

where n=2 for direct allowed transition.

The optical band gap energies E_g for thin films of different composition parameters can be determined from intercepts on hv -axis.

The band gap values are as shown in table below.

Composition parameter(x)	Material $CdZnSe_{2x}Te_{2(1-x)}$	E_g(eV)
0	$CdZnTe_2$	2.04
.25	$CdZnSe_{.5}Te_{1.5}$	2.27
.50	$CdZnSe_1Te_1$	2.4
.75	$CdZnSe_{1.5}Te_{.5}$	2.43
1	$CdZnSe_2$	2.52

These values are found to be in good agreement with that obtained by Zunger at.el.and Nesheva at.el.[25-26]. It is also found that as composition x increases i.e. Se content increases,optical band gap energy value also goes on increasing. The extinction coefficient (k) and refractive index(n) are also calculated for $CdZnSe_{2x}Te_{2(1-x)}$ thin films of different composition parameters (x=0 to 1) The graph is plotted between extinction coefficient and wavelength as shown in **fig.3**.From graph it is seen that extinction coefficient decreases with increasing wavelength.

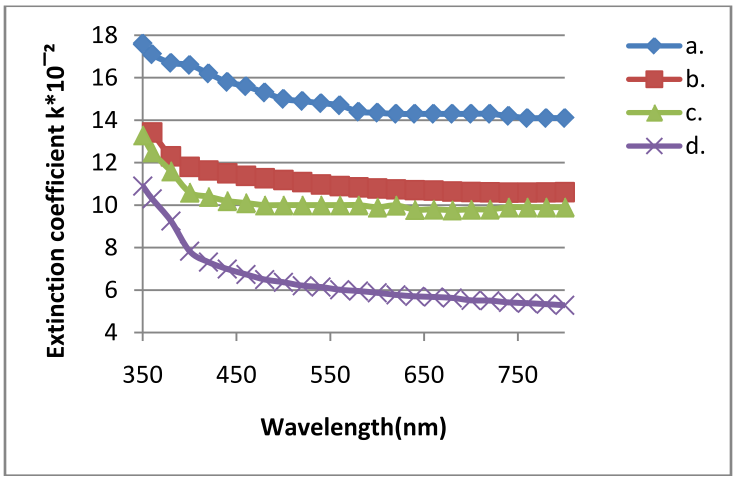

Fig. 3.Variation of extinction coefficient (k) of $CdZnSe_{2x}Te_{2(1-x)}$ thin films w ith wavelength for composition parameter a)x=0, b)x=.25,c)x=.5 ,d)x=1

The graph is also plotted between refractive index and wavelength as shown in **fig. 4**. Graph shows that refractive index decreases with increasing wavelength. It is also found that both extinction coefficient and refractive index decreases as '**Se**' content goes on increasing

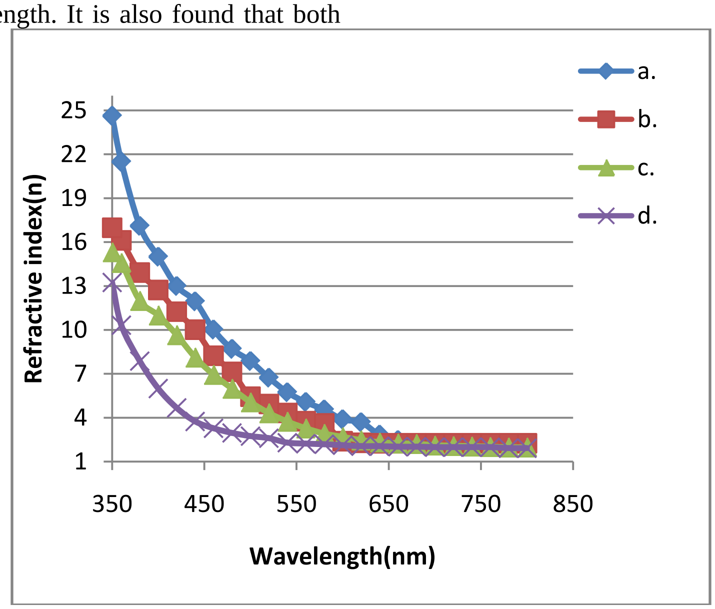

Fig. 4.Variation of refractive index (n) of of $CdZnSe_{2x}Te_{2(1-x)}$ thin films with wavelength for composition parameter a)=0 ,b)x=.25, c)x=.5, d)x=1.

We also calculated real and imaginary parts of dielectric constant.The variation of real (ε_1) and imaginary (ε_2) parts of dielectric constant with wavelength are shown in **figs.5 and 6** respectively. Both ε_1 and ε_2 decreases with wavelength.It is found that values of real part are higher than those of imaginary parts. Thus increasing selenium content causes important changes in optical constants.

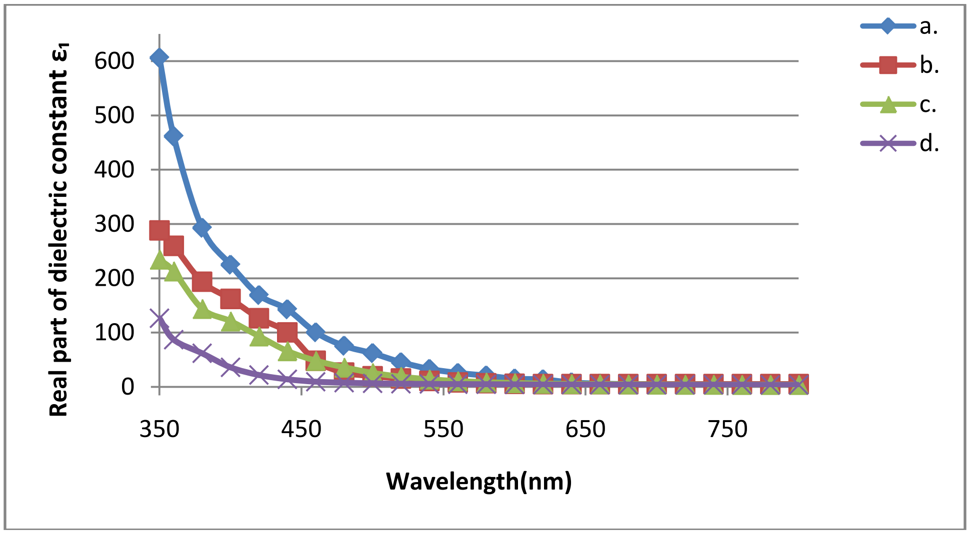

Fig. 5.Variation of real part of dielectric constant(ε_1) of $CdZnSe_{2x}Te_{2(1-x)}$ thin films with wavelength for composition parameter a)x=0, b)x=.25, c)x=.50, and d)x=1.

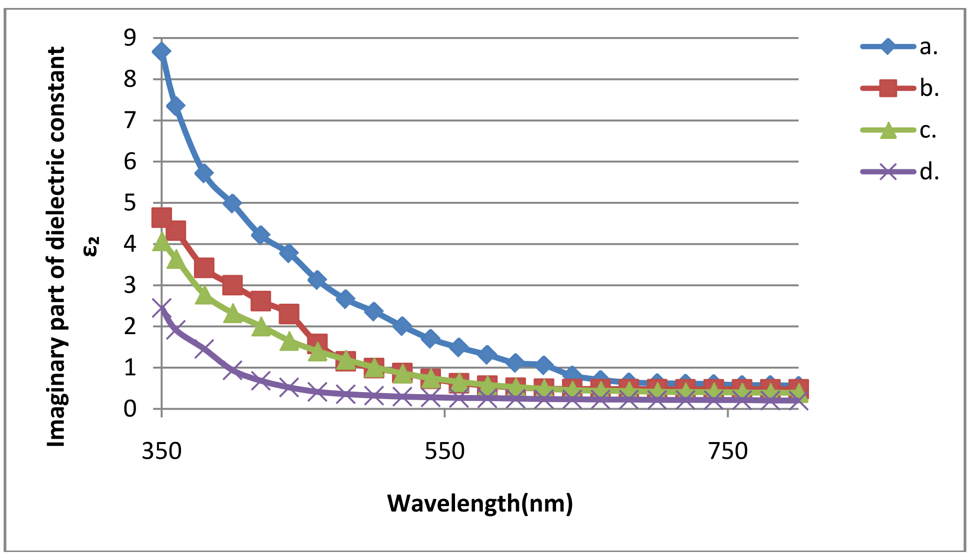

Fig. 6. Variation of imaginary part of dielectric constantε_2 of $CdZnSe_{2x}Te_{2(1-x)}$ thin films with wavelengthfor composition parameter a)x=0, b)x=.25, c)x=.50, and d)x=1

IV. Conclusions

$CdZnSe_{2x}Te_{2(1-X)}$ thin films of composition parameter x= 0, .25, .50, .75, 1 have been deposited on glass substrate by spray pyrolysis method at substrate temperature 300°C.The average transmission values are found to vary from 75.5% to92% for x=0,.25,.50,.75 and 1.The optical constants such as optical band gap, absorption coefficient, extinction coefficient, refractive index, real and imaginary parts of dielectric constant were calculated. The optical band gap increases with Selenium content. The optical band gap vary from 2.04eV to 2.52eV for thin films with composition parameter x=0 to 1 .Absorption spectra shows that absorption is due to direct transition .The extinction coefficient, refractive index, real and imaginary parts of dielectric constant for thin films decreases with wavelength. Thus the influence of selenium content on optical properties of $CdZnSe_{2x}Te_{2(1-X)}$ thin films is noticeable.

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